Physics 114 Statistical Mechanics Spring 2021
Week 11 Conceptual Overview

Concept checklist from Readings:

- **Fermions ...** Electrons in solids can be surprisingly well treated, despite the fact that they are charged, as noninteracting. This is a *free electron model.*

- You might think the simplest place to start the topic of fermi gasses is to treat them at high temperature. But no, fermions are simpler to understand when T=0, since then $\bar{n}_{FD}(\epsilon)$ is a step or "heaviside" function: $\bar{n}_{FD}(\epsilon, T = 0) = \Theta(\mu - \epsilon)$. As one of the problems this week shows for electrons in copper, room temperature is virtually a $T = 0$ situation for electrons in a solid, because the quantum volume λ^3 is very much larger than the volume per electron. These particles truly act as waves, and quantum mechanics is needed.

- Looking at the distribution function $f_{FD}(\epsilon)$ (Fig. 1 below) shows that the step from 1 to 0 occurs at $\epsilon = \mu(T = 0)$. We need to write $T = 0$ because we know that $\mu(T)$ is in general a function of T. (For example, $\mu \propto T^{3/2}$ for a classical ideal gas.) The *Fermi energy* ϵ_F is defined as $\epsilon_F = \mu(T = 0)$.

- Terminology: There are lots of Fermi things. k_F is the *Fermi wave number*, with $\epsilon_F = \frac{\hbar^2 k_F^2}{2m}$. The *Fermi temperature* comes from $\epsilon_F = kT_F$ Also, $p_F = \hbar k_F$ is the *Fermi momentum*, and $\lambda_F = h/p_F$ is the Fermi wavelength, which as we mention above, is much larger than the interatomic spacing in a crystal. There is also the *Fermi surface*, which for free electrons is just the surface of a $3N$ dimensional sphere in k (or p) space, with radius k_F (or p_F).

- The size of the Fermi energy is controlled by the number of particles, N, via
$$N = \int_0^{k_F} g(\mathbf{k}) d\mathbf{k} = \int_0^{\epsilon_F} g(\epsilon) d\epsilon$$
This math is easy with $g(\epsilon) \propto \epsilon^{1/2}$ in 3d (Fig. 1 below). For spin 1/2 particles (electrons, neutrons, ...) where we can have 2 spin states per energy, we get
$$\epsilon_F = \frac{\hbar^2}{2m} (3\pi^2 \frac{N}{V})^{2/3}$$

- The take home is that the Fermi level is an increasing function of the density of fermions: ϵ_F and T_F are proportional to $\rho^{2/3}$, while $p_F \propto \rho^{1/3}$. (Here, G&T use ρ for a number density, $\rho = N/V$.)

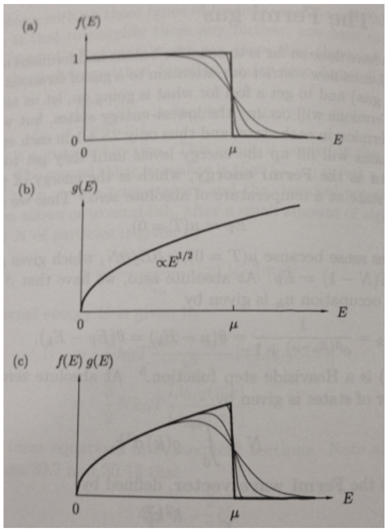

Figure 1: Occupation number (aka distribution function) , density of states, and their product for fermions. Note: μ on these graphs is $\mu(T=0)$.

- The energy, U can be found in the usual way: we take the integral of ϵ weighted by $\bar{n}(\epsilon)g(\epsilon)$. Above are graphs showing $\bar{n}$ and g; bold curves are for $T=0$, where we'd find $U=\frac{3}{5}\epsilon_F N$. Pressure is, as we've seen before for massive particles, $P=\frac{2}{3}\frac{U}{V}$. Thus $P=\frac{2}{5}\frac{N}{V}\epsilon_F$, and the bulk modulus, $-V\partial P/\partial V=\frac{2}{3}\frac{N}{V}\epsilon_F$.

- Now let's think about finite temperatures. In particular, $0 < T << T_F$. A big victory for the free electron gas model is that it gives a linear dependence of heat capacity on T as $T \to 0$. One can find C_V qualitatively by arguing that only an effective number $N_{eff} \propto N(T/T_F)$ of particles near the Fermi energy can get excited by temperature. This argument relies on asserting $\mu(T) \approx \epsilon_F$ when $T << T_F$. Thus $C_V \approx Nk(T/T_F)$.

