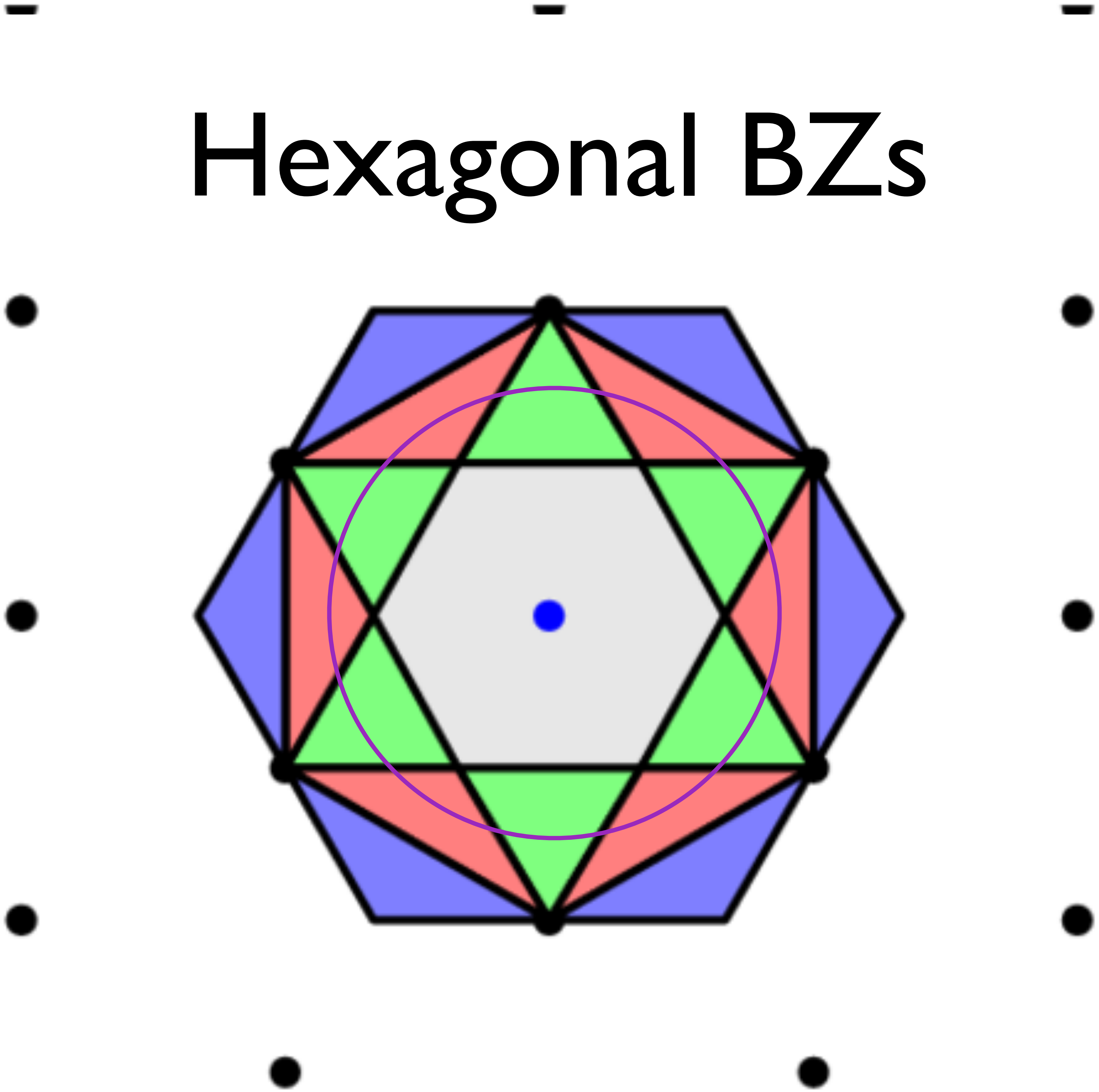
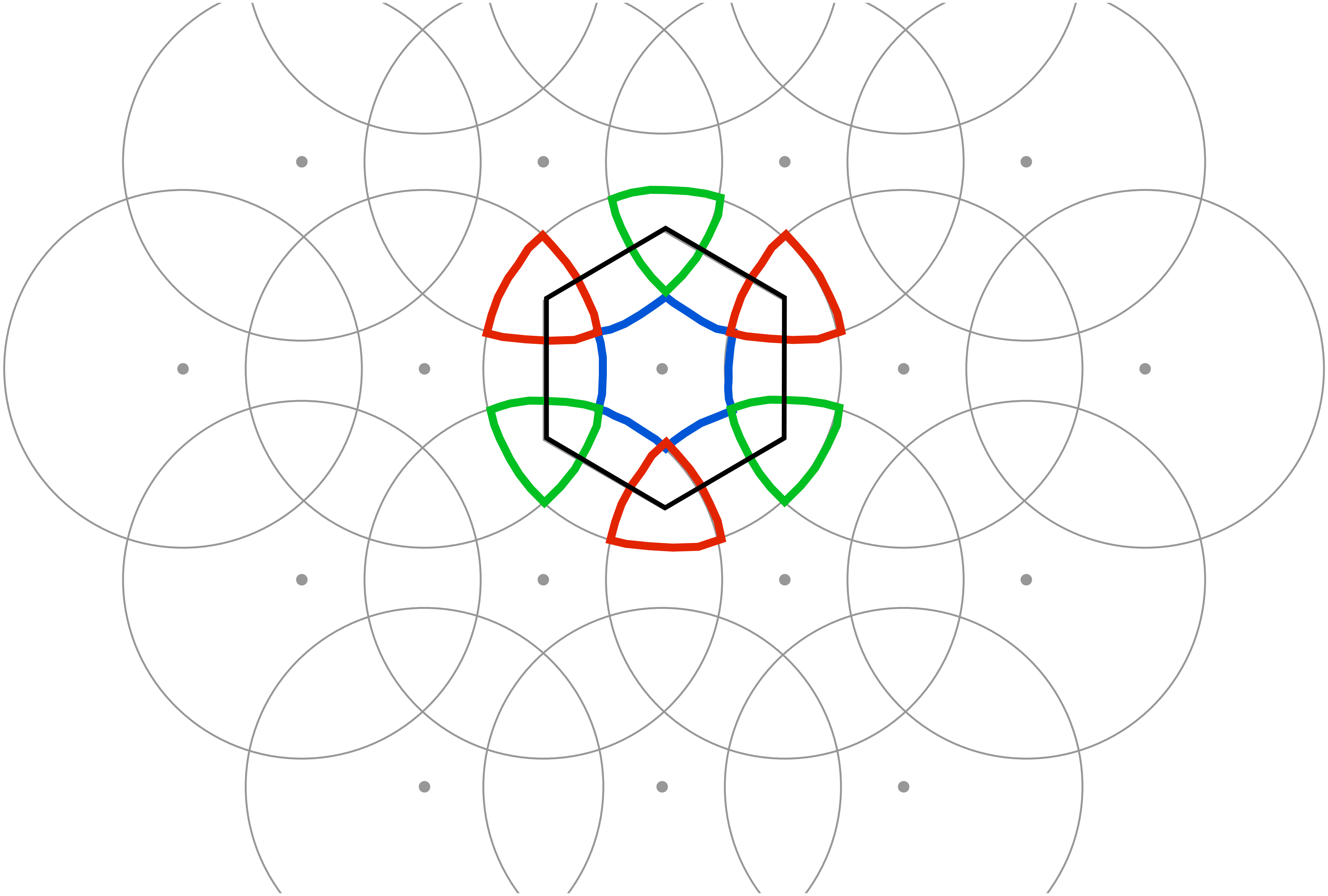
