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

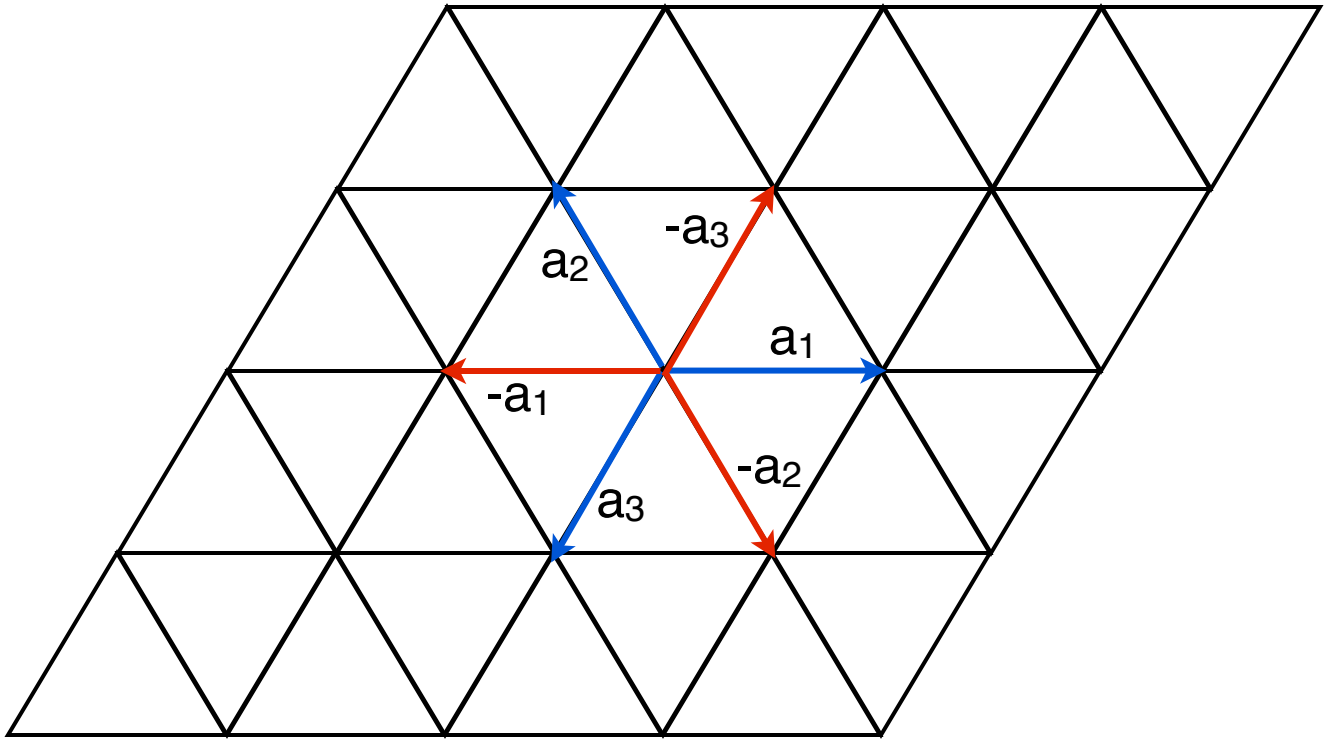
$$\hat{H}\psi_x = \epsilon_0\psi_x - \gamma(\psi_{x+a} + \psi_{x-a}) = \epsilon\psi_x$$

