Lecture 18: review

- Content on Final
- Review of last two chapters
- Questions for the class
- Derivations you should be able to reproduce, understand, and apply to new systems
- Reminder: same office hours, or just stop by my office when the door is open to discuss exam prep

Since the midterm, we have covered Ch 3-6 in the textbook and this will be the focus of the final. However, some of these concepts do have prerequisites in Ch 1-2. For example, when we derive properties of the phonon and electron gas, we usually need information about the number of atoms in the basis. And the concept of a brillouin zone, for which you need to know what a reciprocal lattice is, comes into play when we treat lattice vibrations as quantum particles. Moreover, the final will focus on the last two chapters we covered—5 and 6—because these are concepts that are used heavily in solid state physics research and are strong prerequisites for next quarter. That doesn't mean that Chs 3-4 will not be on the exam, but they will not be emphasized as much.

Below is a flow chart of the topics we covered in chapters 3-6 and why:



why: electrons are important in most materials and this formalism describes their quantum nature; can be directly applied to monovalent materials like Cu, and can be used with minor modifications to describe many metals and semiconductors

•gas of free fermions
•Fermi (-Dirac function, sphere, velocity, momentum, energy)
•Applications to electrical conductivity, hall conductivity, and thermal conductivity

The table below summarizes some of the key aspects of a phonon gas (Ch 5) and a Fermi gas (Ch 6)

	Classical gas (molecules)	Phonon gas	Fermi gas
Number	fixed	Population depends on frequency of mode and temperature: $\langle n \rangle = \frac{1}{e^{\hbar \omega/k_BT} - 1}$ (What are the limits of this expression for very small T and for very large T)? Small T: $e^{\hbar \omega/k_BT} \gg 1 \rightarrow$ $\langle n \rangle \sim e^{-\hbar \omega/k_BT}$ Large T: $e^{\frac{\hbar \omega}{k_BT}} \sim 1 + \frac{\hbar \omega}{k_BT}$ $\langle n \rangle \sim k_BT/\hbar \omega$	fixed

Type of particle	Point-like	boson	Fermion; not necessarily charged (but electrons have
Relationship between energy and momentum	$KE = p^2/2m$ For each particle	Depends on which branch you are considering (see chapter 4), but for acoustic phonons near $k=0, \omega \sim v_s k$ where k is crystal momentum and $v_s$ is speed of sound	$\epsilon_k = \hbar^2 k^2 / 2m$ For free or nearly free electrons
Effect of temperature	Increases the mean kinetic energy of particles (Maxwell- boltzmann distribution)	Occupation number of phonon modes with a given frequency increases	Fermi-dirac function; occupation probability just below or just above the Fermi energy is no longer simply 1 or 0, but it can be some fractional falue in between these numbers
Relationship between temperature and total internal energy	For an N-particle gas $U = 3Nk_BT$	$U = \sum_{K} \sum_{p} < n_{K,p} > \hbar \omega_{K,p} =$ $= \sum_{K} \sum_{p} \frac{\hbar \omega_{K,p}}{e^{\hbar \omega_{K,p}/k_{B}T} - 1}$	The total kinetic energy of electrons at any temperature is given by: U $= \int_{0}^{\infty} dE \ E \ D(E) f(E)$ Where D(E) is the density of states and f(E) is the Fermi-Dirac function, which encodes temperature effects
Density of states	$4\pi \frac{V}{h^3}p^2$ Where $h^3$ is volume in phase space	$D(\omega) = \frac{dN}{d\omega} = \frac{dN}{dk} \frac{dk}{d\omega}$ In 3D: $D(\omega) = \sum_p \frac{K(\omega)^2 V}{2\pi^2} \frac{dK}{d\omega_p}$ Where the sum is taken over all phonon branches (polarizations, p)	$D(E) = \frac{dN}{dE} = \frac{dN}{dk}\frac{dk}{dE}$ In 3D: $D(E) = \frac{V}{2\pi^2} \left(\frac{2m}{\hbar^2}\right)^{3/2} E^{1/2}$
Collisions	Molecules collide with each other and with walls of vessel	Phonons collide with each other, with surface of crystal, and with impurities	In this course, we discussed electrons colliding with phonons and with impurities
Particles can be used to transport	heat	heat	Charge (if they are charged particles) and heat