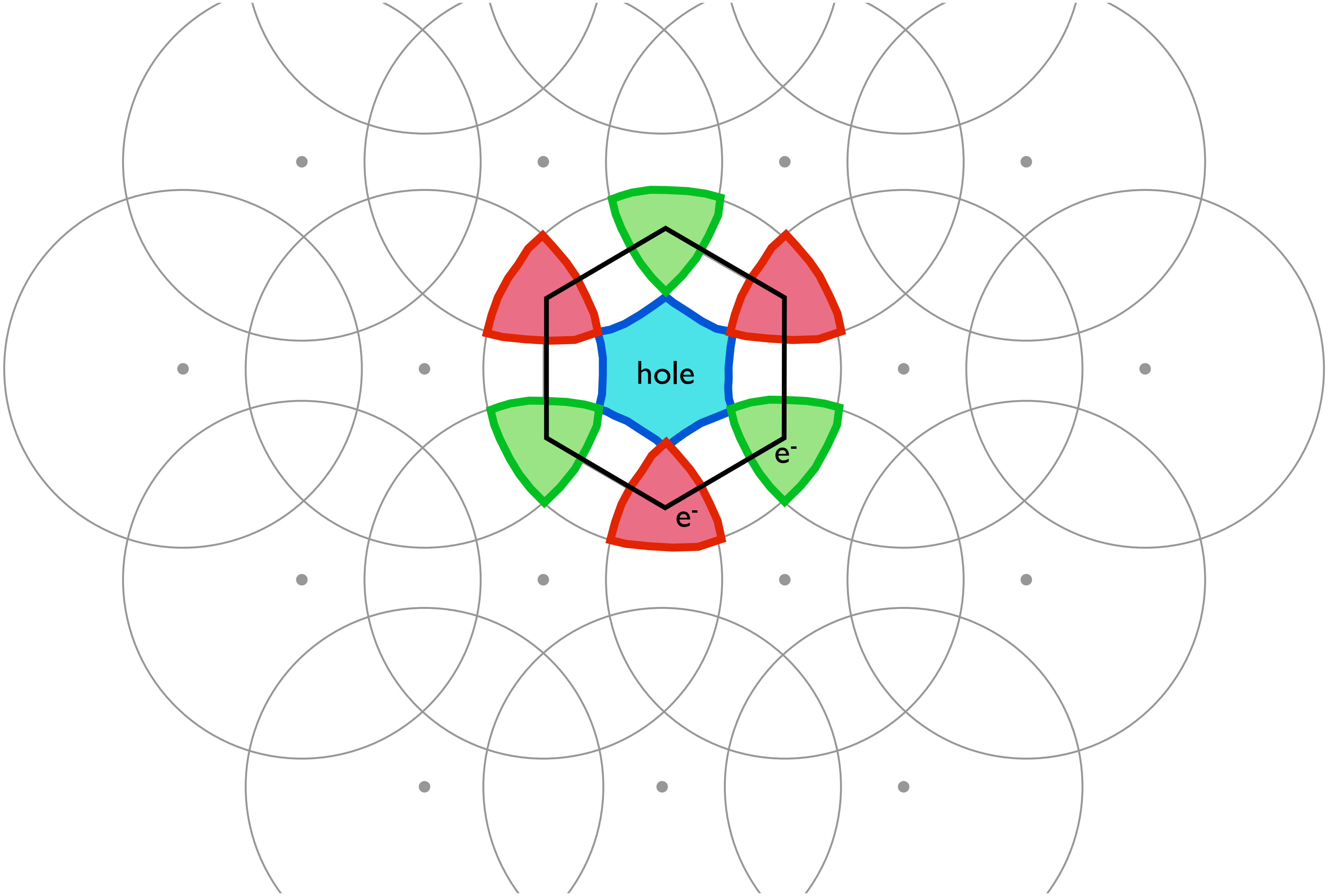
Hexagonal BZs



