

From Canonical ensemble to Grand canonical ensemble
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We summarize the content of Chapter 8 of the textbook (R. Baierlein).

1. Approach from the canonical ensemble (occupation number representation)

The partition function of canonical ensemble (occupation number representation), is given by

$$Z_C(\bar{N}) = \sum_{n_1, n_2, \dots} e^{-\beta(n_1 \varepsilon_1 + n_2 \varepsilon_2 + \dots)} \delta(n_1 + n_2 + \dots, \bar{N})$$

where

$$E = n_1 \varepsilon_1 + n_2 \varepsilon_2 + \dots \quad (\text{the energy of the system})$$

$$N = n_1 + n_2 + \dots \quad (\text{the number of particles in the system, fixed})$$

2. Fermi-Dirac distribution function

We consider the fermion system obeying the Pauli exclusion principle

$$\begin{aligned} \langle n_1 \rangle &= \frac{1}{Z_C(\bar{N})} \sum_{n_1, n_2, \dots} n_1 e^{-\beta(n_1 \varepsilon_1 + n_2 \varepsilon_2 + \dots)} \delta(n_1 + n_2 + \dots, \bar{N}) \\ &= \frac{1}{Z_C(\bar{N})} \sum_{n_2, n_3, \dots} e^{-\beta(\varepsilon_1 + n_2 \varepsilon_2 + n_3 \varepsilon_3 + \dots)} \delta(1 + n_2 + \dots, \bar{N}) \\ &\quad + \frac{1}{Z_C(\bar{N})} \sum_{n_2, n_3, \dots} 0 e^{-\beta(n_2 \varepsilon_2 + n_3 \varepsilon_3 + \dots)} \delta(0 + n_2 + \dots, \bar{N}) \\ &= \frac{1}{Z_C(\bar{N})} e^{-\beta \varepsilon_1} \sum_{n_2, n_3, \dots} e^{-\beta(n_2 \varepsilon_2 + n_3 \varepsilon_3 + \dots)} \delta(n_2 + n_3 + \dots, \bar{N} - 1) \end{aligned}$$

where $n_i = 0, 1$ for fermions. We also Note that

$$\begin{aligned}
& \frac{1}{Z_C(\bar{N})} e^{-\beta \varepsilon_1} \sum_{n_1, n_2, \dots} (1-n_1) e^{-\beta(n_1 \varepsilon_1 + n_2 \varepsilon_2 + \dots)} \delta(n_1 + n_2 + \dots, \bar{N}-1) \\
&= \frac{1}{Z_C(\bar{N})} e^{-\beta \varepsilon_1} \sum_{n_2, n_3, \dots} (1-0) e^{-\beta(0 \varepsilon_1 + n_2 \varepsilon_2 + \dots)} \delta(0 + n_2 + \dots, \bar{N}-1) \\
&+ \frac{1}{Z_C(\bar{N})} e^{-\beta \varepsilon_1} \sum_{n_2, n_3, \dots} (1-1) e^{-\beta(1 \varepsilon_1 + n_2 \varepsilon_2 + \dots)} \delta(1 + n_2 + \dots, \bar{N}-1) \\
&= \frac{1}{Z_C(\bar{N})} e^{-\beta \varepsilon_1} \sum_{n_2, n_3, \dots} e^{-\beta(n_2 \varepsilon_2 + \dots)} \delta(n_2 + n_3 + \dots, \bar{N}-1) \\
&= \langle n_1 \rangle
\end{aligned}$$

From the definition of the partition function, we have

$$Z_C(\bar{N}) = \sum_{n_1, n_2, \dots} e^{-\beta(n_1 \varepsilon_1 + n_2 \varepsilon_2 + \dots)} \delta(n_1 + n_2 + \dots, \bar{N})$$

and

$$Z_C(\bar{N}-1) = \sum_{n_1, n_2, \dots} e^{-\beta(n_1 \varepsilon_1 + n_2 \varepsilon_2 + \dots)} \delta(n_1 + n_2 + \dots, \bar{N}-1)$$

