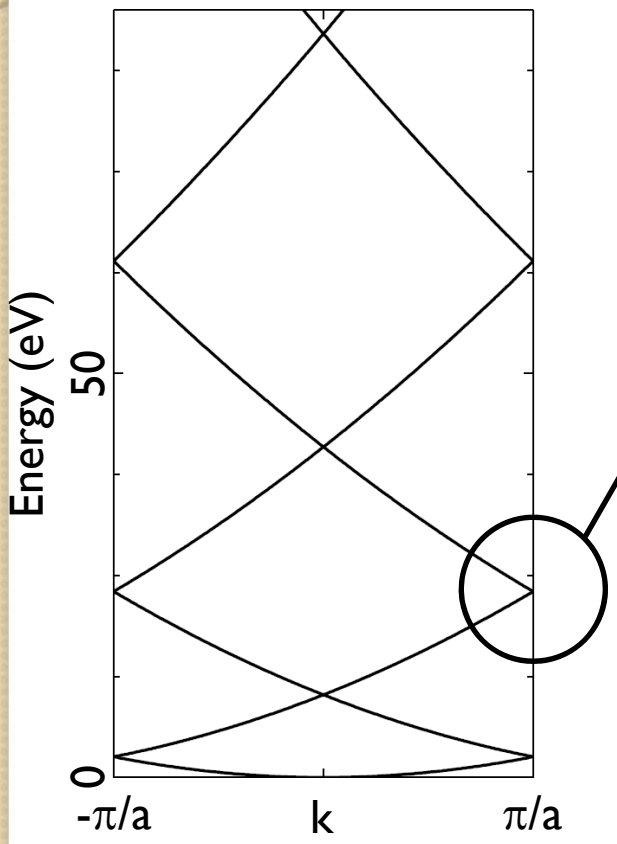
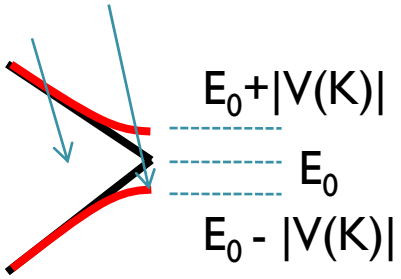
Lecture 11
AE Electron Band Theory I

Some general properties of band theory
("Wilson's rule")
Nearly free electron band

In the limit of weak potential (2x2 approx)

At k=π/a, wave function is equal mix of k and k+K
→ Standing Wave (group velocity = 0)
→ dE / dk = 0



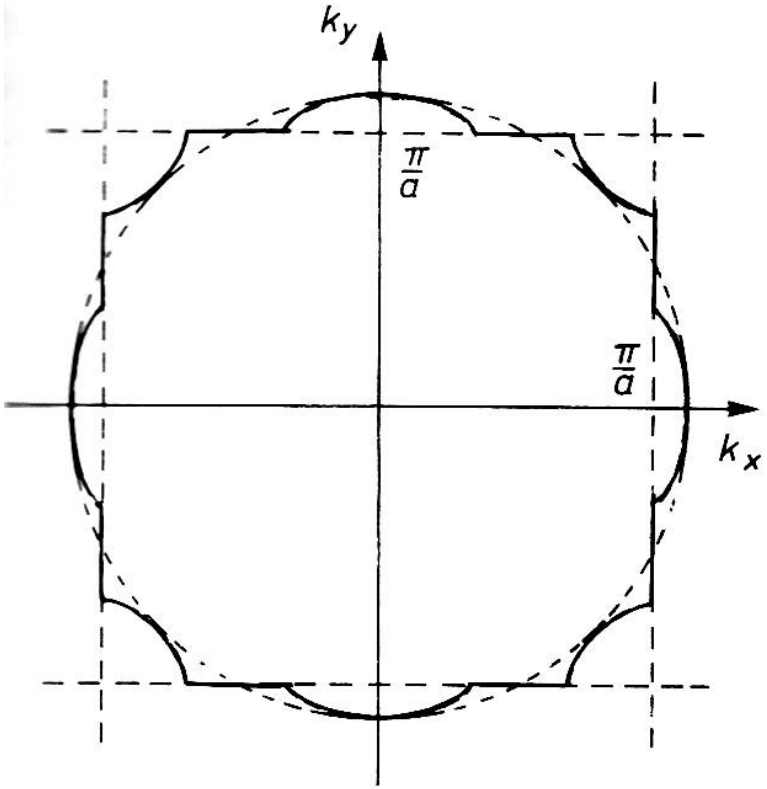


General condition that energies are the same

$$|\mathbf{k}| = |\mathbf{k}-\mathbf{K}|$$

Perpendicular bi-sector planes that we used in defining the BZ (Wigner Seitz Cell)!