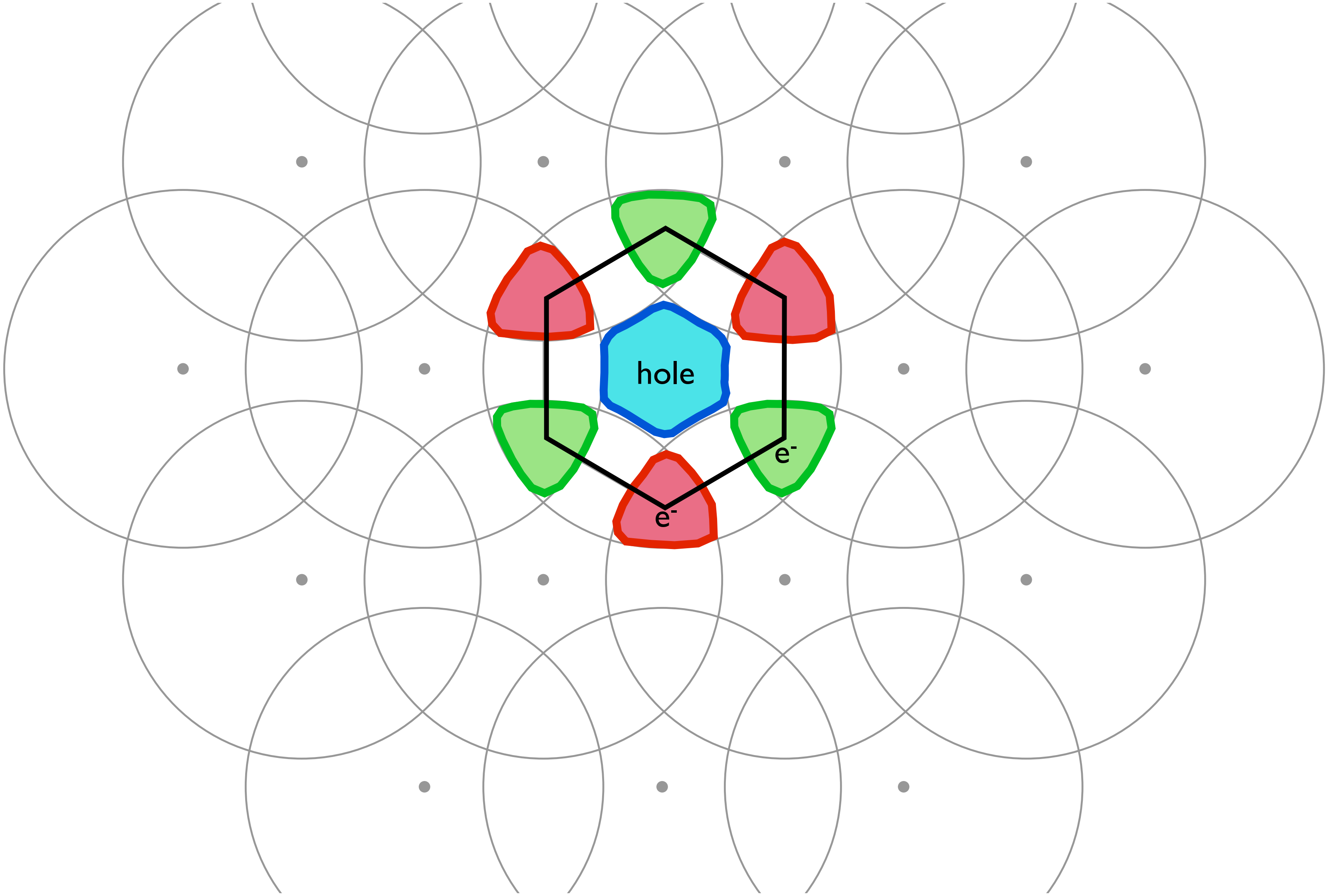
Fermi surface pockets



Fermi surface pockets



w/ periodic potential

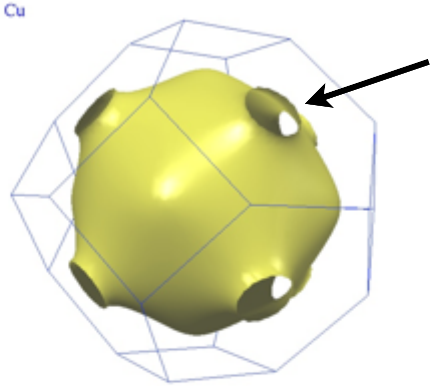


Lessons

- If Fermi sphere extends past first Brillouin zone, several pieces of Fermi surface will exist in multiple bands in free electron limit
- Once weak interactions are added, “cuspy” Fermi surfaces become rounded, and usually do not intersect

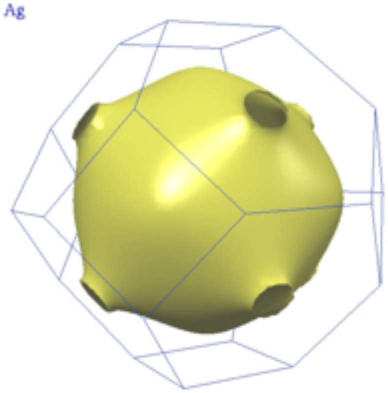
Free electron-like FSs

Cu

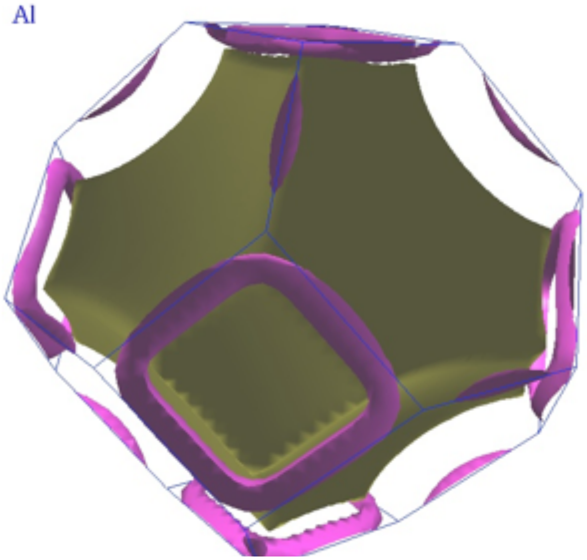


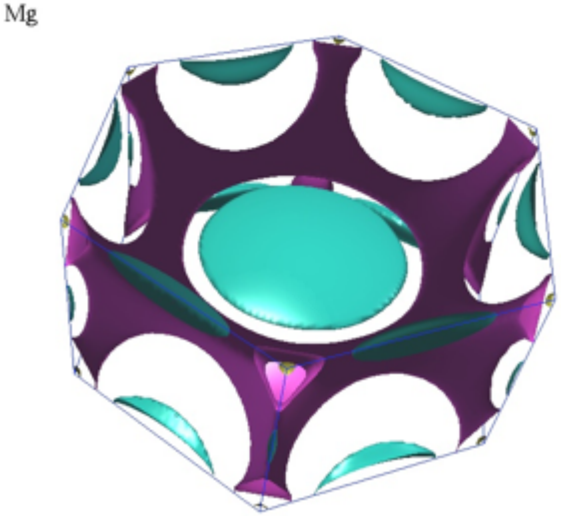
point inside the “neck” is on Bragg plane. Band gap opened at this k, lowering the energy of valence band so it moved inside the Fermi surface. This explains tendency to “necking”

