HW #7 Solutions

Problems 8.1, 8.2, 8.4, 8.5

8.1)

8.1 Find the density matrix for a partially polarized incident beam of electrons in a scattering experiment, in which a fraction f of the electrons are polarized along the direction of the beam and a fraction $1 - f$ is polarized opposite to the direction of the beam.

In general, we can express a mixed state of N particles with a density matrix

$$\rho = \sum_{i=1}^{n} \frac{N_i}{N} |\chi_i\rangle\langle\chi_i|$$

where $|\chi_i\rangle$ indicates the i^{th} state, where N_i particles are in this state. The "n" refers to the number of mixed states that make-up the system. For this problem there are two states, which I will denote by $|\uparrow\rangle$ & $|-\rangle$, where $|+\rangle$ denotes electrons polarized in the direction of the beam & $|-\rangle$ denotes electrons polarized in the opposite direction.

$$\Rightarrow \boxed{\rho = f|\uparrow\rangle\langle\uparrow| + (1-f)|-\rangle\langle-|}$$

8.2) **8.2** Derive the equations of state (8.67) and (8.71), using the microcanonical ensemble.

Section 8.5 steps us through most of the derivation of ideal Bose & Fermi gases using microcanonical ensemble theory, so I will just begin where they left off.

So let's start w/

$$\frac{S}{k} = \sum_i g_i\left[\frac{\beta\epsilon_i - \ln z}{z^{-1}e^{\beta\epsilon_i} \pm 1} \pm \ln(1 \pm z e^{-\beta\epsilon_i})\right]$$

(Huang 8.48)

$(\,) = \left(\begin{matrix}\text{Fermi}\\ \text{Bose}\end{matrix}\right)$

Additionally, since we know

$$\langle n_i \rangle = \frac{1}{z^{-1}e^{\beta\epsilon_i} \pm 1}$$

$(+)$ = Fermi
$(-)$ = Boson

We also have

$$\langle E \rangle = \sum_i g_i \epsilon_i n_i = \sum_i \frac{g_i \epsilon_i}{z^{-1}e^{\beta\epsilon_i} \pm 1}$$

For the purposes of this problem $g_i = 1$. To solve for the pressure, we consider that

$$P = -\left(\frac{\partial A}{\partial V}\right) \quad \& \quad A = U - TS = \langle E \rangle - TS$$

$$\Rightarrow A = \sum_i \cancel{\frac{\epsilon_i}{z^{-1}e^{\beta\epsilon_i} \pm 1}} - \sum_i\left[\cancel{\frac{\epsilon_i}{z^{-1}e^{\beta\epsilon_i} \pm 1}} - \frac{kT\ln z}{z^{-1}e^{\beta\epsilon_i} \pm 1} \pm kT\ln(1 \pm z e^{-\beta\epsilon_i})\right]$$

$$A = \sum_i \frac{kT\ln z}{z^{-1}e^{\beta\epsilon_i} \pm 1} \mp kT\ln(1 \pm z e^{-\beta\epsilon_i})$$

$$= kT\ln z \underbrace{\sum_i\left(\frac{1}{z^{-1}e^{\beta\epsilon_i} \pm 1}\right)}_{=N} \mp \sum_i \ln(1 \pm z e^{-\beta\epsilon_i})\, kT$$

$$= NkT\ln z \mp \sum_i \ln(1 \pm z e^{-\beta\epsilon_i})\, kT$$

As $V \to \infty$, we can consider the continuum limit. For Fermi statistics we get

$$\frac{A_F}{kT} = N \ln z - \frac{V}{h^3}\int_0^\infty 4\pi p^2 dp \ln\left(1+ze^{-\beta p^2/2m}\right)$$

Then we can take the derivative wrt V to get the pressure, but we must keep in mind that z is a function of V

$$\Rightarrow \frac{P}{kT} = -\frac{N}{z}\frac{\partial z}{\partial V} + \frac{4\pi}{h^3}\int_0^\infty p^2 dp \ln\left(1+ze^{-\beta p^2/2m}\right)$$

$$+ \underbrace{\frac{4\pi V}{h^3}\int_0^\infty p^2 dp \frac{z^{-1}}{z^{-1}e^{-\beta p^2/2m}+1}}_{=N}\left(\frac{\partial z}{\partial V}\right)$$

So the first & last term cancel, so that we arrive @

$$\boxed{\frac{P}{kT} = \frac{4\pi}{h^3}\int_0^\infty p^2 dp \ln\left(1+ze^{-\beta p^2/2m}\right)}$$

I don't know if this is explicitly stated in the book but the chemical potential is essentially given by

$$\mu N = G \longleftarrow \text{Gibbs free energy}$$

$$\therefore \quad N d\mu = V dp - S dT \quad \text{for } N \text{ held-constant}$$

$$\Rightarrow \frac{N}{V} = \left(\frac{dP}{d\mu}\right)_T = \frac{\partial P}{\partial \ln z}\frac{1}{kT} = \frac{z}{kT}\frac{\partial P}{\partial z}$$

$$\Rightarrow \boxed{\frac{1}{v} = \frac{4\pi}{h^3}\int_0^\infty dp\, p^2 \frac{1}{z^{-1}e^{\beta p^2/2m}+1}}$$