Change in the Fermi Surface



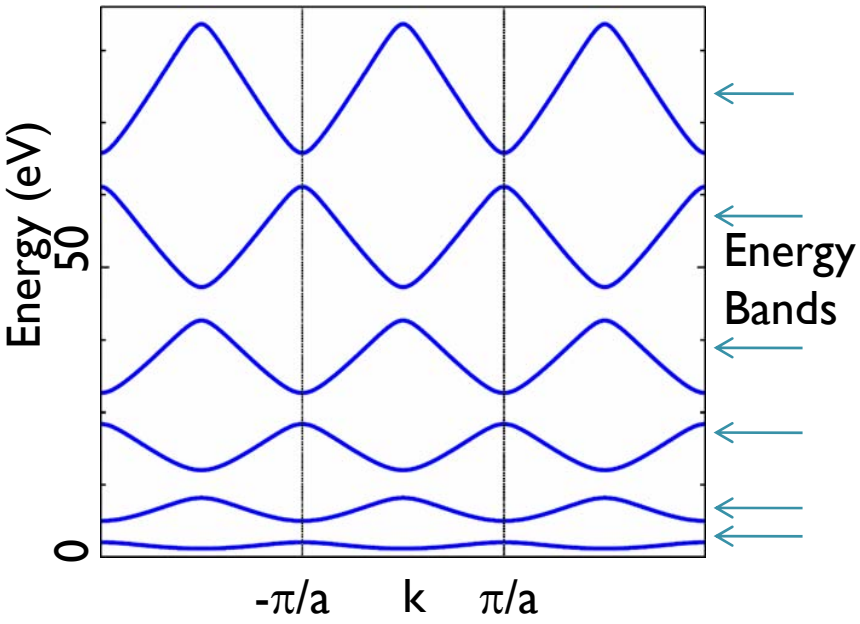
Gradient of E(k) is parallel to the BZ face, i.e. the group velocity perpendicular to the BZ face is zero.

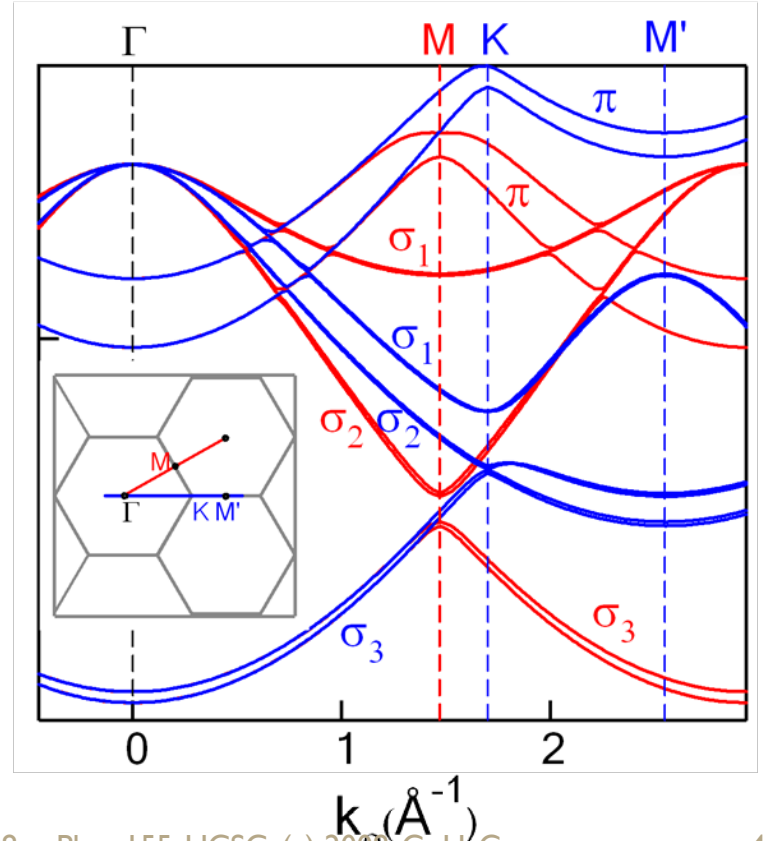
Constant energy contour intersects BZ at right angle

Metals, Insulator, Semi-conductors, Semi-metals

No band gap (at T=0 μ)	Gap >~ 1 eV,	Gap <~ 1 eV,	No Gap
Partially filled bands	All bands filled		Small number of e-s and holes
T=0 FS	No T=0 FS		No or very small T=0 FS

To entirely fill a band, need 2 electrons per unit cell. Bands can also overlap.