Ag

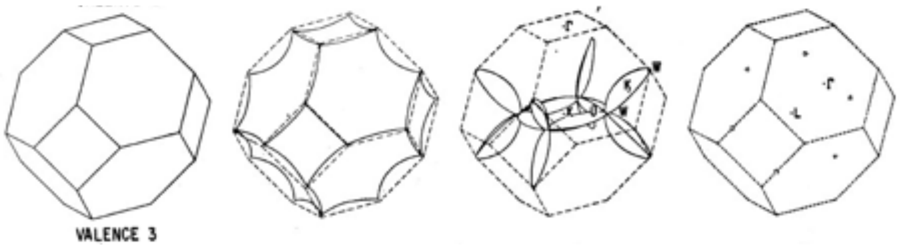


Free electron-like FSs

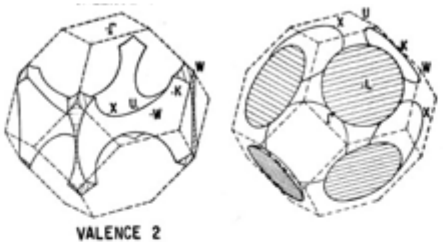




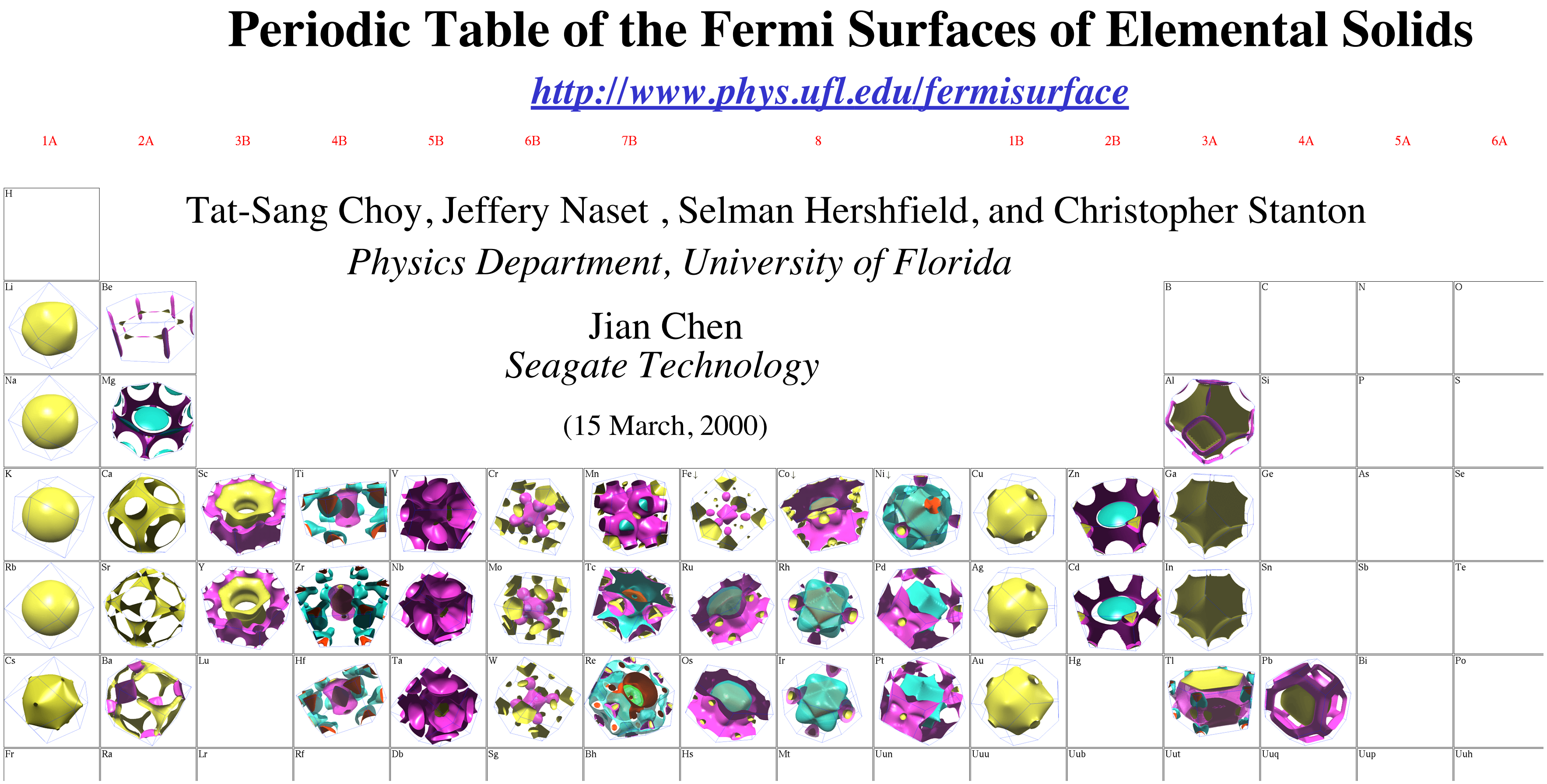
apparently, at least the larger Fermi surface of Al is free-electron-like.