Then we get

$$\begin{aligned}
\langle n_1 \rangle_{\bar{N}} &= \frac{1}{Z_C(\bar{N})} e^{-\beta \varepsilon_1} \sum_{n_1, n_2, \dots} (1-n_1) e^{-\beta(n_1 \varepsilon_1 + n_2 \varepsilon_2 + \dots)} \delta(n_1 + n_2 + \dots, \bar{N}-1) \\
&= \frac{1}{Z_C(\bar{N})} e^{-\beta \varepsilon_1} [Z_C(\bar{N}-1) - Z_C(\bar{N}-1) \langle n_1 \rangle_{\bar{N}-1}] \\
&= \frac{Z_C(\bar{N}-1)}{Z_C(\bar{N})} e^{-\beta \varepsilon_1} [1 - \langle n_1 \rangle_{\bar{N}-1}]
\end{aligned}$$

where

$$Z_C(\bar{N}-1) = \sum_{n_1, n_2, \dots} e^{-\beta(n_1 \varepsilon_1 + n_2 \varepsilon_2 + \dots)} \delta(n_1 + n_2 + \dots, \bar{N}-1)$$

$$\langle n_1 \rangle_{\bar{N}-1} = \frac{1}{Z_C(\bar{N}-1)} \sum_{n_1, n_2, \dots} n_1 e^{-\beta(n_1 \varepsilon_1 + n_2 \varepsilon_2 + \dots)} \delta(n_1 + n_2 + \dots, \bar{N}-1)$$

Here we use $N \rightarrow \bar{N}$. The average number $\bar{N} = \langle N \rangle_G$ is the same for both the canonical ensemble and the grand canonical ensemble. The chemical potential is defined by

$$\begin{aligned}\mu &= \left(\frac{\partial F}{\partial \bar{N}} \right)_{T,V} \\ &= F(\bar{N}) - F(\bar{N} - 1) \\ &= -\frac{1}{\beta} \ln \left[\frac{Z_C(\bar{N})}{Z_C(\bar{N} - 1)} \right]\end{aligned}$$

in the canonical ensemble, where $dF = -SdT - PdV + \mu dN$ and

$$F(\bar{N}) = -k_B T \ln Z_C(\bar{N}) = -\frac{1}{\beta} \ln Z_C(\bar{N})$$

From the above equation, we get

$$e^{\beta\mu} = \frac{Z_C(\bar{N} - 1)}{Z_C(\bar{N})} = \frac{(z)^{-(\bar{N}-1)} Z_G(z)}{(z)^{-\bar{N}} Z_G(z)} = z$$

In the limit $\bar{N} \rightarrow \infty$, we have $\langle n_1 \rangle_{\bar{N}} \approx \langle n_1 \rangle_{\bar{N}-1}$

$$\begin{aligned}\langle n_1 \rangle_{\bar{N}} &= \frac{Z_C(\bar{N} - 1)}{Z_C(\bar{N})} e^{-\beta\epsilon_1} [1 - \langle n_1 \rangle_{\bar{N}-1}] \\ &\approx \frac{Z_C(\bar{N} - 1)}{Z_C(\bar{N})} e^{-\beta\epsilon_1} [1 - \langle n_1 \rangle_{\bar{N}}] \\ &= e^{\beta(\mu - \epsilon_1)} [1 - \langle n_1 \rangle_{\bar{N}}]\end{aligned}$$

Thus we can derive the expression of the Fermi-Dirac distribution function,

$$\langle n_1 \rangle_{\bar{N}} \approx \langle n_1 \rangle_{\bar{N}-1} = \frac{1}{e^{\beta(\epsilon_1 - \mu)} + 1} \quad (\text{Fermi-Dirac distribution function})$$

In general, we have

$$\langle n_a \rangle_{\bar{N}} = \frac{1}{e^{\beta(\epsilon_a - \mu)} + 1}$$

((Note))

Here we use the approximation that

$$Z_G(z) = \sum_{N=0}^{\infty} z^N Z_C(N) \approx z^{\bar{N}} Z_C(\bar{N})$$

where $z = e^{\beta\mu}$. We note that $z^N Z_C(N)$ has a very sharp peak at $N = \bar{N}$. In other words,

$$g(N) = \ln[z^N Z_C(N)] = N \ln z + \ln[Z_C(N)]$$

has a local maximum at $N = \bar{N}$.