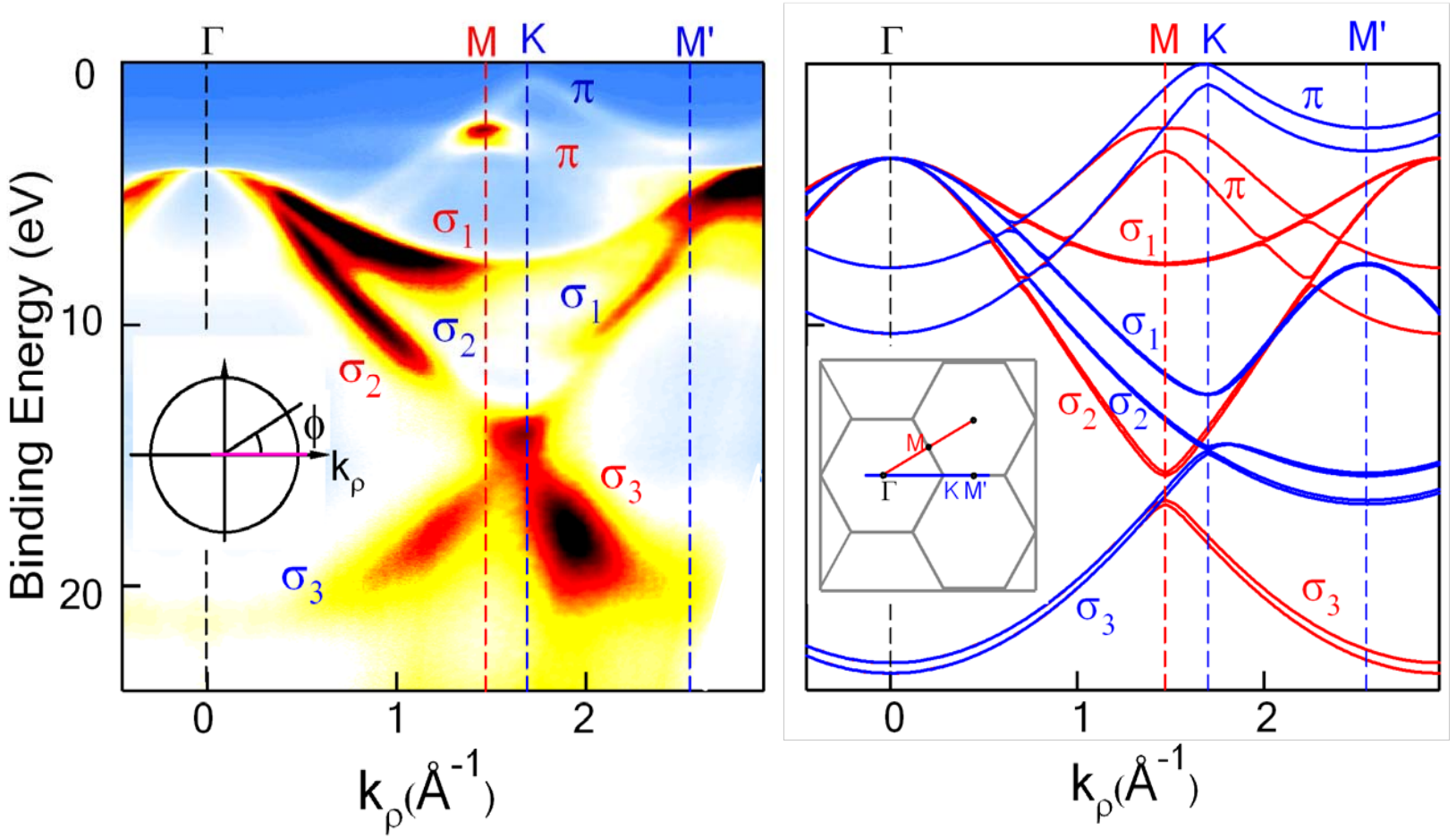




These are GENERAL arguments going beyond nearly free electron or other models!

Bands from Real Stuff (Graphite, Graphene)

Note overlap between bands



Zhou, GHG *et al*, Phys. Rev. B, 2005

Question

So, Fermi surface and band fillings are important to predict metals and non-metals. (remember "unit cell" means "primitive unit cell")

- Cu can be thought of as an fcc crystal with one nearly free electron per unit cell. Is this a metal?
- Diamond (or Si) is an fcc crystal with 8 nearly free electrons per unit cell. Metal or non-metal?
- Graphene has 2 nearly free electrons. What about it?

