Ideal Fermion & Boson

Jian Qin

January 7, 2017

1.1 Equation of state for ideal Fermion and Boson.

The energy dispersion relation for the ideal gas is

$$\epsilon_{\mathbf{k}} = \frac{\hbar^2 \mathbf{k}^2}{2m}.$$

The energy level occupation function is

$$f(\epsilon_{\mathbf{k}}) = \frac{1}{\exp\left(\frac{\epsilon_{\mathbf{k}} - \mu}{k_{\mathrm{B}} T}\right) \pm 1}.$$

Summation over all energy levels gives the equation of state

$$n = \frac{N}{V} = \frac{g}{(2\pi)^3} \int \mathrm{d}\mathbf{k}\, f(\epsilon_{\mathbf{k}}) = \frac{g}{2\pi^2} \int_0^\infty \mathrm{d}k\, k^2 f(\epsilon_k)$$

where g is the degeneracy. For electron with spin-degeneracy, $g = 2$. Setting $f(\epsilon_k) = 1$ and introducing an upper cutoff k_{F} gives

$$k_{\mathrm{F}} = \left(\frac{6\pi^2 n}{g}\right)^{1/3}.$$

Chaning k to ϵ, and normalizing ϵ, $k_{\mathrm{B}}T$ & μ by the Fermi level $\epsilon_{\mathrm{F}} \equiv \hbar^2 k_{\mathrm{F}}^2/(2m)$ gives

$$\frac{2}{3} = \left(\frac{k_{\mathrm{B}}T}{\epsilon_{\mathrm{F}}}\right)^{3/2} \int_0^\infty \mathrm{d}z\, \frac{z^{1/2}}{\mathrm{e}^z \exp\left(-\frac{\mu}{k_{\mathrm{B}}T}\right) \pm 1} = \mp \frac{\sqrt{\pi}}{2} \left(\frac{k_{\mathrm{B}}T}{\epsilon_{\mathrm{F}}}\right)^{3/2} \mathrm{Li}_{3/2}\big(\mp \mathrm{e}^{\mu/(k_{\mathrm{B}}T)}\big).$$

Here $\mathrm{Li}_{3/2}$ is the polylog function of order 3/2. Introducing the shorthand notation $t \equiv k_{\mathrm{B}}T/\epsilon_{\mathrm{F}}$ and $m \equiv \mu/(k_{\mathrm{B}}T)$, the above can be written

$$\frac{4}{3\sqrt{\pi}} t^{-3/2} = \mp \mathrm{Li}_{3/2}\big(\mp \mathrm{e}^m\big).$$

Temperature t can be solved for arbitrary values of m, which relates chemical potential to temperature. The $-$ sign works for Fermion and the $+$ sign works for Boson.

The classical limit is achieved for $m \simeq -\frac{3}{2}\ln(T) \to -\infty$. The polylog function behaves as $\mathrm{Li}_s(z) = z$ for z in the neighborhood of 0, which gives

$$\frac{4}{3\sqrt{\pi}} t^{-3/2} = \mathrm{e}^{\mu/(k_{\mathrm{B}}T)} \to \mu = -k_{\mathrm{B}}T \ln\left[\frac{3\sqrt{\pi}}{4}\left(\frac{k_{\mathrm{B}}T}{\epsilon_{\mathrm{F}}}\right)^{3/2}\right].$$

(November 10, 2016)

1.2 Classical partition function in occupation number representation.

Classical partition function for indistinguishable particles is given by

$$Q_{\rm C}(N,V,T) = \frac{1}{N!}\{\text{partition function for distinguishable particles}\}.$$

This allows one to follow the energy state of each particle separately. For ideal gas, we can write $Q_{\rm C} = q^N/N!$, here the single particle partition function is calculated in the energy representation

$$q = \sum_{\epsilon} \exp\left(-\frac{\epsilon}{k_{\rm B}T}\right).$$

But to derive the Boson and Fermion distribution, we used the occupation number representation, and used

$$Q_{\rm F,B}(N,V,T) = \overbrace{\sum_{n_1}\sum_{n_2}\cdots}^{n_1+n_2+\cdots=N} \exp\left(-\frac{n_1\epsilon_1 + n_2\epsilon_2 + \cdots}{k_{\rm B}T}\right).$$

The range of n_1, n_2, etc. is $\{0,1\}$ for Fermsion and is $\{0,1,2,\cdots\}$ for Boson. What about $Q_{\rm C}$? The range of n_1, n_2 is $\{0,1,2,\cdots\}$, the same as for Boson. But to correct for the effects of particle distinguishability, we have

$$Q_{\rm C}(N,V,T) = \frac{1}{N!}\overbrace{\sum_{n_1}\sum_{n_2}\cdots}^{n_1+n_2+\cdots=N} \frac{N!}{n_1!\,n_2!\,\cdots} \exp\left(-\frac{n_1\epsilon_1 + n_2\epsilon_2 + \cdots}{k_{\rm B}T}\right).$$

The combinatorial factor accounts for the number of ways of distributing particles. So finally,

$$Q_{\rm C}(N,V,T) = \overbrace{\sum_{n_1}\sum_{n_2}\cdots}^{n_1+n_2+\cdots=N} \frac{1}{n_1!\,n_2!\,\cdots} \exp\left(-\frac{n_1\epsilon_1 + n_2\epsilon_2 + \cdots}{k_{\rm B}T}\right).$$

The distinction from the cases of Fermion and Boson vanishes when $n_\alpha = 0$ or 1 at high temperature, or when the level is either occupied or empty.