compare to Ch. 9, Fig. 1



More zoology



Periodic Table of the Fermi Surfaces of Elemental Solids

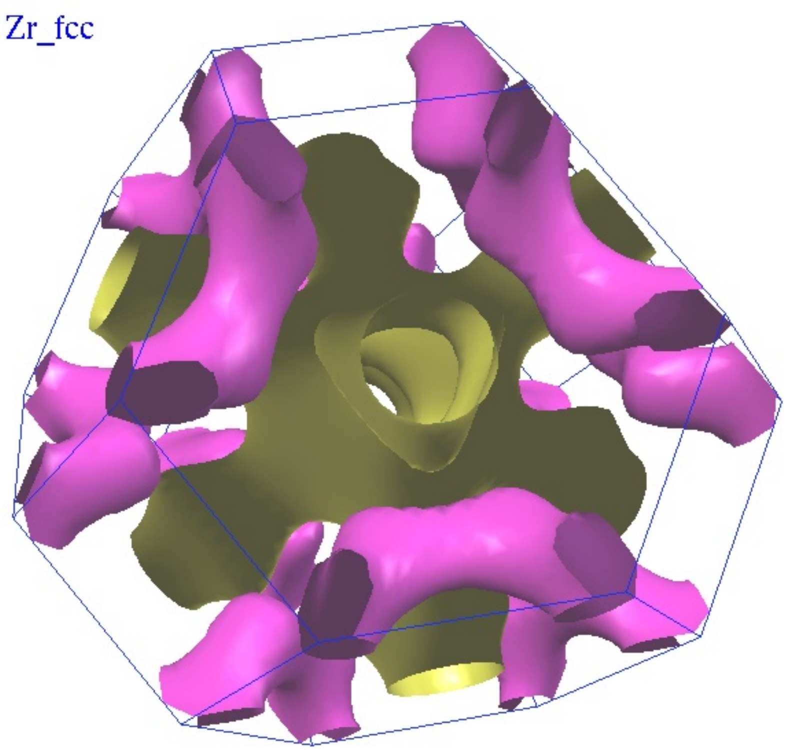
http://www.phys.ufl.edu/fermisurface

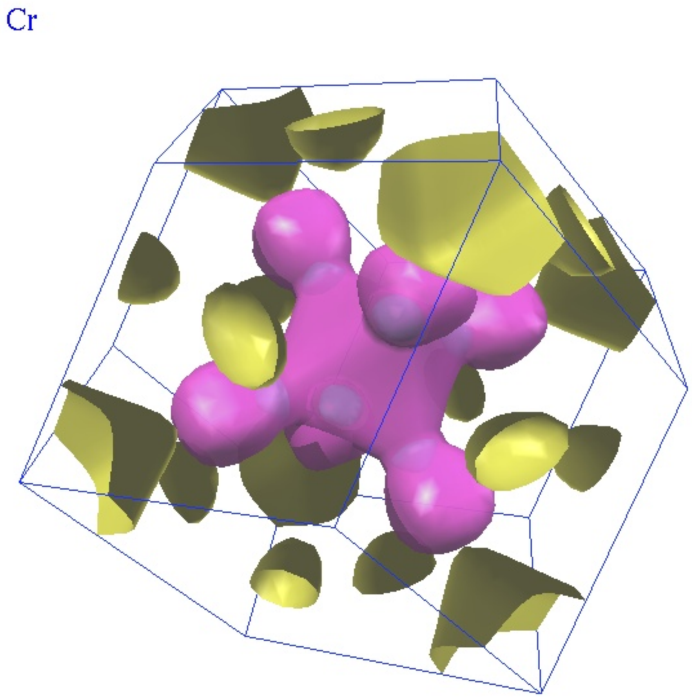
Tat-Sang Choy, Jeffery Naset , Selman Hershfield, and Christopher Stanton
Physics Department, University of Florida

Jian Chen
Seagate Technology

(15 March, 2000)

Wild stuff





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

