Physics 112 Fall 2017 Professor William Holzapfel Homework 9 Solutions

Problem 1, Kittel 7.13: Chemical Potential versus Concentration

(a) We know for a classical ideal gas $\mu/\tau = \ln\left(\frac{n}{n_Q}\right)$, so for $\frac{n}{n_Q} \ll 1$ we expect a logarithmic behavior of the chemical potential. We've also seen that for a degenerate Bose gas $\left(\frac{n}{n_Q}\gg 1\right)$ the chemical potential acts like $\mu/\tau \approx -\frac{1}{N}$. In the thermodynamic limit, $N\gg 1$ so we essentially have $\mu\approx 0$ for $\frac{n}{n_Q}>1$. This behavior is plotted in figure 1.

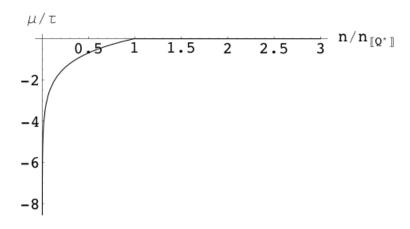


Figure 1: μ/τ vs. n/n_Q is plotted for a Bose gas.

(b) For fermions we have the same ideal gas behavior for $\frac{n}{n_Q} \ll 1$, but for $\frac{n}{n_Q} \gg 1$, we will have a degenerate Fermi gas with $\mu \simeq \epsilon_F$. We can rewrite the expression for the Fermi energy in terms of $\frac{n}{n_Q}$, using $n_Q \equiv \left(\frac{m\tau}{2\pi\hbar^2}\right)^{3/2}$:

$$\epsilon_f = \frac{\hbar^2}{2m} (3\pi^2 n)^{2/3}$$
$$= \frac{\tau}{4\pi} (3\pi^2)^{2/3} \left(\frac{n}{n_Q}\right)^{2/3}$$

So we see that $\mu/\tau \sim \left(\frac{n}{n_Q}\right)^{2/3}$ for a Fermi gas with $\frac{n}{n_Q} \gg 1$. We've graphed this behavior in figure 2.

The important thing to notice is that in a Bose gas, the chemical potential is always negative (as measured from the ground state energy) or close to zero (when Bose-Einstein condensation

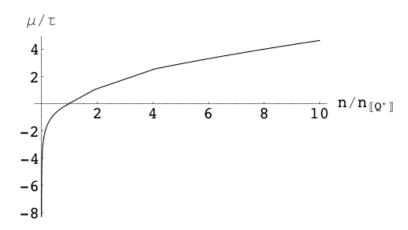


Figure 2: μ/τ vs. n/n_Q for a Fermi gas.

occurs), whereas in a Fermi gas, the chemical potential becomes positive in the quantum (degenerate) limit.

Problem 2, Kittel 7.14: Two Orbital Boson System

If the occupation of the ground state $(\epsilon_0 = 0)$ is twice that of the first excited state $(\epsilon_1 = \epsilon)$, then because there are only two states we have $f(\epsilon_0, \tau) + f(\epsilon_1, \tau) = N$ and hence

$$f(\epsilon_0, \tau) = \frac{2}{3}N$$

$$f(\epsilon_1, \tau) = \frac{1}{3}N.$$

The occupation of each state is given by the Bose-Einstein distribution function:

$$f(\tau,0) = \frac{1}{e^{-\mu/\tau} - 1} = \frac{2}{3}N,$$
 (1)

$$f(\tau, \epsilon) = \frac{1}{e^{(\epsilon - \mu)/\tau} - 1} = \frac{1}{3}N. \tag{2}$$

Solving equation (??) for $e^{-\mu/\tau}$ gives

$$e^{-\mu/\tau} = 1 + \frac{3}{2N}.$$

We can plug this into (??) and solve for $\tau(\epsilon)$, yielding

$$e^{\epsilon/\tau} = \frac{1+\frac{3}{N}}{1+\frac{3}{2N}} \approx \left(1+\frac{3}{N}\right)\left(1-\frac{3}{2N}\right) \approx 1+\frac{3}{2N}.$$

We can take the log of both sides, and expand the log using $\log(1+x) \approx x$ for $x \ll 1$:

$$\epsilon/\tau \approx \ln\left(1 + \frac{3}{2N}\right) \approx \frac{3}{2N}.$$

Thus the temperature at which the first excited state has half the number of particles as the ground state is

 $\tau \approx \frac{2N\epsilon}{3}$

which is much higher than ϵ !

