Physics 123B

Leon Balents

Winter 2015

Course Organization

- Grading: HW 30%, Mid-term 30%, Final 40%
- Office hours
  - Thurs, 2:30-4:00, Kohn 2315 (KITP)

Review questions 1

- What is a crystal?
  - A: a periodic arrangement of atoms
- How do we describe this structure mathematically?
  - A: through Bravais lattice (primitive vectors) + Basis; symmetry; unit cell
- How do we study structure experimentally?
  - A: x-rays; neutrons; AFM/STM...

Review Questions 2

- What does (elastic) x-ray scattering measure?
  - A: reciprocal lattice. define it.
- What are phonons?
  - A: normal modes of small oscillations of atoms
- What are acoustic and optical phonons? How many branches of each are there in NaCl?
  - A: acoustic modes have $\omega \sim k$; 3 of each per unit cell.

Review Questions 3

- How does the phonon heat capacity depend on T at low and high T, i.e. what is the power law?
  - A: $C \sim T^3$ at low T, C = const. at high T.
- What is the characteristic temperature separating these two limits called?
  - A: DeBye temperature
- Give an example of another physical property phonons contribute to
  - A: thermal conductivity, sound, thermal expansion

Review Questions 4

- In the free electron model, what is the Fermi energy, and what is a typical value for it in a metal?
  - A: E_F separates occupied and empy states. It is of order a few eV = 10^4-10^5 K
- What is the temperature dependence of the electronic heat capacity at low T?
  - A: it is linear in T
- Which of the electronic or phononic contribution to the heat capacity of a metal is typically larger at room temperature? Why?
  - A: phonons. Because all the phonon entropy is released over the DeBye temperature, while the electron entropy is released over the Fermi energy, and $E_F >> kT_D$

Review Questions 5

- What is the "Drude model"/Ohm's law expression for the conductivity of the free electron gas?
  - A: $\sigma = n e^2 \tau/m$, where τ is a collision time/relaxation time
- What determines the collision time at room temperature and at low temperature?
  - A: usually phonons at room temperature, and impurities at low temperature.
- What is the Hall coefficient, and what does it measure, in the free electron model?
  - A: it is the ratio of the hall resistivity to magnetic field, and it measures -1/(the density of electrons)

Review Questions 6

- Is the electronic or phononic contribution to thermal conductivity usually more important in metals at room temperature?
  - A: electronic. This might be surprising since the phonon heat capacity dominates. But there is an extra factor of velocity v in the thermal conductivity, $K = C\ v\ l$, and $v_F >> v_{sound}$.
- What is the form of the wavefunction of an electron in an ideal periodic solid?
  - A: It has the Bloch form of a plane-wave times a periodic function
- What is the crystal momentum, and how is it different from the true momentum?
  - A: The crystal momentum is defined as hbar times the wavevector appearing in the Bloch form. It is different from the true momentum because the electron scatters off of the lattice, and therefore is in a superposition state of many momenta which differ by reciprocal lattice vectors. So the crystal momentum is only defined up to a Bragg momentum

Review Questions 7

- What is an energy band?
  - A: Electronic states have energies $\varepsilon_n(k)$ which are periodic in wavevector/ crystal momentum and have discrete n. Each such function is a band, and spans a finite range of energy.
- How many orbitals are there in a band?
  - A: Each band contains 2 orbitals (including electron spin) per primitive unit cell of the lattice. Equivalently, there is one crystal momentum per p.u.c.
- Both Francium and Radium (atomic number 87 and 88, respectively) have b.c.c. crystal structures in elemental form. Can you say whether either one is metallic?
  - A: Fr *must* be metallic in b.c.c. form, since it has an odd number of electrons per atom and bcc is a Bravais lattice with one atom per p.u.c. (Here we assume it does not become magnetic). In fact radium is also metallic, though it does not need to be.