$$\psi(r) = \sum_{R} \psi_R \, \phi(r - R)$$

amplitude

orbital of atom at R

- Amplitudes obey "discrete Schrodinger equation"

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

atomic energy

"hopping" amplitude - decays rapidly with distance

Tight binding

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

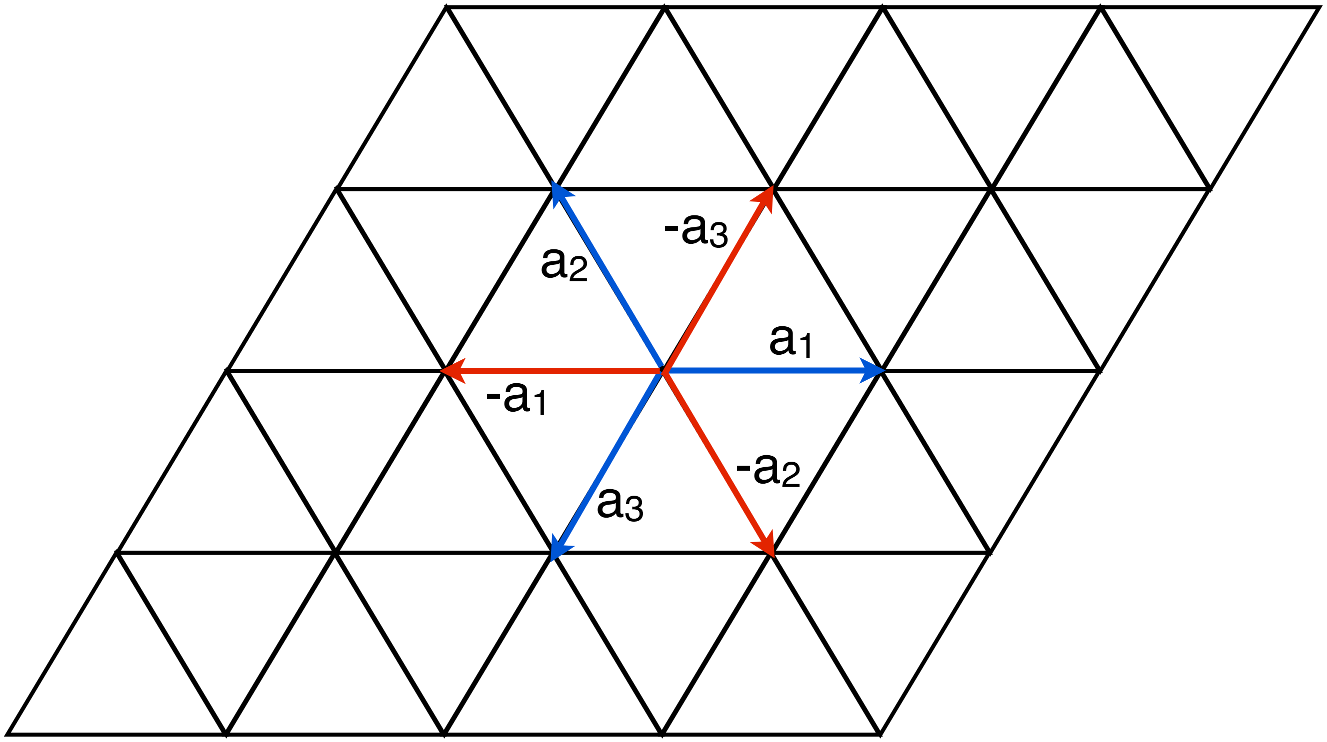
$$\hat{H}\psi_x = \epsilon_0\psi_x - \gamma(\psi_{x+a} + \psi_{x-a}) = \epsilon\psi_x$$