$$g'(\bar{N}) = \ln z + \frac{\partial \ln[Z_C(\bar{N})]}{\partial \bar{N}} = 0$$

which means that

$$\mu = \left(\frac{\partial F(N)}{\partial N} \right)_{N=\bar{N}} = \left(\frac{\partial F(\bar{N})}{\partial \bar{N}} \right)$$

3. Bose-Einstein distribution function

We start with the canonical ensemble

$$\langle n_1 \rangle = \frac{1}{Z_C(\bar{N})} \sum_{n_1, n_2, \dots} n_1 e^{-\beta(n_1 \epsilon_1 + n_2 \epsilon_2 + \dots)} \delta(n_1 + n_2 + \dots, \bar{N})$$

where $n_1 = 0, 1, 2, 3, 4, \dots, \bar{N}$. We put $n_1 = n_1' + 1$.

$$\begin{aligned} \langle n_1 \rangle_{\bar{N}} &= \frac{1}{Z_C(\bar{N})} e^{-\beta \epsilon_1} \sum_{n_1', n_2, \dots} (n_1' + 1) e^{-\beta(n_1' \epsilon_1 + n_2 \epsilon_2 + \dots)} \delta(n_1' + n_2 + \dots, \bar{N} - 1) \\ &= \frac{1}{Z_C(\bar{N})} e^{-\beta \epsilon_1} \sum_{n_1', n_2, \dots} (n_1' + 1) e^{-\beta(n_1' \epsilon_1 + n_2 \epsilon_2 + \dots)} \delta(n_1' + n_2 + \dots, \bar{N} - 1) \\ &= \frac{1}{Z_C(\bar{N})} e^{-\beta \epsilon_1} [Z_C(\bar{N} - 1) + Z_C(\bar{N} - 1) \langle n_1 \rangle_{\bar{N}-1}] \\ &= \frac{Z_G(\bar{N} - 1)}{Z_C(\bar{N})} e^{-\beta \epsilon_1} [1 + \langle n_1 \rangle_{\bar{N}-1}] \end{aligned}$$

We use the relation

$$e^{\beta\mu} = \frac{Z_C(\bar{N}-1)}{Z_C(\bar{N})},$$

We also assume that

$$\langle n_1 \rangle_{\bar{N}-1} \approx \langle n_1 \rangle_{\bar{N}}$$

in the limit of $\bar{N} \rightarrow \infty$. Thus we get

$$\langle n_1 \rangle_{\bar{N}} = e^{\beta(\mu-\varepsilon_1)} [1 + \langle n_1 \rangle_{\bar{N}}]$$

or

$$\langle n_1 \rangle_{\bar{N}} [1 - e^{\beta(\mu-\varepsilon_1)}] = e^{\beta(\mu-\varepsilon_1)}$$

or

$$\langle n_1 \rangle_{\bar{N}} = \frac{e^{\beta(\mu-\varepsilon_1)}}{1 - e^{\beta(\mu-\varepsilon_1)}} = \frac{1}{e^{\beta(\varepsilon_1-\mu)} - 1} \quad (\text{Bose-Einstein distribution})$$

In general, we have

$$\langle n_a \rangle_{\bar{N}} = \frac{1}{e^{\beta(\varepsilon_a-\mu)} - 1}$$

4. Limits: classical and semi-classical

$$\langle n_a \rangle = e^{-\beta(\varepsilon_a-\mu)} = e^{\beta\mu} e^{-\beta\varepsilon_a}$$

$$\bar{N} = \sum_a \langle n_a \rangle = e^{\beta\mu} \sum_a e^{-\beta\varepsilon_a} = e^{\beta\mu} Z_C(1)$$

or

$$e^{\beta\mu} = \frac{\bar{N}}{Z_c(1)}$$

or

$$\beta\mu = -\ln\left(\frac{Z_c(1)}{\bar{N}}\right)$$

or

$$\mu = -k_B T \ln\left(\frac{Z_c(1)}{\bar{N}}\right)$$

Using this expression for the chemical potential, the above expression of $\langle n_a \rangle$ can be rewritten as

$$\langle n_a \rangle = \frac{\bar{N}}{Z_c(1)} e^{-\beta\epsilon_a} \quad (\text{Maxwell-Boltzmann distribution function})$$