Review Questions 8

- How do you distinguish metals and insulators according to band theory?
  - A: a metal has partially filled bands, and an insulator has all bands either filled or empty
- What is the Fermi surface?
  - A: it is the boundary between occupied and unoccupied Bloch states in a metal, which forms a surface in momentum space
- What is the Fermi surface of a free electron gas?
  - A: a sphere

Review Questions 9

- What is a semiconductor?
  - A: it is a material which is an insulator at T=0 with a relatively small (usually <2eV) band gap.
- What is a direct and indirect gap?
  - A: a direct gap is the minimum energy needed to go from the valence to conduction band conserving k. An indirect gap is a smaller energy transition which does not conserve k.
- How can the gap be measured?
  - A: optics can measure both direct and indirect gap. Activation energy of the conductivity can measure the gap.

Review Questions 10

- What are electrons and holes in semiconductors, and what does their effective mass mean?
  - A: They are occupied or empty states at the bottom of the conduction or top of the valence band, respectively. The effective mass is the inverse of the band curvature at its minimum/maximum.
- Are effective masses in semiconductors smaller or larger than the electron mass, usually?
  - A: usually smaller.

Review Questions 11

- What are donors and acceptors?
  - A: They are impurity atoms in a semiconductor which tend to ionize, forming a charged ionic center and an oppositely charged "doped" electron or hole.
- How does the binding energy and Bohr radius of a donor depend on effective mass and dielectric constant?
  - A: The binding energy is $E = Ry\ (m^*/m)\ 1/(\varepsilon^2)$, and the radius is $a = a_B\ \varepsilon\ (m/m^*)$
- What measurements determine the sign and density of charge carriers?
  - A: Hall effect, and thermopower

Fermi surfaces

- I want to talk about Fermi surfaces
- Every metal has one*, and they are all unique
- We're going to lead into talking about an exceptional case between a metal and an insulator, where there is *no* Fermi surface: graphene

* Well, almost. Except for effects of randomness of atomic positions.

Fermi surfaces

- Key result of band theory: electrons occupy quantum states described by continuous crystal momentum and discrete "band index" quantum numbers
- Energies of each band are smooth functions of quasi-momentum, $\varepsilon_n(k)$
- Fermi statistics: states below E_F are occupied, others empty
- Condition $\varepsilon_n(k)=E_F$ generally describes a surface (when it has solutions). This is the Fermi surface.

Why Fermi surfaces?

- Any time we weakly perturb a system, we excite mainly low energy excitations
  - in metals, the characteristic energy scale is $E_F \sim$ eV, so most perturbations are weak
  - In a metal, the low energy excitations are adding or removing electrons near the Fermi energy (or moving them from below to above).
  - In some cases, one can think of the excitation as a deformation of the surface (c.f. displacement in E field)
- It is remarkable that this geometric object *in reciprocal space* becomes essential to the physics of something as simple as a piece of metal!
  - manifests both wavelike nature of electrons and quantum statistics!

Whence Fermi surfafes

- They are determined by the bands, i.e. solving $\varepsilon_n(k)=E_F$.
- Can try to understand via:
  - Nearly free electron theory
  - Tight binding
  - *ab initio* electronic structure
  - measurement

Tight binding method

- The opposite limit from NFEA - assume the ionic potential strongly confines electrons
  - only a small number of atomic orbitals are important
- We can try to construct Bloch states from these orbitals only
  - conceptually similar to making "bonding" and "anti-bonding" orbitals on molecules
  - but with 10^{23} atoms instead of 2!

Tight Binding

- Write the wavefunction as a superposition

$$\psi(r) = \sum_R \psi_R \, \phi(r - R)$$

ψ_R: amplitude

$\phi(r - R)$: orbital of atom at R

- Amplitudes obey "discrete Schrodinger equation"

"γ" here is "t" in many texts, including Simon

$$\hat{H}\psi_R = \epsilon_0 \psi_R - \sum_{R'} \gamma_{R,R'} \psi_{R'} = \epsilon \psi_R$$