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

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

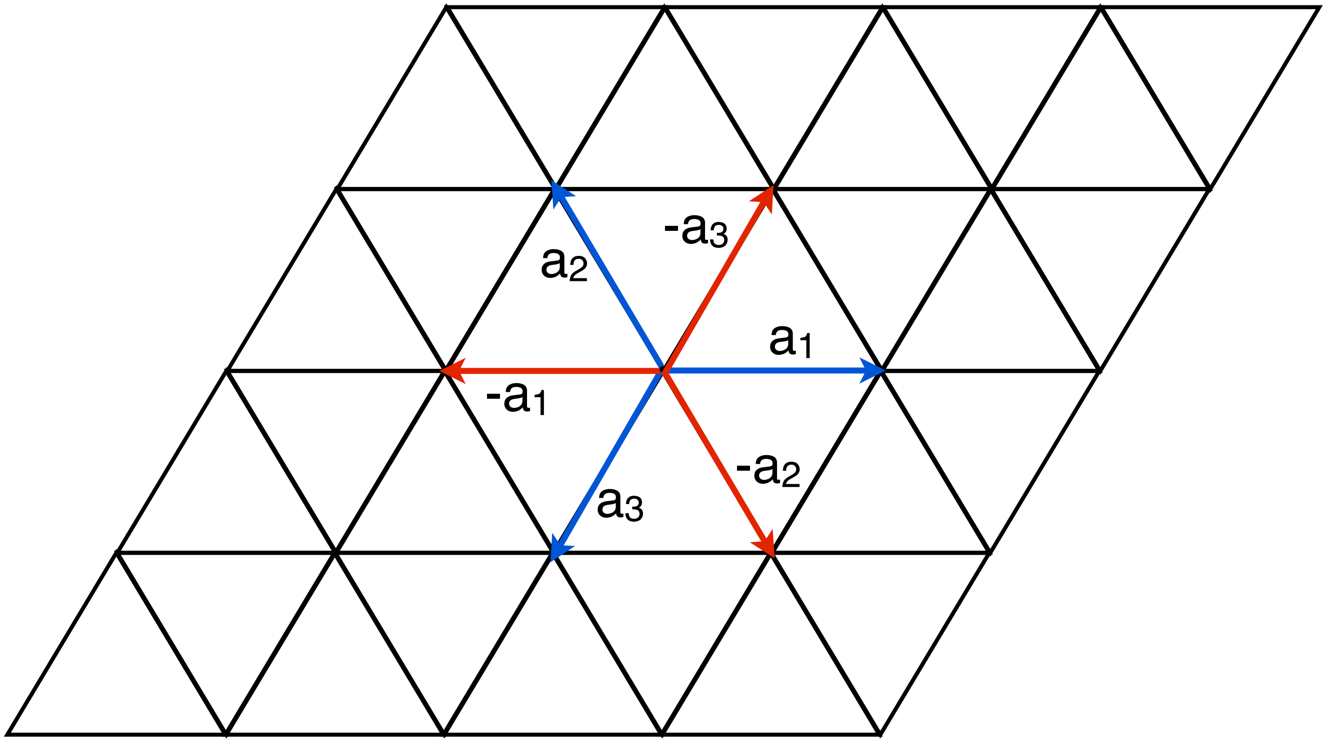
- Easily generalized to 2d and 3d lattices (see Kittel)

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:

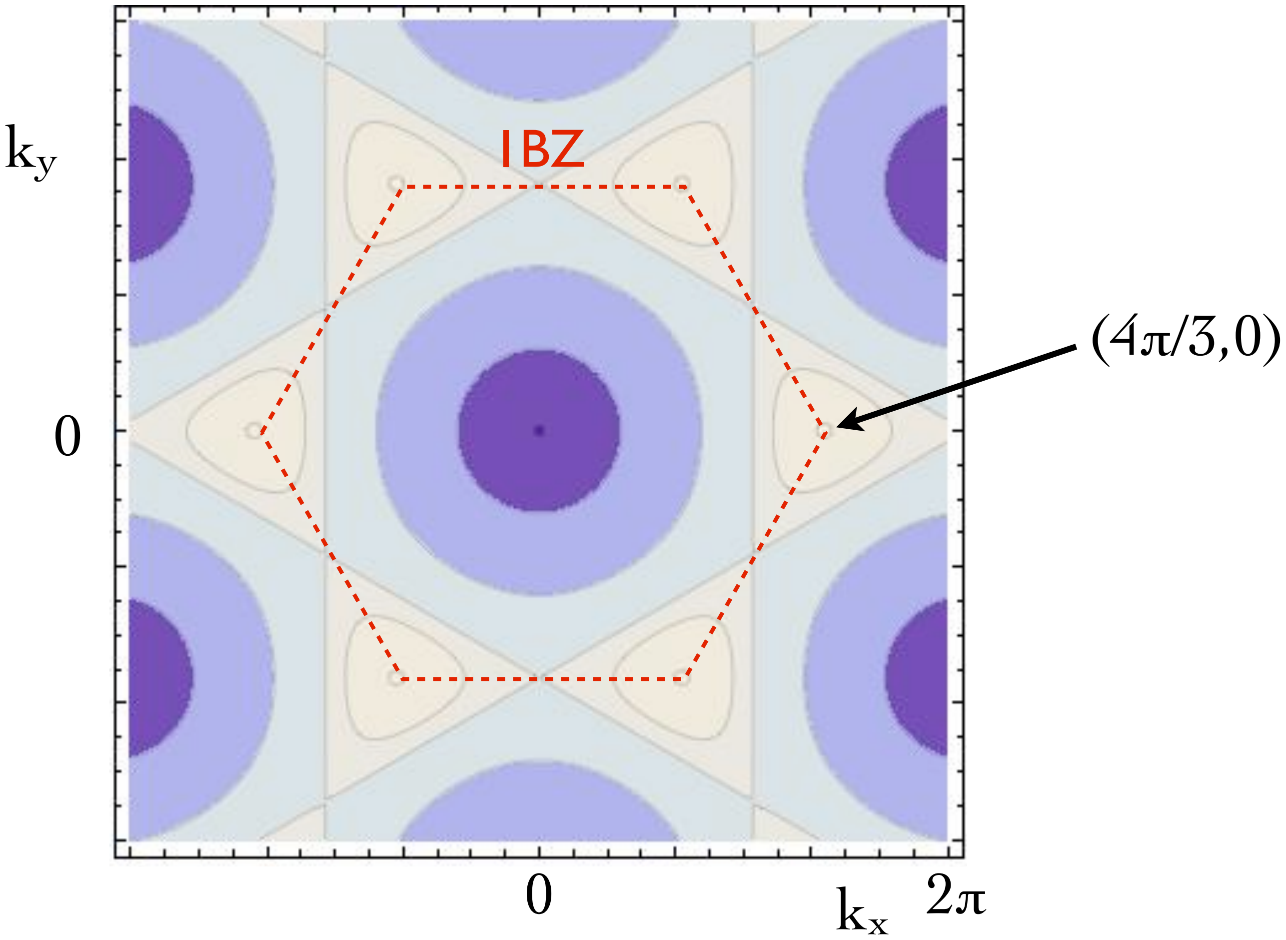
$$\epsilon(k) = \epsilon_0 - 2\gamma \sum_{i=1}^{3} \cos \mathbf{k} \cdot \mathbf{a}_i$$

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

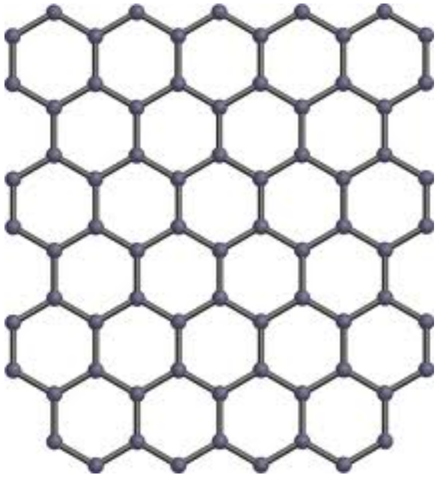
$$\epsilon(k) = \epsilon_0 - 2\gamma \left(\cos k_x + 2 \cos \frac{k_x}{2} \cos \frac{\sqrt{3} k_y}{2} \right)$$

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



- 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*