Problem 3: Bose Einstein Condensation with Rb 87

(a) For a particle in a 3D box $\epsilon_{\vec{n}} = \frac{\hbar^2 \pi^2}{2mL^2} (n_x^2 + n_y^2 + n_z^2)$. The ground state has $\vec{n} = (1, 1, 1)$ with corresponding energy

$$\epsilon_0 = \frac{\hbar^2 \pi^2}{2mL^2} \cdot 3 = \frac{3 \times \pi^2 \times (1.05 \times 10^{-34})^2}{2 \times 87 \times 1.66 \times 10^{-27} \times 10^{-10}}$$

$$= 1.13017 \times 10^{-32} \text{ J.}$$
(3)

(b) The Bose-Einstein condensation temperature is given by the expression derived in lecture:

$$\tau_E = \frac{2\pi\hbar^2}{m} \left(\frac{N}{2.612V}\right)^{2/3} = \frac{2\pi \times (1.05 \times 10^{-34})^2}{87 \times 1.66 \times 10^{-27}} \left(\frac{10^4}{2.612 \times 10^{-15}}\right)^{2/3}$$
$$= 1.17 \times 10^{-30} \text{ J}$$
$$\implies T_E = 8.50 \times 10^{-8} \text{ K}.$$

This is about two orders of magnitude larger than the ground state energy. This emphasises the point that Bose-Einstein condensation is a special feature of the statistics of many bosons, and occurs at a much higher temperature than the temperature at which single particle is likely to be in the ground state on its own.

(c) In lecture (and the book) we derived the relation for a Bose gas below the Einstein temperature: $\frac{N_e}{N} \approx \left(\frac{\tau}{\tau_E}\right)^{3/2}$, so the number of particles in the ground state is:

$$N_0 = N - N_e = N \left(1 - \left(\frac{\tau}{\tau_E} \right)^{2/3} \right) = 10^4 \times \left(1 - (0.9)^{2/3} \right)$$

 $\approx 1.460 \text{ Atoms.}$

The Bose-Einstein distribution function relates the occupation of the ground state to the chemical potential:

$$f(\epsilon_0, \tau, \mu) = \frac{1}{e^{(\epsilon_0 - \mu)/\tau} - 1} = N_0$$
 (4)

This can be solved for the chemical potential,

$$\mu = \epsilon_0 - \tau \ln \left(1 - \frac{1}{N_0} \right) \approx \epsilon_0 - \frac{\tau}{N_0}$$
$$= 1.058 \times 10^{-32} \text{ J}$$

which combined with (??) tells us that $\epsilon_0 - \mu \approx 8 \times 10^{-34}$ J, over ten times smaller than ϵ_0 itself.

Now that we have the chemical potential and the temperature, we can plug them into the distribution function to find the occupation of one of the first excited states using $\epsilon_1 = \frac{\hbar^2 \pi^2}{2mL^2} \left(n_x^2 + n_y^2 + n_z^2 \right) = \frac{\hbar^2 \pi^2}{2mL^2} \cdot 6 = 2\epsilon_0$:

$$N_1 = \frac{1}{e^{(\epsilon_1 - \mu)/\tau} - 1} \approx 93 \text{ Atoms}$$

So there are 93 atoms in each of the three degenerate states with energy ϵ_1 . (Remember, the distribution function tells us the occupancy of a *single* orbital with energy ϵ , not the total occupancy of all degenerate orbitals with energy ϵ ; if there are n degenerate orbitals with energy ϵ , the total occupancy of the entire energy level is $n \cdot f(\epsilon)$. We saw this in problem 1 on problem set 6).

(d) Repeating the above calculations for 10^6 atoms, the Einstein temperature is:

$$\tau_E = \frac{2\pi \times (1.05 \times 10^{-34})^2}{87 \times 1.66 \times 10^{-27}} \left(\frac{10^6}{2.612 \times 10^{-15}}\right)^{2/3} = 2.5 \times 10^{-29} \text{ J},$$

$$T_E = 2.8 \times 10^{-6} \text{ K}.$$

The number of particles in the ground state at $\tau = .9\tau_E$ is given by

$$N_0 = N - N_e = N \left(1 - \left(\frac{\tau}{\tau_E} \right)^{2/3} \right) = 10^6 \times \left(1 - (0.9)^{2/3} \right) = 146,000 \text{ Atoms}$$

and the chemical potential is:

$$\mu = \epsilon_0 - \tau \ln \left(1 - \frac{1}{N_0} \right) \approx \epsilon_0 - \frac{\tau}{N_0} = 1.115 \times 10^{-32} \text{ J}.$$

The number of particles in the first excited state is then

$$N_1 = \frac{1}{e^{(2\epsilon_0 - \mu)/\tau} - 1}$$

$$\approx 2,000 \text{ atoms.}$$
(5)