ϵ_0: atomic energy

$\gamma_{R,R'}$: "hopping" amplitude - decays rapidly with distance

Tight binding

- Often we assume just nearest-neighbor hopping
- Example: one dimensional chain

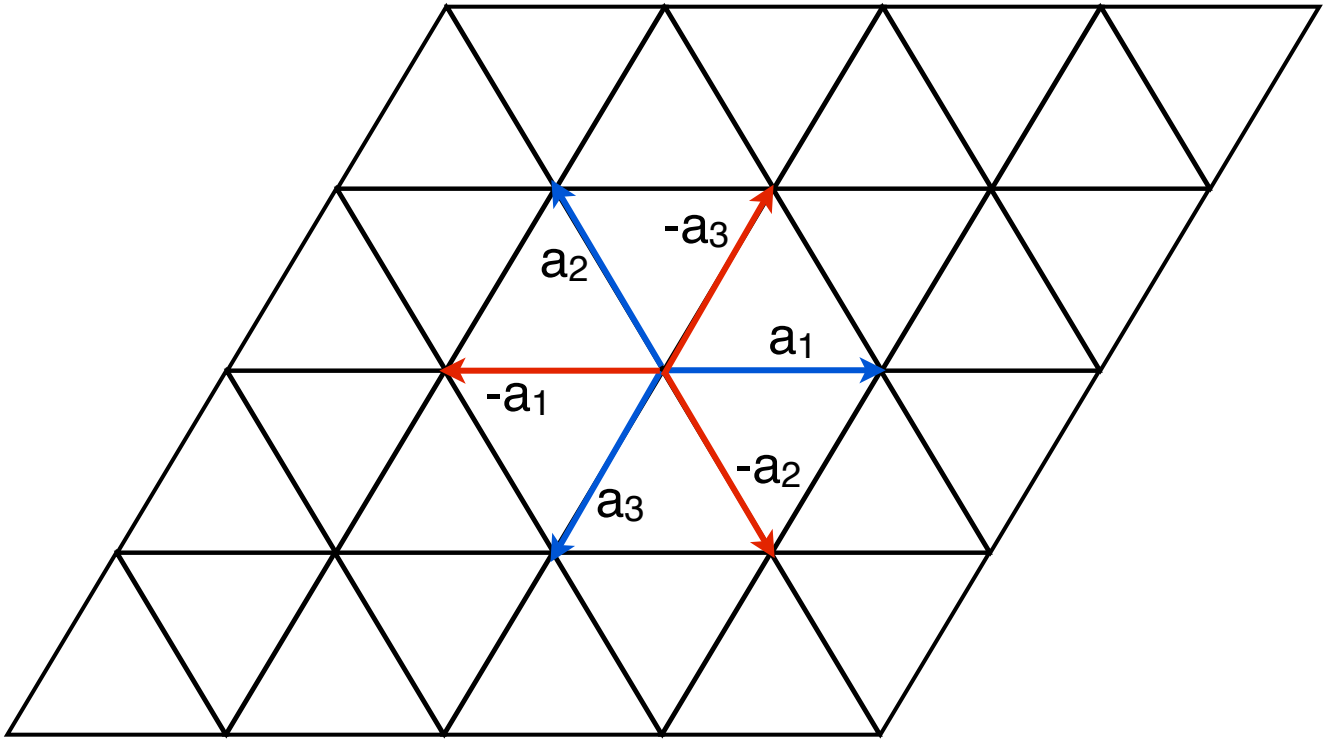
$$\hat{H}\psi_x = \epsilon_0\psi_x - \gamma(\psi_{x+a} + \psi_{x-a}) = \epsilon\psi_x$$