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

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

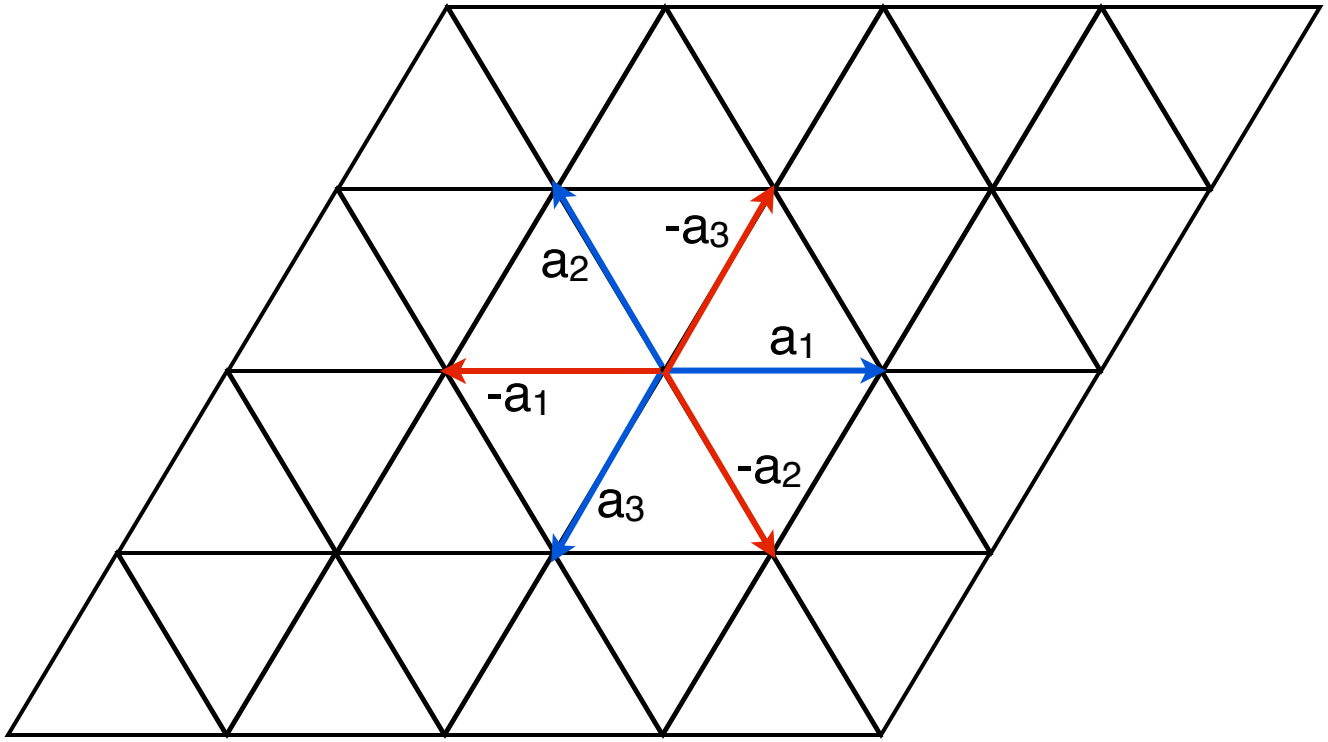
- Easily generalized to 2d and 3d lattices (see Kittel)

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:

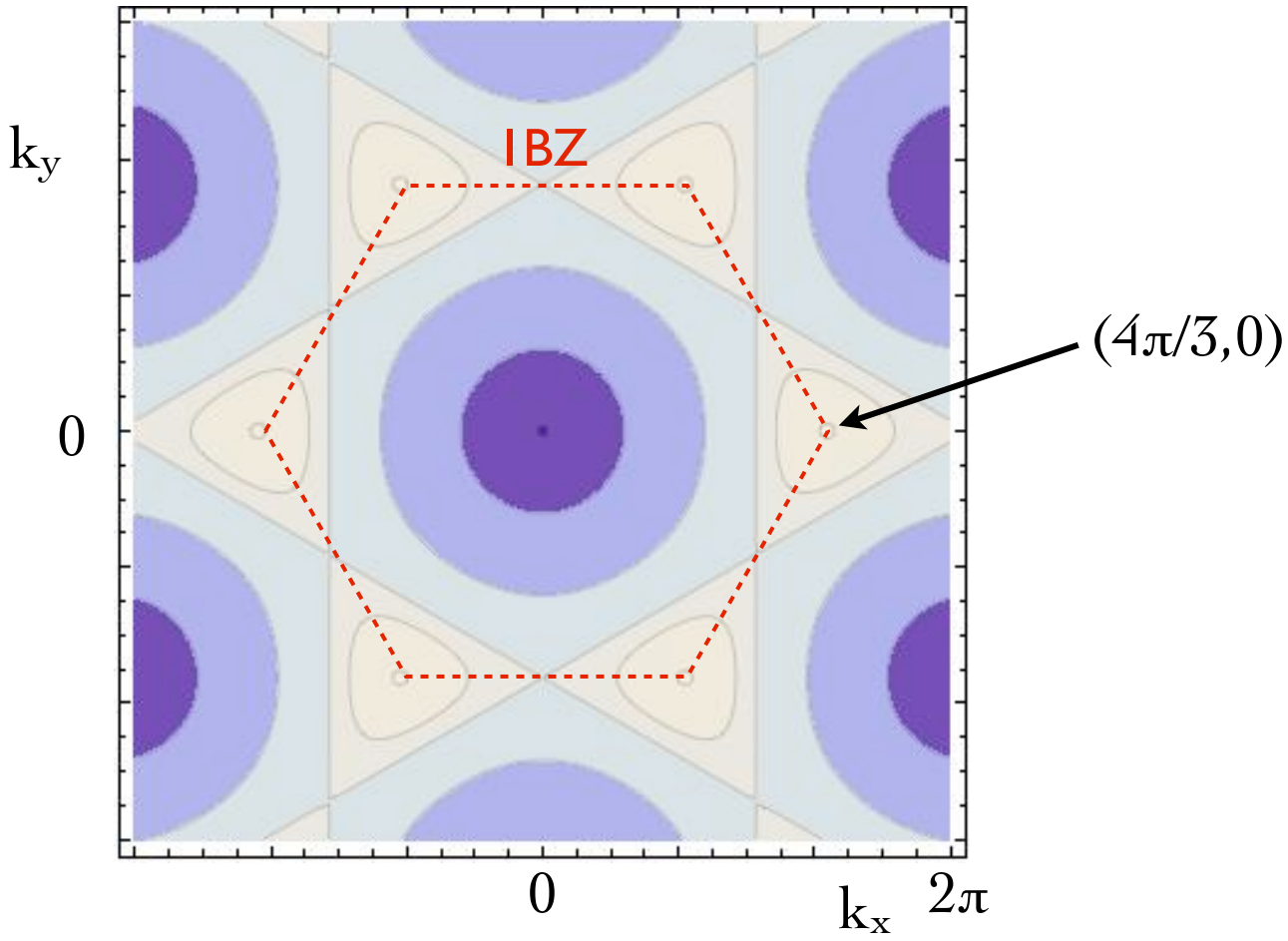
$$\epsilon(k) = \epsilon_0 - 2\gamma \sum_{i=1}^{3} \cos \mathbf{k} \cdot \mathbf{a}_i$$

