PHYS4031 STATISTICAL MECHANICS

SAMPLE QUESTIONS FOR DISCUSSION IN WEEK 12 EXERCISE CLASSES (21, 23 November 2016)

You may want to think about them before attending exercise class.
SQ28 - Applying and making sense of the Sommerfeld expansion
SQ29 - How does $\mu \to 0$ from below in Bose gas and the concept of macroscopic occupation of single-particle ground state

SQ28 **The Sommerfeld expansion - Using it and making sense of it.**

Summary on Key Equations: In studying ideal Fermi gas, the key equations are

$$N = \sum_{s.p.\ states\ i} \frac{1}{e^{(\epsilon_i - \mu)/kT} + 1} \tag{1}$$

$$E = \sum_{s.p.\ states\ i} \frac{\epsilon_i}{e^{(\epsilon_i - \mu)/kT} + 1} \tag{2}$$

$$pV = kT \sum_{s.p.\ states\ i} \ln\left(1 + e^{-(\epsilon_i - \mu)/kT}\right) \tag{3}$$

where the summations are **over all single-particle states**. Equations (1) and (2) have clear physical interpretation as the Fermi-Dirac distribution gives the number of fermion in a single-particle state. Equation (3) follows from $pV = -\Omega = kT \ln Q_F$. **These equations are general** in that they can be used to study ideal Fermi gas in any spatial dimension with any $\epsilon(k)$ dispersion relation.

In applying these equations to ideal Fermi gas, we turn the summations into integrals by invoking the **density of states** $g(\epsilon)$, as discussed in Chapter VIII. In doing so, we encounter integrals of the following form

$$\boxed{\int_0^\infty \frac{f(\epsilon)}{e^{(\epsilon-\mu)/kT} + 1}\, d\epsilon} \tag{4}$$

where $f(\epsilon)$ is some function of the single-particle energy ϵ. For example, Eq. (1) gives $f(\epsilon) = g(\epsilon)$, Eq. (2) gives $f(\epsilon) = \epsilon g(\epsilon)$, and Eq. (3) gives $f(\epsilon) = g(\epsilon)\ln\left(1 + e^{-(\epsilon-\mu)/kT}\right)$. If you understand everything up to here, you are in good shape.

Sommerfeld Expansion: In Fermi gas physics, the $T = 0$ physics and $kT \ll \mu$ (low-temperature) physics are the most important. It is because the Pauli Exclusion Principle imposes an energy scale E_F that is usually high comparing with the ordinary temperature (thus kT) that we want to study the system. For $kT \ll \mu$, the following Sommerfeld formula can be used

$$\boxed{\int_0^\infty \frac{f(\epsilon)}{e^{(\epsilon-\mu)/kT} + 1}\, d\epsilon \approx \int_0^\mu f(\epsilon) d\epsilon + \frac{\pi^2}{6}(kT)^2 f'(\mu)} \tag{5}$$

where

$$\boxed{f'(\mu) \equiv \left(\frac{df(\epsilon)}{d\epsilon}\right)\Bigg|_{\epsilon=\mu}} \tag{6}$$

In our course, you are not expected to know how to derive the formula, but you are expected to know how to apply the formula.

(a) **Applying the formula:** Let's say there is a situation in which the density of states has the form $g(\epsilon) = \mathcal{A}\epsilon^2$, **illustrate** how Eq. (1) and Eq.(2) can be treated by the Sommerfeld expansion. [Don't need to work out the Fermi gas physics. Just show clearly how to apply Eq. (5).]

(b) **Making sense of it: Show** Eq. (5) (in a more physical than mathematical way).

SQ29 **How does $\mu \to 0$ from below in Bose gas? (Related to Ch.VII, Ch.XII and Ch.XIV)**

In Ch.VII and Ch.XII, we derived the Bose-Einstein distribution (twice) and stressed that its physical meaning is the number of bosons in a single-particle state of energy ϵ. **Such a number cannot be negative.** This simple physical sense has important implication.

The general expression for the number of bosons N in a Bose gas is given by

$$N = \sum_{s.p.\ states\ i} \frac{1}{e^{(\epsilon_i - \mu)/kT} - 1} \tag{7}$$

where the summation is over single-particle states. As the expression in the summation cannot be negative, it follows that the chemical potential μ must obey $\mu < \epsilon_i$ for *all* single-particle states i. Let ϵ_{lowest} be the lowest energy of the single-particle states (ground state), μ is then restricted to $\mu < \epsilon_{lowest}$ to make sure that the number of bosons in any state will NOT be negative. Practically, ϵ_{lowest} (recall particle-in-a-BIG-box) can be taken as zero. **Therefore, $\mu < 0$ and this statement must be true at all temperatures.** Observe that for fermions (see Eq. (1)), we don't need to worry because of the "+1" in the denominator. Thus the "-1" in the Bose-Einstein distribution makes a lot of differences.

Here, TA will show the mathematical form of how $\mu \to 0$ from below.

(a) Let N_0 be the number of bosons in the lowest single-particle state, i.e., the state with $\epsilon_{lowest} = 0$. Single out N_0 from Eq.(7) and **show that**

$$\mu = -kT \ln \left(1 + \frac{1}{N_0}\right) . \tag{8}$$

Immediately, one sees $\mu < 0$ for all temperatures.

(b) For bosons, any number of them could occupy a single-particle state. In the limit of $T \to 0$, we would expect $N_0 \to N$, as all the bosons can occupy the single-particle ground state and thus μ becomes 0. Fine! But here is the **key point**. In many cases, we don't need to go to $T = 0$. Instead for a range of low-temperatures $T < T_c$, N_0 becomes **a macroscopic number**. What it really means is that **a finite fraction of bosons** in the system go into the single-particle ground state. Thus, in the thermodynamic limit, $N \to \infty$ and $V \to \infty$ with N/V = finite, a finite fraction implies $N_0 \to \infty$. Show that in this case,

$$\mu \sim -kT \frac{1}{N_0} \to 0 \tag{9}$$

for $T < T_c$. In technical jargon, when the ground state is **macroscopically occupied** at sufficient low temperatures, we have **Bose-Einstein condensation**. In other words, Bose-Einstein condensation refers to the macroscopic occupation of the ground state at low temperatures.

[Remark: The idea of **macroscopic occupation** of the ground state is important. When there is a bit of inter-particle interaction between the bosons, even the $T = 0$ state may not consist of all the bosons in the ground state. However, as long as there is a macroscopic occupation (a finite fraction of the whole system of bosons) of the ground state, there is Bose-Einstein condensation. In contrast, we could have one or two fermions (spin) in the single-particle ground state even as $T \to 0$, thus no macroscopic occupation of single-particle ground state for a Fermi gas.]

(c) Hence, put the information together and sketch schematically $\mu(T)$ for an 3D ideal Bose gas.