4. The semi-classical limit of the partition function

We start with the above relations

$$e^{\beta\mu} = \frac{\bar{N}}{Z_c(1)}$$

and

$$e^{\beta\mu} = \frac{Z_c(\bar{N}-1)}{Z_c(\bar{N})}$$

Form these equation we get the recursion formula for $Z_c(\bar{N})$

$$e^{\beta\mu} = \frac{Z_c(\bar{N}-1)}{Z_c(\bar{N})} = \frac{\bar{N}}{Z_c(1)}$$

or

$$Z_c(\bar{N}) = \frac{Z_c(1)}{\bar{N}} Z_c(\bar{N}-1)$$

Using this relation, we get

$$\begin{aligned} Z_c(\bar{N}) &= \frac{Z_c(1)}{\bar{N}} \frac{Z_c(1)}{\bar{N}-1} Z_c(\bar{N}-2) \\ &= \frac{Z_c(1)}{\bar{N}} \frac{Z_c(1)}{\bar{N}-1} \frac{Z_c(1)}{\bar{N}-2} \dots \frac{Z_c(1)}{2} Z_c(1) \\ &= \frac{Z_{c1}^{\bar{N}}}{\bar{N}!} \end{aligned}$$

or

$$Z_c(\bar{N}) = \frac{Z_{c1}^{\bar{N}}}{\bar{N}!}$$

which is the partition function of identical N particles. Note that

$$Z_{c1} = Z_c(1)$$

5. Pressure

From the thermodynamics property

$$dU = TdS - PdV$$

the pressure can be obtained as

$$P = -\frac{\partial U}{\partial V} = -\frac{1}{Z} \sum_j \left(\frac{\partial E_j}{\partial V} \right) e^{-\beta E_j} = -\sum_j \left(\frac{\partial E_j}{\partial V} \right) \frac{e^{-\beta E_j}}{Z}$$

For the energy eigenvalue for the one-particle energy

$$\varepsilon_a = \frac{\hbar^2}{2m} k^2 = \frac{\hbar^2}{2m} \left(\frac{2\pi}{L} n \right)^2 = \frac{\hbar^2 (2\pi n)^2}{2m} L^{-2} = \frac{\hbar^2 (2\pi n)^2}{2m} V^{-\frac{2}{3}} \quad \text{with} \quad k = \frac{2\pi}{L} n$$

$$\frac{\partial \varepsilon_a}{\partial V} = -\frac{2}{3} \frac{\varepsilon_a}{V}$$

For the energy eigenvalue for the N -particle energy,

$$\frac{\partial E_j}{\partial V} = -\frac{2}{3} \frac{E_j}{V}$$

Thus we have the pressure as

$$P = \frac{2}{3V} \sum_j E_j \frac{e^{-\beta E_j}}{Z} = \frac{2U}{3V}$$

or

$$PV = \frac{2}{3} U.$$

We now calculate the internal energy

$$\begin{aligned} U &= \frac{1}{Z(N)} \sum_{n_1, n_2, n_3, \dots} (n_1 \varepsilon_1 + n_2 \varepsilon_2 + \dots) e^{-(\beta n_1 \varepsilon_1 + \beta n_2 \varepsilon_2 + \dots)} \delta(n_1 + n_2 + \dots, N) \\ &= \varepsilon_1 \langle n_1 \rangle + \varepsilon_2 \langle n_2 \rangle + \dots \\ &= \sum_a \varepsilon_a \langle n_a \rangle \end{aligned}$$

or

$$U = \sum_a \varepsilon_a \langle n_a \rangle = \sum_a \frac{\varepsilon_a}{e^{\beta(\varepsilon_a - \mu)} \pm 1}$$

Note that

$$\langle n_a \rangle = \frac{1}{e^{\beta(\varepsilon_a - \mu)} \pm 1} = e^{\beta(\varepsilon_a - \mu)} \mp e^{2\beta(\varepsilon_a - \mu)}$$

The chemical potential is determined by the condition that

$$N = \sum_a \langle n_a \rangle = \sum_a e^{\beta(\varepsilon_a - \mu)} \mp \sum_a e^{2\beta(\varepsilon_a - \mu)}$$