Energy conserved in collisions?	Yes	Yes	yes
Momentum conserved in collisions?	Yes, except for at walls	Yes, modulo a reciprocal lattice vector <b>G</b>	Yes, modulo a reciprocal lattice vector <b>G</b>
Number of particles conserved in collision?	Yes	No	Yes

## Questions for class (answers at end of this set of lecture notes):

- 1. What can this formalism of a free electron gas apply to?
- 2. What is the general procedure for finding a density of states?
- 3. When do we use density of states?
- 4. Thermal conductivity: what are intuitive explanations for why each term is included? ( $K = \frac{1}{3}Cv\ell$ )
- 5. Electrical conductivity: intuitive explanation for various terms ( $\sigma = \frac{ne^2\tau}{m}$ )
- 6. Why are we justified in modeling a crystal lattice as masses connected by springs for the purposes of deriving dispersion relations of elastic waves?
- 7. If I give you an atomic potential energy, U(r) = f(r), how do you find a spring constant from this?
- 8. Phonons: what is an intuitive connection between dispersion relations and density of states?
- 9. Phonons: how many phonon modes are there for a D dimensional crystal with p atoms in the basis and why?
- 10. Why are only electrons close to the fermi energy relevant for thermal and transport properties of free electron gas ?
- 11. What is a dispersion relation and what is it useful for ?
- 12. What is the first brillouin zone and what is its significance for the topics we discussed in this part of the course ?

## Derivations that you should be able to reproduce:

- Dispersion relations for elastic waves in solids from masses-on-springs model
- Density of states for phonon and fermion gas in any dimension
- Aggregate properties of phonon gas (for example, but not limited to, total internal energy)
- Fermi-anything in arbitrary gas of free fermions (e.g. Fermi energy, fermi momentum, fermi velocity, density of states at fermi energy)
- Also, you should aim to understand the 'practical' applications of the concepts we have covered so far: thermal conduction, electrical conduction, stress/strain relationships

Hint: try to explain what you are doing at every step and why, so that you can apply it to an arbitrary system

## Answers to questions:

- 1. electrons in a metal, liquid helium 3 or some other condensate of fermions, neutron star
- # of particle=(Volume of sphere in k-space with radius k)/(size of each box); use dispersion relation to solve for energy or frequency as a function of k, and take derivative of N wrt to energy or frequency
- 3. when we want to do an integral over energy to determine collective properties of a phonon or electron gas; the density of states tells us how many states are contained in each energy slice
- 4. Thermal conductivity:
  - a. K describes the effectiveness of transmitting heat from one side of a specimen to another
  - b.  $\ell$  is a mean free path between phonon scattering events; when a phonon scatters it loses information about what direction it was moving, and this inhibits the transport of heat)
  - c. v is the velocity that phonons travel at between scattering events, typically the speed of sound; faster velocity means that a phonon can get to the cooler side of the sample faster
  - d. *C* is the heat capacity per volume; it is included because the process of heat transfer is identical to the process of heating up a portion of the specimen some distance away
- Electrical conductivity describes the ease of transmitting charge from one end of the specimen to the other (note: this real space picture will not work for a more sophisticated treatment of electrical conduction). Larger τ corresponds to higher conductivity because it gives electrons more travel time between scattering events. Larger n corresponds to higher conductivity because more electrons can transport the same amount of charge in a faster amount of time
- 6. interatomic potential is roughly quadratic for small displacements from minimum
- take 1<sup>st</sup> deriv and set to zero to get equilibrium separation, take 2<sup>nd</sup> derivative and plug in result from previous step, if needed
- density of states, is sort of an integral over momentum of the dispersion relations; for every momentum, you count how many 'boxes'—quantized energy values originating from quantized momentum values—you encounter
- There are Dp total phonon modes, because each atom in the basis can move independently in D dimensions; D of these phonon modes are acoustic, and the remaining D(p-1) are optical
- 10. energy can be transported by electrons that can be promoted to a higher energy state. The temperature sets a rough value for  $\Delta E$  that an electron can acquire. For an electron buried deep inside the Fermi sphere, a thermal energy kick can only promote it to an energy that is already occupied by other electrons
- 11. Energy vs k or frequency vs k; used to calculate group velocity and density of states. Group velocity sets the maximum speed at which a particle can transmit 'information.';

density of states is important for determining all aggregate properties of Fermi and Bose gas

12. Wigner-Seitz cell in momentum space; uniquely defines phonon dispersion; any larger K can be translated back to first BZ by reciprocal lattice vector **G**