Physics 114 Statistical Mechanics Spring 2018
Seminar 11

Overview:

This is our second week studying *Fermi-Dirac* or *Bose-Einstein* particles in stat mech. Last week, we began with the general formalism: counting states of the system, finding free energy $\Omega = \Sigma_k \Omega_k$, and the occupation number $\bar{n}_k$ for states labelled with wave number $\vec{k}$. These led us, in a familiar way, to calculating statistical properties of interest. This week, we apply our understanding of boson statistics to quantized vibrations, or *phonons* in solids. We do the *Einstein solid* (familiar to us) and the *Debye solid* (new). (Next week, when we talk about phase transitions, we will do the *Bose Einstein Condensate (BEC)* .)

We also focus on fermions, half-integer spin particles, no two of which can occupy a single quantum state. The *ideal Fermi gas* is a starting place from which to model electrons moving in a solid, or the degeneracy pressure that keeps a neutron star from collapsing. A key idea is the *Fermi level* ... the highest energy level which N fermions fill at $T = 0^*$. We will look at this ground-state situation, and also look at higher temperatures, with particles excited beyond the Fermi level ... for example, the electrons which carry current in a conductor.

*Schroeder Problem 7.10, done as a warmup last week, had you filling energy levels separated by $\hbar\omega$. You did this for three kinds of particles. You hopefully saw that the lowest energy state for 5 fermions consisted of filling levels 0, 1, 2, 3, 4. So the "fermi energy" of this system was $10\hbar\omega$.

Required Reading:

G&T Sections

- 6.8, 6.9
- 6.11.2

B&B Sections

- Ch. 24
- 30.2 - 30.3

Schroeder Sections

- 7.3, 7.5

Presentations:

If life gets dull, Amy might talk about *Fermi surfaces* ... which bring stat mech and solid state physics together.

Concept checklist from Readings:

- **Quantized vibration in solids ...** Recall the Einstein model of solids. Now we have a new perspective on it. The q quanta of energy shared among the N oscillators are like q bosons. The expected energy per oscillator, e, is the ground state energy, $\hbar\omega/2$, plus the energy of $\bar{n}$ bosons ... each one carrying energy $\bar{\omega}$. That is:

  $$Z_1 = e^{-\beta\hbar\omega/2}\frac{1}{1-e^{-\beta\hbar\omega}}$$
  $$=> \ e = (1/2+\bar{n})\hbar\omega \ \ with \ \ \bar{n} = \frac{1}{e^{\beta\hbar\omega}-1}$$

  These new bosons are quanta which carry vibrational energy. Like photons, they have $\mu = 0$.

- We introduce a relevant, new temperature $T_E = \hbar\omega/k_B$. If we do the familiar calculation of C_v for the Einstein solid, we notice that for for $T >> T_E$ we are in the high T limit known as "Dulong-Petit" . This limit is just what we'd get from *equipartition*: $C_v = 3Nk_B$. (Notation alert: We have wave vectors k floating around now, so I have tried to write Boltzmann's constant as k_B ... but look out for typos.)

- The problem with the Einstein crystal's C_v is that it falls to zero much too fast as $T \to 0$. Not a theoretical problem, but an experimental one. Experiments give $C_v \propto T^3$ as $T \to 0$.

- The *Debye model* is an improvement. The same kind of summing over modes as we've done a couple times before, is now applied to lattice vibrations. Now our quantized vibrations are not independent oscillators as in the Einstein model, but the *normal modes* of a lattice of N atoms. Every quantized wave vector $\vec{k}$ is converted to a frequency based on the average speed of sound, $\bar{c}$, in the lattice:

  $$k\bar{c} = \omega$$

  This allows us to get the density of states:

  $$g(\omega)d\omega = \frac{3V\omega^2 d\omega}{2\pi^2\bar{c}^3}$$

- U can be found in the usual way, by integrating $\hbar\omega$ weighted by $\bar{n}(\omega)g(\omega)$ over all ω. However, we need to think about the limits of integration. Unlike E&M radiation in a box, solid vibrations have a shortest wavelength λ_D equal to the typical spacing between atoms. This is shown in problem G&T 6.35, which is assigned this week. It's equivalent to arguing that there is a high frequency cutoff ω_D, so we don't count more modes than there are. There can only be $3N$ *normal modes* of vibration in a 3d crystal with N atoms.

- This high energy low wavelength cutoff leads us to define an equivalent temperature, the *Debye temperature* $T_D = \hbar\omega_D/k_B$. We thus get:

$$U = N\ 9\frac{(k_B T)^4}{(k_B T_D)^3}\int_0^{T_D/T}\frac{x^3}{e^x - 1}dx$$

- At low T, $C_v \propto T^3$ which is what experiments show. Schroeder reminds us that in a metal, there is another contribution at low temperatures proportional to T, which is something we discuss below, the contribution from the "free electron gas" (i.e. the conduction electrons). At high T, the law of Dulong and Petit, $C_v = 3Nk$ is obeyed, just as for an Einstein solid. Hooray!