For the one-particle state with the free energy:

$$\sum_a = \sum_k$$

$$\begin{aligned} D(\varepsilon) d\varepsilon &= \frac{(2s+1)V}{(2\pi)^3} 4\pi k^2 dk \\ &= \frac{(2s+1)V}{4\pi^2} \left(\frac{2m}{\hbar^2} \right)^{3/2} \sqrt{\varepsilon} d\varepsilon \end{aligned}$$

The density of states:

$$D(\varepsilon) = \frac{(2s+1)V}{4\pi^2} \left(\frac{2m}{\hbar^2} \right)^{3/2} \sqrt{\varepsilon}$$

where $s = \frac{1}{2}$ for electron

$$\varepsilon = \frac{\hbar^2 k^2}{2m}$$

((Note)) Classical limit

$$\langle n_a \rangle = e^{-\beta(\varepsilon_a - \mu)} = e^{\beta\mu} e^{-\beta\varepsilon_a}$$

$$N = \sum_a \langle n_a \rangle = e^{\beta\mu} \sum_a e^{-\beta\varepsilon_a} = e^{\beta\mu} Z_{C1}$$

$$e^{\beta\mu} = \frac{N}{Z_{C1}}$$

or

$$\beta\mu = -\ln\left(\frac{Z_{C1}}{N}\right)$$

or

$$\mu = -k_B T \ln \left(\frac{Z_{C1}}{N} \right)$$

Note that

$$U = -N \frac{\partial}{\partial \beta} \ln Z_{C1} = \sum_a \varepsilon_a \langle n_a \rangle = \frac{N}{Z_{C1}} \sum_a \varepsilon_a e^{-\beta \varepsilon_a} = N \sum_a \varepsilon_a P_a$$

and

$$\langle n_a \rangle = \frac{N}{Z_{C1}} e^{-\beta \varepsilon_a}$$

We now calculate the partition function Z_{C1} as

$$\begin{aligned} Z_{C1} &= \frac{V(2s+1)}{(2\pi)^3} \int_0^\infty 4\pi k^2 dk e^{-\frac{\beta \hbar^2 k^2}{2m}} \\ &= \frac{V(2s+1)}{2\pi^2} \left(\frac{2m}{\beta \hbar^2} \right)^{3/2} \int_0^\infty dx x^2 e^{-x^2} \\ &= \frac{V(2s+1)}{\pi^2} \left(\frac{2m}{\beta \hbar^2} \right)^{3/2} \frac{\sqrt{\pi}}{2^3} \\ &= V(2s+1) \left(\frac{mk_B T}{2\pi \hbar^2} \right)^{3/2} \\ &= V(2s+1) \lambda_{th}^{-3} \end{aligned}$$

or

$$Z_{C1} = \frac{V(2s+1)}{n_Q}$$

where the thermal wavelength is

$$\lambda_{th} = \left(\frac{2\pi \hbar^2}{mk_B T} \right)^{1/2} \quad n_Q = \frac{1}{\lambda_{th}^3}$$

(i) Internal energy

$$U = -N \frac{\partial}{\partial \beta} \ln Z_{C1} = \frac{3}{2} N k_B T$$

(ii) Helmholtz free energy

$$F = -N k_B T \ln Z_{C1} = -N k_B T \ln \left[\frac{V(2s+1)}{n_Q} \right]$$

(iii) Pressure

$$P = - \left(\frac{\partial F}{\partial V} \right)_T = \frac{N k_B T}{V}$$

(iv) Chemical potential

$$\mu = k_B T \ln \left[(2s+1) \frac{n}{n_Q} \right]$$

(v) Helmholtz free energy and chemical potential depend on the number of spin s .