- This argument can be made quantitative. In G&T 6.8, a long derivation yields (hooray)
$$C_V=\frac{\pi^2}{2}Nk\frac{T}{T_F}$$

- For $T >> 0$, we need $\mu(T)$ to decrease. Arguing qualitatively: The area under $\bar{n}(\epsilon)g(\epsilon)$ remains constant ... we want to discuss a constant number N of fermions. The fact that $\mu(T)$ changes by decreasing, is because $g(\epsilon)$ is an increasing function of ϵ. Figure 7.14 of Schroeder might be helpful to view here.

- The details of how $\mu(T)$ varies: hangs close to ϵ_f near $T=0$ but then starts to decrease, can be made quantitative as well. We can also find how $\bar{E}(T)$ and $C_v(T)$ vary with increasing temperature. Schroeder and B&B call this the *Sommerfeld expansion*. Please try to follow the arguments in these texts. The gist is that we expand $\bar{n}(\epsilon)$ in a Taylor expansion around ϵ_F. The expansion parameter can ultimately be recast as $\frac{T}{T_F}$. The end results are:

$$\mu(T) = \epsilon_F[1 - \frac{\pi^2}{12}(\frac{T}{T_F})^2 + ...] \quad T << T_F$$

$$E(T) = \frac{3}{5}N\epsilon_F[1 + \frac{5\pi^2}{12}(\frac{T}{T_F})^2 + ...] \quad T << T_F$$

$$C_v(T) = \frac{\pi^2}{2}Nk\frac{T}{T_F} \quad T << T_F$$

- Sometimes we want to go above T_F, though if the fermions are in a metal, it might melt first :-o. Both G&T problem 6.30 and Schroeder problem 7.32 fund $\mu(T)$ numerically. The chemical potential goes through zero at $T = T_F$, and becomes negative for higher temperatures (as we'd expect in a classical ideal gas :-).

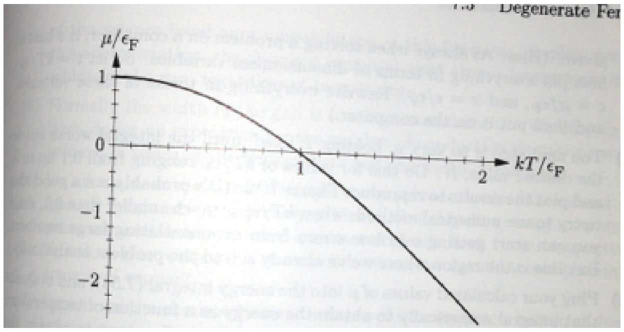

Figure 2: Figure 7.16 of Schroeder, chemical potential of ideal Fermi gas.

- **Quantum gasses at high and low temperatures ...** G&T problem 6.60 is about finding $P(T)$ for the ideal Fermi gas. G&T 6.61 is similar, for the ideal Bose gas. The gist is that there is a correction to $PV = NkT$, which is *positive* for Fermions, raising the pressure from the classical result:

$$PV = NkT\ [1 + \frac{\lambda_{th}^3}{2^{7/2}}\ (\frac{N}{V})\ + ...]$$

  and is *negative* for Bosons, lowering the pressure:

$$PV = NkT\ [1 - \frac{\lambda_{th}^3}{2^{5/2}}\ (\frac{N}{V})\ + ...]$$

- G&T Section 6.11.2 goes over the low temperature expansion of a Fermi gas. This is also done in both the B&B and Schroeder readings.

- **Bose-Einsten condensation ...** is weird and wonderful. When a boson gas has its temperature reduced past T_c, a substantial number of particles begin to occupy the same state, the ground quantum state. They stop contributing to pressure or viscosity . To understand why this transition occurs, we first we might think about how the chemical potential changes with T. Fixing N, the total number of bosons, we can in principle find μ via:

  $$N = \int_0^\infty \frac{1}{e^{\beta(\epsilon-\mu)} - 1} g(\epsilon) d\epsilon$$

  Calculated this way, using the classical density of states, $g(\epsilon) \propto \epsilon^{1/2}$, we find that the chemical potential rises to a value extremely close to zero as T gets very low. When μ actually reaches zero (or ϵ_0, the ground state energy ... which is close to zero in a real system, there will be one temperature $T = T_c$ that satisfies this equation.

  $$N = V\ \lambda_{th}^{-3}\ \frac{2}{\sqrt{\pi}} \int_0^\infty \frac{x^{1/2}}{e^x - 1} dx \quad with\ \lambda_{th} = \frac{h^2}{\sqrt{2\pi m k T_c}}$$