We see that these expressions match (8.67). We can use a similar process for the ideal Bose gas

For Bose Statistics, we first split off the $\vec{p}=0$ contribution, since in the limit $p\to 0$ & $z\to 1$, $\ln(1-ze^{-\beta\epsilon_p})$ diverges & therefore can dominate contributions to the free energy

$$\Rightarrow \frac{A_B}{kT} = N\ln z + \ln(1-z) + \frac{V}{h^3}\int_0^\infty 4\pi p^2 \ln(1-ze^{-\beta p^2/2m})$$

However, we see that, because of the 2^{nd} term we will not get a cancellation of all $\partial z/\partial V$ terms after taking derivatives w.r.t. V. So I'll highlight a different approach. Instead begin w/

$$N = \sum_p \frac{ze^{-\beta\epsilon_p}}{1-ze^{-\beta\epsilon_p}} \simeq \frac{z}{1-z} + \frac{V}{h^3}\int_0^\infty 4\pi p^2 dp \frac{1}{z^{-1}e^{\beta p^2/2m}-1}$$

using the same logic as before. Immediately we get

$$\boxed{\frac{1}{v} = \frac{1}{V}\frac{z}{1-z} + \frac{4\pi}{h^3}\int_0^\infty p^2 dp \frac{1}{z^{-1}e^{\beta p^2/2m}-1}}$$

Recalling that

$$\frac{1}{v} = \frac{z}{kT}\left(\frac{\partial P}{\partial z}\right)_T \Rightarrow \frac{P}{kT} = \int \frac{dz}{z}\frac{1}{v}$$

$$\Rightarrow \boxed{\frac{P}{kT} = -\frac{4\pi}{h^3}\int_0^\infty dp\, p^2 \ln(1-ze^{-\beta p^2/2m}) - \frac{1}{V}\ln(1-z)} \; *$$

We see that this is the same as (8.71)

* Technically there is a constant of integration that depends on temperature, but you could show that it doesn't contribute.

8.4)

8.4 Verify (8.49) for Fermi and Bose statistics, i.e., the fluctuations of cell occupations are small.

Solution is given in the book

8.5)

8.5 Calculate the grand partition function for a system of N noninteracting quantum mechanical harmonic oscillators, all of which have the same natural frequency ω_0. Do this for the following two cases:

(*a*) Boltzmann statistics

(*b*) Bose statistics.

Suggestions. Write down the energy levels of the N-oscillator system and determine the degeneracies of the energy levels for the two cases mentioned.

(a) I will start off with Boltzmann statistics. The energy levels of the Quantum Harmonic Oscillator is given by

$$\varepsilon_k = (k+1/2)\hbar\omega$$

Therefore we can write the partition function for a single particle using Boltzmann statistics as

$$Q_1 = \sum_k e^{-\beta\varepsilon_k} = \frac{1}{e^{+\beta\hbar\omega/2} - e^{-\beta\hbar\omega/2}} = \frac{1}{2\sinh(\beta\hbar\omega/2)}$$

For N-independent (indistinguishable) QHO's, we have

$$Q_N = \frac{1}{N!} Q_1^N$$

$$\therefore \mathcal{Z} = \sum_{N=0}^{\infty} z^N Q_N = \sum_{N=0}^{\infty} \frac{(zQ_1)^N}{N!} = \exp[zQ_1]$$

$$\Rightarrow \boxed{\ln\mathcal{Z} = zQ_1 = \frac{z}{2\sinh(\beta\hbar\omega/2)}}$$

(b) To address the Bose statistics, we go the usual route of writing the grand partition function as

$$\mathcal{Z} = \sum_{N=0}^{\infty} \sum_{\substack{\{n_k\} \\ \Sigma n_k = N}} z^N e^{-\beta E[\{n_k\}]} \quad \text{where} \quad E[\{n_k\}] = \sum_k \varepsilon_k n_k$$

$$= \sum_{N=0}^{\infty} \sum_{\substack{\{n_k\} \\ \Sigma n_k = N}} \exp\Big[\beta \sum_k n_k(\mu - \varepsilon_k)\Big]$$

$$\mathcal{Z} = \sum_{N=0}^{\infty} \sum_{\substack{\{n_k\} \\ \sum n_k = N}} \prod_k \exp\left[-\beta n_k(\varepsilon_k - \mu)\right]$$

Recall that we can rearrange the products & sums as

$$\mathcal{Z} = \prod_k \sum_{n=0}^{\infty} \exp\left[-\beta n(\varepsilon_k - \mu)\right]$$

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

Note that if we used this same process w/ Boltzmann statistics, we would have an additional factor of $1/n!$, which would give us the same answer as before

$$\Rightarrow \boxed{\ln \mathcal{Z} = -\sum_{k=0}^{\infty} \ln\left(1 - z e^{-\beta\hbar\omega(k+1/2)}\right)}$$