6. Probability

The probability is defined as

$$P[E_s(N), N] = \frac{1}{Z_G} z^N e^{-\beta E_s(N)}$$

$E_s(N)$ is the energy eigenvalue of N -particle eigenfunction.

$$\sum_{N,s} P[E_s(N), N] = \frac{1}{Z_G} \sum_{N,s} z^N e^{-\beta E_s(N)} = 1$$

where the partition function of the grand canonical ensemble,

$$Z_G = \sum_{N,s} z^N e^{-\beta E_s(N)} = \sum_{N,s} e^{\mu N} e^{-\beta E_s(N)}$$

with

$$z = e^{\beta\mu}$$

$E_s(N)$ is the energy eigenvalue for the N particles. The average number of particle number:

$$\langle N \rangle = \sum_{N,s} N z^N e^{-\beta E_s(N)}$$

$$\langle N \rangle = \frac{1}{\beta} \frac{\partial}{\partial \mu} \ln Z_G = \frac{1}{\beta Z_G} \frac{\partial Z_G}{\partial \mu} = \frac{1}{Z_G} \sum_{N,s} N z^N e^{-\beta E_s(N)}$$

We note that the partition function of the N particle (canonical ensemble) is defined by

$$Z_C(N) = \sum_s e^{-\beta E_s(N)}$$

Thus Z_G is expressed by

$$Z_G = \sum_N e^{\beta\mu N} Z_C(N)$$

7. Occupation number representation:

$$E_s(N) = n_1 \varepsilon_1 + n_2 \varepsilon_2 + \dots$$

$$N = n_1 + n_2 + \dots$$

where $\varepsilon_1, \varepsilon_2, \dots$ are the energy eigenvalues of one-particle system.

$$\begin{aligned} Z_G &= \sum_N \sum_{\{n_1, n_2, \dots\}} e^{\mu(n_1 + n_2 + \dots)} e^{-\beta(\varepsilon_1 n_1 + \varepsilon_2 n_2 + \dots)} \delta[n_1 + n_2 + \dots - N] \\ &= \sum_N \sum_{\{n_1, n_2, \dots\}} e^{\mu(n_1 + n_2 + \dots)} e^{-\beta(\varepsilon_1 n_1 + \varepsilon_2 n_2 + \dots)} \delta[n_1 + n_2 + \dots - N] \\ &= \sum_{\{n_1, n_2, \dots\}} e^{\beta(\mu - \varepsilon_1) n_1} e^{\beta(\mu - \varepsilon_2) n_2} \dots \\ &= \sum_{n_1} e^{\beta(\mu - \varepsilon_1) n_1} \sum_{n_2} e^{\beta(\mu - \varepsilon_2) n_2} \dots \end{aligned} \tag{1}$$

It is difficult to perform the summation in Eq.(1) in the canonical ensemble, because of the restriction $N = n_1 + n_2 + \dots$. In the grand partition function with the summation $\sum_N$ the calculation can be made much more easier. The problem is reduced to one-particle problem.

For fermions; $n = 0$ and 1

$$Z_G = [1 + e^{\beta(\mu - \varepsilon_1)}][1 + e^{\beta(\mu - \varepsilon_2)}] \dots$$

$$\begin{aligned} \ln Z_G &= \ln[1 + e^{\beta(\mu - \varepsilon_1)}] + \ln[1 + e^{\beta(\mu - \varepsilon_2)}] + \dots \\ &= \sum_k \ln[1 + e^{\beta(\mu - \varepsilon_k)}] \end{aligned}$$

$$\begin{aligned} \frac{1}{\beta} \frac{\partial}{\partial \mu} \ln Z_G &= z \frac{\partial}{\partial z} \ln Z_G \\ &= \sum_k \frac{e^{\beta(\mu - \varepsilon_k)}}{1 + e^{\beta(\mu - \varepsilon_k)}} \\ &= \sum_k \frac{1}{e^{\beta(\varepsilon_k - \mu)} + 1} \end{aligned}$$

The Fermi-Dirac distribution function;

$$f_k = \frac{1}{e^{\beta(\varepsilon_k - \mu)} + 1}$$

For bosons; $n = 0, 1, 2, \dots$

$$Z_G = [1 - e^{\beta(\mu - \varepsilon_1)}]^{-1} [1 - e^{\beta(\mu - \varepsilon_2)}]^{-1} \dots$$

$$\begin{aligned} \ln Z_G &= -\ln[1 - e^{\beta(\mu - \varepsilon_1)}] - \ln[1 - e^{\beta(\mu - \varepsilon_2)}] - \dots \\ &= -\sum_k \ln[1 - e^{\beta(\mu - \varepsilon_k)}] \end{aligned}$$

$$\begin{aligned}
\frac{1}{\beta} \frac{\partial}{\partial \mu} \ln Z_G &= z \frac{\partial}{\partial z} \ln Z_G \\
&= - \sum_k \frac{-e^{\beta(\mu - \varepsilon_k)}}{1 - e^{\beta(\mu - \varepsilon_k)}} \\
&= \sum_k \frac{1}{e^{\beta(\varepsilon_k - \mu)} - 1}
\end{aligned}$$