- The dimensionless integral above has the value 2.315, so

  $$N = 2.612\ V\lambda_{th}^{-3}\ \ \equiv Li_{3/2}(z=0)\ V\lambda_{th}^{-3}$$

  (The second expression follows the polylogarithm treatment in B&B.) This can only be true for one value of λ_{th}, hence one temperature, the *BEC transition temperature.* It will depends on the mass of particles and their density. From above:

  $$kT_c = 0.527\ \frac{h^2}{2\pi m}\ (\frac{N}{V})^{2/3}$$

- Why can't we have bosons with lower temperatures than T_c? We can, but we have to fix a problem in our formalism. We tried to find the temperature that gave us the known density N/V, by integrating energies from 0 to ∞. But below T_c we have *significant numbers of particles occupying the ground quantum state.* These are not accounted for in our integral weighted by $g(\epsilon)$, which happens to be zero at $\epsilon = 0$. We have to count low-lying quantum states using a sum, not an integral. The population of the ground state rises in a new way below T_c. A phase transition!

- The expressions for N above are correct, but only for the population of particles in the excited state. We thus write:

  $$N_0 = N - N_{excited} = N[1 - (\frac{T}{T_c})^{3/2}]$$

The N_0 particles that are "condensed" are in the ground energy state. So rather than thinking of them like a drop of water in a gas vapor, we should think of them as all slowed to their zero-point state of motion. In experiments, the atoms are localized in a magnetic trap. Here is a link to the Nobel prize lecture of Wolfgang Ketterle, who participated in the first experiment that found a BEC in ultra cold alkali halide atoms. Here's an MIT video about creating the BEC: `https://www.youtube.com/watch?v=u8wNSVxYZGI`.

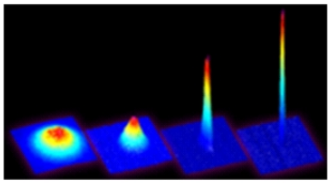

Figure 3: False color image of velocity space of Rubidium gas undergoing BEC -BaRbiE project, Univ. Ulm

- One can explore the thermodynamics of the $N_{excited}$ particles, as one moves through the BEC phase transition. B&B Fig. 30.6 plots z, $U(T)$, and $C_V(T)$, and problem 30.4 (not assigned) allows us to derive the inflection at $C_V(T = T_c)$ which heralds the transition.

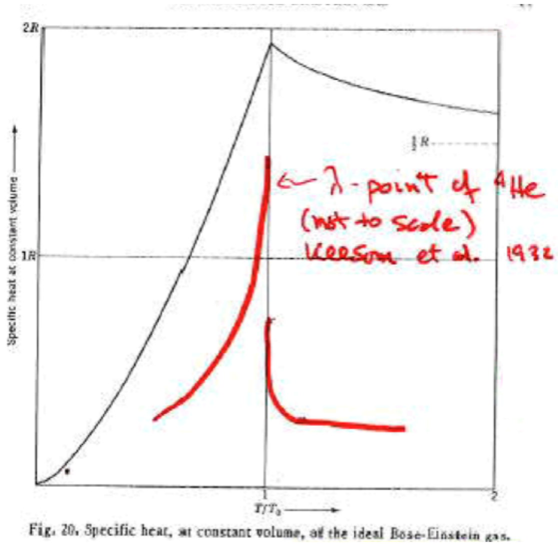

Figure 4: Specific heat of ideal bose gas, with superfluid helium specific heat cartooned in G. Baym lecture notes, Tokyo. 2004

- *Superfluidity* is a phenomenon related to BEC, though the differences are subtle. Superfluid bosons also share a quantum state, allowing them to escape through nanoscopic pores, move without viscosity, and

follow each other in gravity-defying streams. Cool videos of superfluids exist: e.g. `https://www.youtube.com/watch?v=2Z6UJbwxBZI` .
A Bose-Einstein condensate is not quite identical to a superfluid. Superfluids require interatomic interactions, whereas Bose-Einstein condensation is a result that emerges for noninteracting bosons.

- Bose-Einstein condensation is a *collective phenomenon*. A large number of bosons follow each other into the ground state. Were they distinguishable, there would be a very tiny fraction in the ground state, due to the many ways to distribute them among the many, many excited states around energy kT. (This is the essence of the canonical distribution. Because $E - TS$ is minimized, the large S of having particles in higher energy states fights with the low E of having them in lower energy states. The compromise for distinguishable, classical particles is that they hover around energy kT.) However, for bosons, there are far fewer excited state configurations available. The larger the number of bosons, N, the more important is the smallness of $e^{-\epsilon N/kT} \approx e^{-N}$, the probability of occupying a state of energy around kT. So the bosons lower their free energy by falling into the ground state. Like the degeneracy pressure of fermions, this is truly a result of bosons being identical! It is a demonstration that (as Schroeder says David Griffiths says) “even God cannot tell them apart”.