To find a condition which ensures that $N_0 \gg N_1$, we first invert (??) to get

$$e^{(\epsilon_0 - \mu)/\tau} = 1 + 1/N_0. \tag{7}$$

Plugging this into (??) gives

$$N_{1} = \frac{1}{e^{\epsilon_{0}/\tau}e^{(\epsilon_{0}-\mu)/\tau} - 1}$$

$$= \frac{1}{e^{\epsilon_{0}/\tau}(1 + 1/N_{0}) - 1}$$

$$\approx \frac{1}{(1 + \epsilon_{0}/\tau)(1 + 1/N_{0}) - 1}$$

$$\approx \frac{1}{\epsilon_{0}/\tau + 1/N_{0}}.$$

Using this, the inequality $N_1 \ll N_0$ becomes

$$1/N_0 \ll \epsilon_0/\tau + 1/N_0 \tag{8}$$

$$\Leftrightarrow \frac{\epsilon_0 N_0}{\tau} \gg 1 \tag{9}$$

$$\Leftrightarrow \epsilon_0 N_0 \gg \tau.$$
 (10)

It's interesting to contrast this result with what we'd get if the particles were distinguishable. In that case, you would only get many more particles in the ground state if $\tau < \epsilon_1 - \epsilon_0 = \epsilon_0$, a much more restrictive condition than (??).

Problem 4: Bose Gas in One Dimension

(a) In 3D we know that Bose-Einstein condensation occurs when $\mu \sim 0$, because the number of particles in the excited states in this regime

$$N_e = \int_0^\infty d\epsilon \, D(\epsilon) f(\epsilon, \tau < \tau_E, \mu \approx 0) \approx 2.61 V \left(\frac{m\tau}{2\pi\hbar^2}\right)^{3/2}$$
 (11)

is a finite number, independent of the total number of particles N in the system. This is the signature of Bose-Einstein condensation; if we put any more particles in the system, they must go into the ground state.

To see if Bose-Einstein condensation occurs in 1D, we can repeat the calculation of the total number of particles in excited states, using the 1D density of states we found in problem set 8, $D = \frac{L}{\pi} \left(\frac{2m}{\hbar^2 \epsilon}\right)^{1/2}$:

$$N_e = \int_0^\infty d\epsilon \, D(\epsilon) f(\epsilon, \tau, \mu \approx 0) = \int_0^\infty d\epsilon \frac{L}{\pi} \left(\frac{2m}{\hbar^2}\right)^{1/2} \frac{\epsilon^{-1/2}}{e^{\epsilon/\tau} - 1}$$

To evaluate this integral, let's first break it up into two pieces: an integral from $\epsilon = 0 \to \alpha$ and an integral from $\alpha \to \infty$, where $\alpha \ll 1$. For $\epsilon = 0 \to \alpha$ we can expand the exponential, and perform the integral:

$$\frac{L}{\pi} \left(\frac{2m}{\hbar^2}\right)^{1/2} \int_0^{\alpha} d\epsilon \frac{\epsilon^{-1/2}}{e^{\epsilon/\tau} - 1} \approx \frac{L}{\pi} \left(\frac{2m}{\hbar^2}\right)^{1/2} \int_0^{\alpha} d\epsilon \frac{\epsilon^{-1/2}}{(1 + \epsilon/\tau) - 1}$$

$$= \frac{L\tau}{\pi} \left(\frac{2m}{\hbar^2}\right)^{1/2} \int_0^{\alpha} d\epsilon \epsilon^{-3/2}$$

$$= \frac{L\tau}{\pi} \left(\frac{2m}{\hbar^2}\right)^{1/2} \left(-2\frac{1}{\epsilon^{1/2}}\Big|_0^{\alpha}\right)$$

$$\to \infty \text{ as } \alpha \to 0.$$

Since this integral diverges at $\epsilon = 0$, we conclude that we can put as many particles as we want in the excited states, which suggests that a Bose-Einstein condensate doesn't form. Don't take this calculation too seriously, though; in 2D the integral diverges but a Bose-Einstein

condensate can still form (see remark in **(b)**), and as Kittel admits, even in 1D this calculation should be done with a discrete sum, not an integral approximation.

(b) A sufficient (but not necessary!) condition for Bose-Einstein condensation to occur is that the integral in part (a) be finite. The potentially divergent piece of the integral is proportional to:

 $\int_0^\alpha d\epsilon \, \frac{\epsilon^a}{e^{\epsilon/\tau} - 1} \sim \tau \int_0^\alpha d\epsilon \, \epsilon^{a-1}$

where a is the power of ϵ in the density of states $D(\epsilon) \sim \epsilon^a$. This integral is convergent at $\epsilon = 0$ when a > 0, so Bose Einstein condensation will occur when the density of states is proportional to a positive power of the energy. In 2D the density of states is independent of the energy and so a = 0, yet Bose-Einstein condensation *still* occurs; the analysis in this case is subtler, however. See Pathria, *Statistical Mechanics*, 2nd. ed., pg. 190 exercise 7.13 for details.