Bose-Einstein distribution function;

$$n_k = \frac{1}{e^{\beta(\varepsilon_k - \mu)} - 1}.$$

REFERENCES

R. Baierlein, Thermal Physics (Cambridge, 1999).

APPENDIX-I

$$z \frac{\partial}{\partial z} = \frac{\partial}{\partial \ln z} = \frac{\partial}{\partial (\beta \mu)} = \frac{1}{\beta} \frac{\partial}{\partial \mu} = k_B T \frac{\partial}{\partial \mu}$$

APPENDIX

(a) Grand canonical ensemble:

$$\langle N \rangle_G = z \frac{\partial}{\partial z} \ln Z_G$$

The partition function of the canonical ensemble:

$$Z_{CN} = \frac{(Z_{C1})^N}{N!}$$

The partition function of the grand canonical ensemble;

$$\begin{aligned}
Z_G &= \sum_N z^N Z_{CN} \\
&= \sum_N z^N \frac{(Z_{C1})^N}{N!} \\
&= \sum_N \frac{(zZ_{C1})^N}{N!} \\
&= \exp(zZ_{C1})
\end{aligned}$$

or

$$\ln Z_G = zZ_{C1}$$

Thus we have

$$\langle N \rangle_G = z \frac{\partial}{\partial z} \ln Z_G = z \frac{\partial}{\partial z} (zZ_{C1}) = zZ_{C1}$$

or

$$\langle N \rangle_G = zZ_{C1} = e^{\beta\mu} Z_{C1}$$

The chemical potential is thus obtained as

$$\mu = k_B T \ln \left(\frac{\langle N \rangle_G}{Z_{C1}} \right)$$

where

$$Z_{C1} = V n_Q(T)$$

$$\mu = k_B T \ln \left(\frac{N}{Z_{C1}} \right) = k_B T \ln \left(\frac{N}{V n_Q} \right) = k_B T \ln \left(\frac{n}{n_Q} \right)$$

with

$$n = \frac{N}{V}$$

(b) Canonical ensemble:

Approximation:

$$Z_G = \sum_N z^N Z_{CN} \approx z^{\bar{N}} Z_{C\bar{N}}$$

where

$$Z_{C\bar{N}} = \frac{(Z_{C1})^{\bar{N}}}{\bar{N}!}$$

$$Z_G \approx z^{\bar{N}} Z_{C\bar{N}} = z^{\bar{N}} \frac{(Z_{C1})^{\bar{N}}}{\bar{N}!}$$

$$\begin{aligned} \ln Z_G &\approx \ln \left[z^{\bar{N}} \frac{(Z_{C1})^{\bar{N}}}{\bar{N}!} \right] \\ &= \bar{N} \ln z + \bar{N} \ln Z_{C1} - \ln \bar{N}! \end{aligned}$$

$$\begin{aligned} \langle N \rangle_G &= z \frac{\partial}{\partial z} \ln Z_G \\ &= z \frac{\partial}{\partial z} [\bar{N} \ln z + \bar{N} \ln Z_{C1} - \ln \bar{N}!] \\ &= \bar{N} \end{aligned}$$

(c) Occupation number representation

$$\begin{aligned} \langle N \rangle_G &= \sum_a \langle n_a \rangle_G \\ &= \sum_a \frac{1}{e^{\beta(\varepsilon_a - \mu)} \pm 1} \\ &\approx \sum_a e^{-\beta(\varepsilon_a - \mu)} \\ &= z \sum_a e^{-\beta \varepsilon_a} \\ &= z Z_{C1} \end{aligned}$$

since

$$\frac{1}{e^{\beta(\varepsilon-\mu)}-1} \approx$$