The grand canonical partition function is not constrained by the total particle number.

$$\begin{aligned}\Xi_{\rm C}(\mu,V,T) &= \sum_{n_1}\sum_{n_2}\cdots \frac{1}{n_1!\,n_2!\,\cdots}\exp\left(-\frac{n_1(\epsilon_1-\mu) + n_2(\epsilon_2-\mu) + \cdots}{k_{\rm B}T}\right) \\ &= \exp\left[\exp\left(-\frac{\epsilon_1-\mu}{k_{\rm B}T}\right) + \exp\left(-\frac{\epsilon_2-\mu}{k_{\rm B}T}\right)\cdots\right].\end{aligned} \tag{1}$$

This is identical to the result obtained directly from the particle representation

$$\Xi_{\rm C}(\mu,V,T) = \sum_N \frac{q^N\,{\rm e}^{\mu N/(k_{\rm B}T)}}{N!} = \exp\left[q\,{\rm e}^{\mu/(k_{\rm B}T)}\right].$$

The pressure thus is given by $pV = k_{\rm B}T\ln\Xi_{\rm C}(\mu,V,T)$, leaving

$$pV_{\rm C} = k_{\rm B}T\sum_\alpha \exp\left(-\frac{\epsilon_\alpha-\mu}{k_{\rm B}T}\right).$$

This can be compared to the correponsinng expression for Fermion and Boson,

$$pV_{\rm F,B} = \pm k_{\rm B}T\sum_\alpha \ln\left[1 \pm \exp\left(-\frac{\epsilon_\alpha-\mu}{k_{\rm B}T}\right)\right]. \tag{2}$$

The average number of particle in a given level at high temperature is $\langle n_\alpha\rangle = \exp\left(-\frac{\epsilon_\alpha-\mu}{k_{\rm B}T}\right)$.

(November 11, 2016)

1.3 The level occupation representation is meaningful only for ideal gas.

From the derivation, it is clear that the occupation numbers

$$f_{\mathrm{F,B}}(\epsilon) = \frac{1}{\exp\left(\dfrac{\epsilon-\mu}{k_{\mathrm{B}}T}\right) \pm 1}$$

as well as the classical limit

$$f_{\mathrm{C}}(\epsilon) = \exp\left(-\frac{\epsilon-\mu}{k_{\mathrm{B}}T}\right)$$

only applies to ideal (non-interacting) particles. Specifically, the partition function for the non-interacting particles reads

$$\Xi_{\mathrm{C}}(\mu, V, T) = \sum_{N=0}^{\infty} \frac{Q(N,V,T)}{N!} \exp\bigl(\mu N/(k_{\mathrm{B}}T)\bigr).$$

The particle number then is given by

$$\begin{aligned}\langle N\rangle &= \frac{1}{\Xi_{\mathrm{C}}} \sum_{N=1}^{\infty} \frac{Q(N,V,T)}{(N-1)!} \exp\bigl(\mu N/(k_{\mathrm{B}}T)\bigr) \\ &= \frac{\exp\bigl(\mu/(k_{\mathrm{B}}T)\bigr)}{\Xi_{\mathrm{C}}} \sum_{N=0}^{\infty} \frac{Q(N+1,V,T)}{N!} \exp\bigl(\mu N/(k_{\mathrm{B}}T)\bigr).\end{aligned}$$

For ideal gases, we have

$$Q(N,V,T) = q(V,T)^N = \left(\sum_i \exp\bigl(-\epsilon_i/(k_{\mathrm{B}}T)\bigr)\right)^N = Q(N+1,V,T)/q(V,T).$$

So the occupation number can be simply written as

$$\begin{aligned}\langle N\rangle &= \frac{\exp\bigl(\mu/(k_{\mathrm{B}}T)\bigr)\, q(V,T)}{\Xi_{\mathrm{C}}} \sum_{N=0}^{\infty} \frac{Q(N,V,T)}{N!} \exp\bigl(\mu N/(k_{\mathrm{B}}T)\bigr) \\ &= \exp\bigl(\mu/(k_{\mathrm{B}}T)\bigr)\, q(V,T) \\ &= \sum_i \exp\left(-\frac{\epsilon_i-\mu}{k_{\mathrm{B}}T}\right).\end{aligned}$$

In retrospect, this is natural since the abover representation used the fact that the single particle state is well-defined. The latter is meaningful only for non-interacting particles.

(November 16, 2016)