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

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

2d hexagonal lattice

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



Graphene

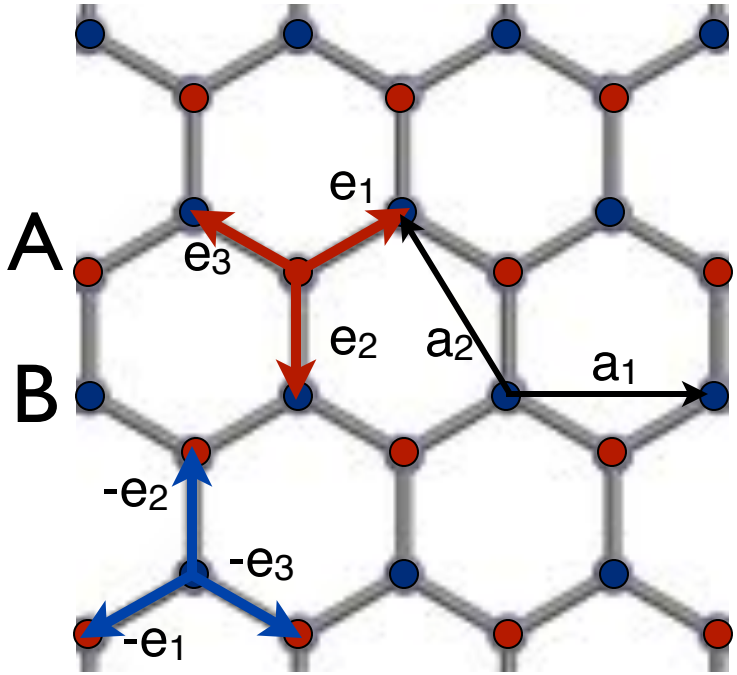
n.b. Prof. Andrea Young
new faculty!

- Single layers of honeycomb lattice of carbon
- First systematically exfoliated and studied by A. Geim + K. Novoselov, 2004.
- Nobel prize, 2011
- Interesting because it intrinsically has a *point Fermi surface*

Graphene

- electronic properties?
- Carbon has Z=6, (He) $2s^2\,2p^2$ = (He) $sp^2\pi$
- 1 π = p^z electron per C atom not tied up in covalent sp^2 bonds
- Can treat this via tight-binding model

Graphene



e_i are replaced by δ_i in many articles (e.g. Leggett notes). Also lattice can be rotated from

Bipartite: A sites hop to B sites, and vice versa

$$\hat{H}\psi_R = \epsilon_0\psi_R - \gamma\sum_{i=1}^{3}\psi_{R+e_i} = \epsilon\psi_R \qquad R \in A$$

$$\hat{H}\psi_R = \epsilon_0\psi_R - \gamma\sum_{i=1}^{3}\psi_{R-e_i} = \epsilon\psi_R \qquad R \in B$$