QUALIFYING EXAMINATION, Part 4

Solutions

Problem 1: Statistical Mechanics I

(a) The classical single-particle partition function z is

$$z = \int \frac{dx\,dp}{2\pi\hbar}\, e^{-\beta E(p,x)} = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dp\, e^{-\frac{\beta p^2}{2m}} \int_a^{\infty} dx\, e^{-\beta V(x)} = \left(\frac{m}{2\pi}\right)^{1/2} \frac{1}{\hbar b \beta^{3/2}} e^{-\beta ab} \ .$$

The partition function of the N identical non-interacting particles is is given by

$$Z = \frac{z^N}{N!} = \frac{1}{N!}\left(\sqrt{\frac{m}{2\pi}}\frac{1}{\hbar b\beta^{3/2}} e^{-\beta ab}\right)^N \ .$$

The free energy is given by

$$\begin{aligned} F &= -k_B T \ln Z \approx -k_B T\left(N \ln \frac{\sqrt{m/2\pi}}{\hbar b \beta^{3/2}} - N\ln N + N\right) + Nab \\ &= -Nk_B T \ln \frac{e\sqrt{m/2\pi}}{\hbar b\beta^{3/2} N} + Nab \ . \end{aligned}$$

(b) If the wall moves by a small distance da, the work done by the gas is $f da$. At constant temperature, this is equal to the decrease in the *free* energy, i.e., $dF = -f da$ (more generally $dF = SdT - f da$). We then have

$$f = -\left(\frac{\partial F}{\partial a}\right)_{T,N} = -Nb \ .$$

(c) The probability of finding a particle at x is proportional to $e^{-\beta V(x)} = e^{-\beta b x}$. The density $n(x)$ should be normalized, $\int_a^\infty n(x) = N$, which gives

$$n(x) = \frac{Nb}{k_B T} e^{-\beta b(x-a)} \ .$$

(d) In terms of $n(x=a)$, we have

$$f = -n(x=a) k_B T \ .$$

This relation is the same as the ideal gas law in 1D, and it holds for any confining potential $V(x)$. One can see that this is the case by considering the gas in a small interval $[x, x+\Delta x]$, where Δx is sufficiently large compared to the mean distance between gas particles near the wall, but much smaller than the length scale on which the potential varies. For such a small interval the variation of the potential can be ignored and the gas should follow the ideal gas law. Therefore $f = -nk_BT$ holds locally.

We can also derive this relation directly. For a general confining potential $V(x)$, the partition function is

$$Z = \frac{1}{N!}\left(\frac{m}{2\pi\hbar^2\beta}\right)^{N/2}\left(\int_a^\infty dx\, e^{-\beta V(x)}\right)^N ,$$

and it follows that the free energy is

$$F = -k_BT\ln Z = -k_BT\left(N\ln\sqrt{\frac{m}{2\pi\hbar^2\beta}} - \ln N!\right) + Nk_BT\ln\left(\int_a^\infty dx\, e^{-\beta V(x)}\right) .$$

The force is then given by

$$f = -\left(\frac{\partial F}{\partial a}\right)_{T,N} = -Nk_BT\frac{e^{-\beta V(a)}}{\int_a^\infty dx\, e^{-\beta V(x)}} .$$

Generalizing the calculation in (c), the density at x is

$$n(x) = \frac{Ne^{-\beta V(x)}}{\int_a^\infty dx\, e^{-\beta V(x)}} .$$

Thus $f = -n(a)k_BT$ for any confining potential.

Problem 2: Statistical Mechanics II

(a) The energy spectrum of the 1D harmonic oscillator is $\epsilon_n = \hbar\omega(n + \frac{1}{2})$, where n is a non-negative integer. At $T = 0$, the single-species fermions occupy each level of the harmonic oscillator up to ϵ_{F}. Hence for N fermions

$$\epsilon_{\mathrm{F}} = \hbar\omega\left(N - \frac{1}{2}\right) .$$

(b) (i) The total energy at $T = 0$ is the sum of all single-particle energies up to ϵ_{F}. Thus

$$\frac{E}{N} = \frac{1}{N}\sum_{j=0}^{\infty}\epsilon_j\langle n_j\rangle = \frac{\hbar\omega}{N}\sum_{j=0}^{N-1}\left(j + \frac{1}{2}\right) = \frac{\hbar\omega}{N}\frac{N^2}{2} = \frac{\hbar\omega N}{2} .$$

(ii) For the 1D harmonic oscillator, the states are equally spaced by $\hbar\omega$, and thus the number of states of energy smaller than ϵ is $N_s(\epsilon) = \epsilon/(\hbar\omega)$. It follows that the *average* density of states is constant, $g(\epsilon) = dN_s/d\epsilon = 1/\hbar\omega$. In the continuum limit, the average energy per particle is then

$$\frac{E}{N} = \frac{1}{N}\int_0^{\epsilon_{\mathrm{F}}}\epsilon g(\epsilon)\mathrm{d}\epsilon = \frac{1}{N}\frac{\epsilon_{\mathrm{F}}^2}{2\hbar\omega} \approx \frac{N\hbar\omega}{2} .$$

(c) The grand-canonical partition function is $Z_{\mathrm{GC}} = \prod_{n=0}^{\infty}\ln(1 + e^{-\beta(\hbar\omega(n+1/2)-\mu)})$ (where $1/\beta = k_{\mathrm{B}}T$), so the grand potential is

$$\Omega(\mu, T) = -k_{\mathrm{B}}T\sum_{n=0}^{\infty}\ln[1 + e^{-\beta(\hbar\omega(n+1/2)-\mu)}] .$$

(d) The average total particle number $\bar{N}$ is

$$\bar{N} = -\left(\frac{\partial\Omega}{\partial\mu}\right)_T = \sum_{n=0}^{\infty}\frac{1}{e^{\beta(\hbar\omega(n+1/2)-\mu)} + 1} .$$

This equation can also be obtained from $\bar{N} = \sum_{j=0}^{\infty}\langle n_j\rangle$, where $\langle n_j\rangle$ is the Fermi-Dirac occupation number of level j.

(e) (i) The high-temperature regime corresponds to $\beta \to 0$ and $z \to 0$. In this case, the EoS reads

$$\lim_{z\to 0 \text{ and } \beta\to 0} N(\mu, T) = \sum_{n=0}^{\infty} ze^{-\beta\hbar\omega(n+1/2)} = \frac{ze^{-\beta\hbar\omega/2}}{1 - e^{-\beta\hbar\omega}} \approx \frac{z}{\beta\hbar\omega} = \frac{kT}{\hbar\omega}z .$$

(ii) The limit in (i) is the classical limit.