- Solve it? $\psi_x = \overline{\psi}e^{ikx}$

$$\epsilon(k) = \epsilon_0 - 2\gamma\cos ka$$

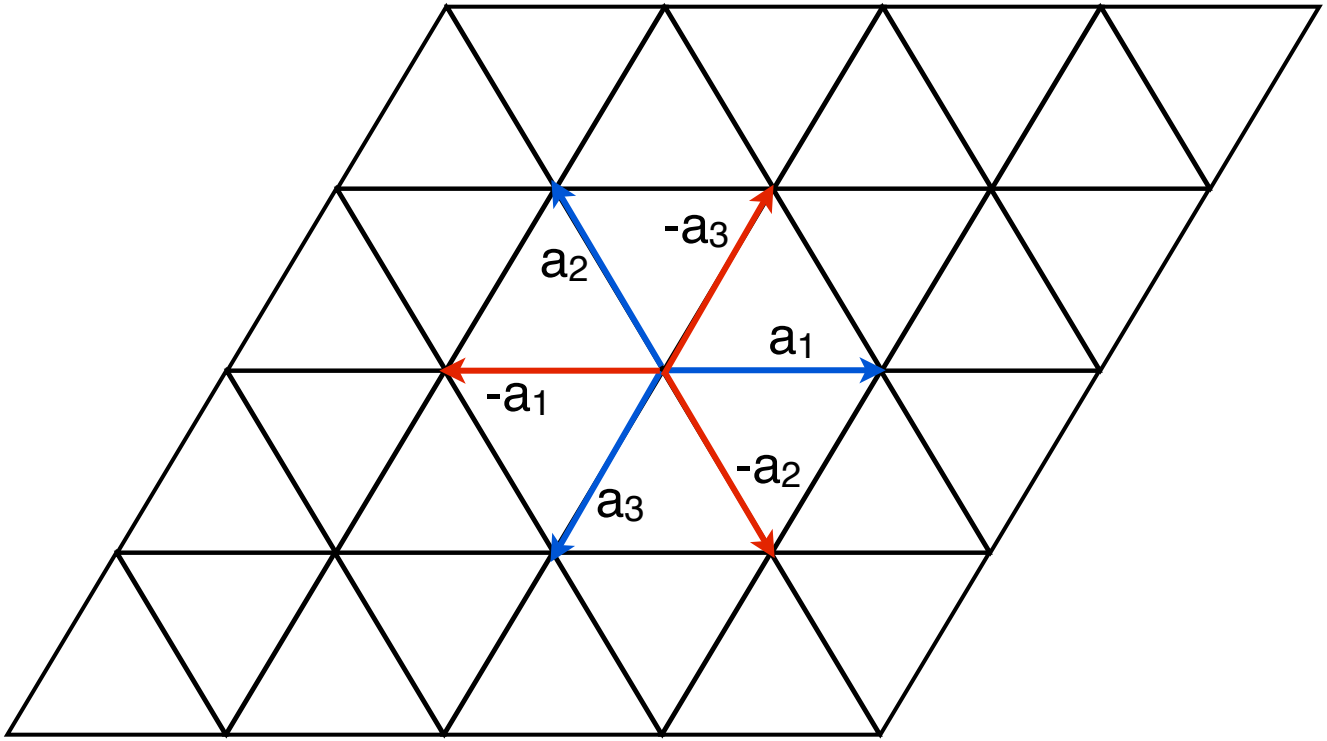
- Easily generalized to 2d and 3d lattices (see Kittel)

2d hexagonal lattice



$$\epsilon_0 \psi_R - \gamma \sum_{\langle R', R \rangle} \psi_{R'} = \epsilon \psi_R$$

2d hexagonal lattice



$$\epsilon_0 \psi_R - \gamma \sum_{i=1}^{3} (\psi_{R+a_i} + \psi_{R-a_i}) = \epsilon \psi_R$$

2d hexagonal lattice

- Spectrum:

$$\epsilon(k) = \epsilon_0 - 2\gamma \sum_{i=1}^{3} \cos \mathbf{k} \cdot \mathbf{a}_i$$

- Primitive vectors: $(1,0)\ (-\frac{1}{2}, \frac{\sqrt{3}}{2})\ \ (-\frac{1}{2}, -\frac{\sqrt{3}}{2})$
- Energy:

$$\epsilon(k) = \epsilon_0 - 2\gamma \left(\cos k_x + 2 \cos \frac{k_x}{2} \cos \frac{\sqrt{3} k_y}{2} \right)$$