- B&B Section 24.3 gives us a glimpse of a situation where we can no longer treat phonons like particles-in-boxes. Now, is *not* the case that the *dispersion relation* is $\omega \propto k$. Nor is the density of states $g(\omega) \propto \omega^2$ in 3d. This analysis probably familiar to you from a Phys 111 seminar, where you looked at the *normal modes* of a system of masses, connected by springs. In this section, we can read the variable q as being like the wave number, k. We see the relationship between ω and q in Eq. (24.33) and Fig. 24.5 for a 1d chain of masses. Because $sin(qa/2) \propto (aq/2)$ for small q, the small-q limit is just like an Einstein or Debye model. For large q, the situation is different. Also different is $g(\omega)$. The low-ω limit is like a particle in a box. But higher ω behavior in Fig. 24.7 shows that $g(\omega)$ depends on the detailed way atoms are bound together in the copper solid.

- **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, $\rho = N/V$.)

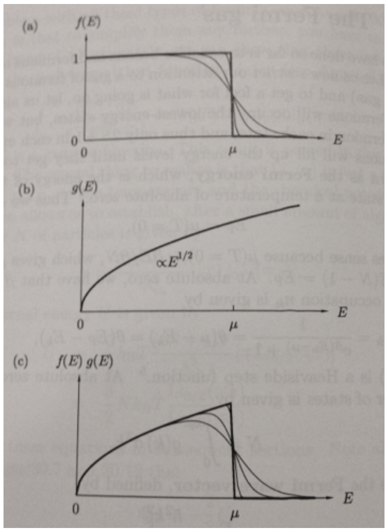

Figure 1: Occupation number (aka distribution function) , density of states, and their product for fermions. Note: μ on these graphs is $\mu(T = 0)$.

- 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 $U = \frac{3}{5}\epsilon_F$. 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 find $\mu(T)$ 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 :-).

- **Quantum gasses at high and low temperatures ...** I want to keep our assignment *short* this week, so I'm not asking you to do G&T problem 6.60 on finding $P(T)$ for the ideal Fermi gas or G&T 6.61 for the ideal Bose gas. I will hope to remember to ask about these when we do "Real Gasses" (Seminar 13) . Though these are ideal

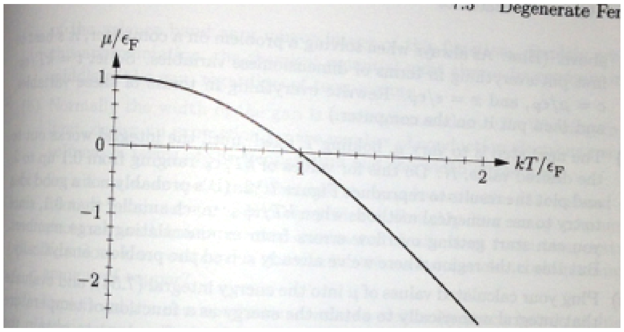

Figure 2: Figure 7.16 of Schroeder, chemical potential of ideal Fermi gas.

gasses, they are nonclassical ones. As a result, there is a correction to $PV = NkT$ so long as the deBroglie wavelength is not negligible compared to the average spacing between particles. This correction is *positive* for Fermions, raising the pressure from the classical result:

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

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

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

- 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.

Warmup Problems: *Due before seminar, Monday or Tuesday at latest … can hand them in as hard copies during seminar*

1: Brainstorming for second presentation In one of our last two seminar meetings (Seminar 13: May 2 or 3 *or* Seminar 14: May 16) you'll give your second presentation. It should be no more than 10 minutes, and it can be as close-to-the book (Chapters 6-10 of B&B) or as beyond-our-syllabus as you wish. Some favored topics of mine would be one of those B&B chapters, how random walks lead to the diffusion equation, density matrices in stat mech, or the Renormalization Group treatment of phase transitions. Do some thinking, and give me one or more stat mech or thermo topics about which you'd be enthusiastic to talk.

2: Counting Fermions Schroeder Problem 7.16

Regular problems:

1: A non-relativistic and a relativistic Fermi gas

i) Each atom in a piece of copper contributes one conduction electron. By looking up the density and atomic mass of copper, find the Fermi energy, Fermi temperature, and the degeneracy pressure. Is room temperature low enough to treat the electrons in copper as a degenerate Fermi gas?

ii) Suppose you have a gas of very high energy, hence relativistic, electrons. In this case, the energy of an electron is $\epsilon = pc$ where p is momentum. Modify the derivation of the Fermi energy of a classical electron gas (found in all three of our textbooks) to show that

$$\mu(T=0) \equiv \epsilon_F = hc(\frac{3N}{8\pi V})^{1/3}$$

Also, please show that the total energy is

$$U = \frac{3}{4} N \epsilon_F$$

for this relativistic Fermi gas. How does this compare with the non relativistic case? (This is Eq. (7.42) of Schroeder, or alternatively Eq. (6.152b) of G&T).

2: Einstein and Debye Theories G&T Problem 6.35

3: A neutron star G&T problem 6.55

4: A Fermi gas at low temperature ($T < T_F$) G&T problem 6.31

5: Chemical potential for a Fermi gas Schroeder problem 7.32

6: Toy system of Fermions G&T Problem 6.57

7: Magnons Schroeder Problem 7.64