Metals, Insulator, Semi-conductors, Semi-metals

No band gap, Partially filled bands, T=0 FS

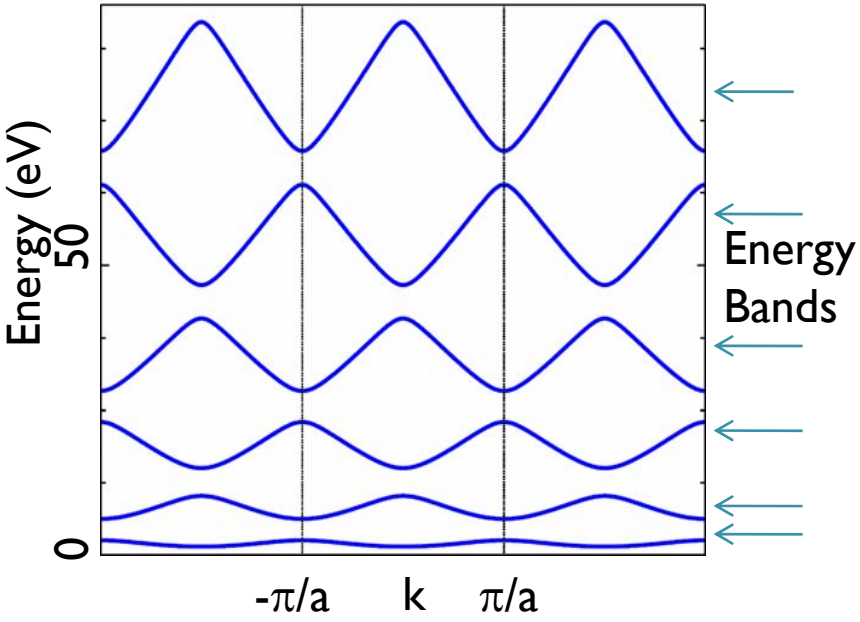
Gap >~ 1 eV, All bands filled, No T=0 FS

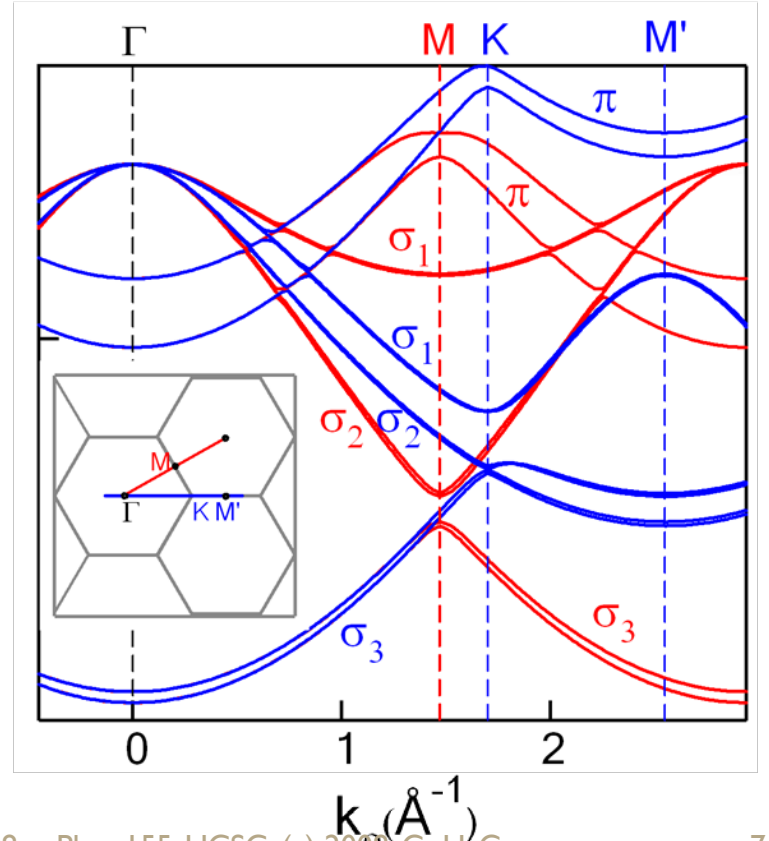
Gap <~ 1 eV, No Gap

Small number of e-s and holes, No or very small T=0 FS

To entirely fill a band, need 2 electrons per unit cell. Bands can also overlap.

Wilson's rule: metal if an odd number of free electrons per unit cell





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