Physics 489 S 04 Lecture 13
Nearly-Free Electrons in Crystals (A&M chapter 9)

1. Key point of course - recall from last lecture
   Electronic bands $\epsilon_n(\mathbf{k})$ are the allowed states for a single particle (an electron) in a periodic potential.
   See figure below for examples of BZ's for well-known crystals
   The starting point (and often an excellent approximate description) for understanding *many* electrons in crystals is to treat the electrons as non-interacting particles that obey the Pauli exclusion principle.

2. The simplest band structure - Free Electron bands
   Derived entirely from a change of variables $\mathbf{q} = \mathbf{k} + \mathbf{G}$, where $\mathbf{q}$ is any vector in reciprocal space, and $\mathbf{k}$ is defined to be in the BZ, with $\mathbf{G}$ a reciprocal lattice vector. This has the effect of 'translating' free electron states with energy $\epsilon(\mathbf{q})$ into the first Brillouin Zone (BZ), and defining the energy $\epsilon(\mathbf{k} + \mathbf{G})$ as a function of $\mathbf{k}$.

   Simple in 1 D
   2D and 3D cases have degenerate points where bands cross.

3. Fourier analysis for "empty lattice" where V(G) = 0
   Free electron bands

4. Nearly Free Electron bands:
   For weak potentials, i.e., small V(G): Use perturbation theory
   Small changes in free electron bands, except at points where degenerate states are mixed
   At BZ boundaries, opens gaps, creates standing waves
   Equivalent to Bragg scattering condition.
   (This shows why BZ is more useful than other primitive cells)

5. 1D cases: opens gaps in the density of states
   Periodic in extended zones

6. Now consider many non-interacting electrons in the crystal
   Electrons fill lowest states up to the Fermi energy
   Simple counting leads to filled or partially-filled bands

7. 2D and 3D cases: Fermi surfaces in k-space
   Example of 2D square lattice
   For 1 electron per primitive cell, FS in first band inside BZ.
   For 2 electrons per primitive cell, FS crosses zone boundary into 2nd band.

8. Extended Zone Scheme: 1st, 2nd BZ, etc.

9. Examples: Na(bcc), Al (fcc), Ge (diamond)

Figure 1: Brillouin zones for several common lattices: a) simple cubic (sc), b) face centered cubic (fcc), c) body centered cubic (bcc) and d) hexagonal (hex). (High symmetry points and lines are labelled according to Bouckaret, Smoluchowski, and Wigner.) The zone center ($\mathbf{k} = 0$) is designated Γ and interior lines by Greek letters, points on the zone boundary by Roman letters. In the case of the fcc lattice, a portion of a neighboring cell is represented by dotted lines. This shows the orientation of neighboring cells that provides useful information, for example, that the line Σ from Γ to K continues to a point outside the first BZ that is equivalent to X. This line is shown for examples such as the bands for Al and GaAs.

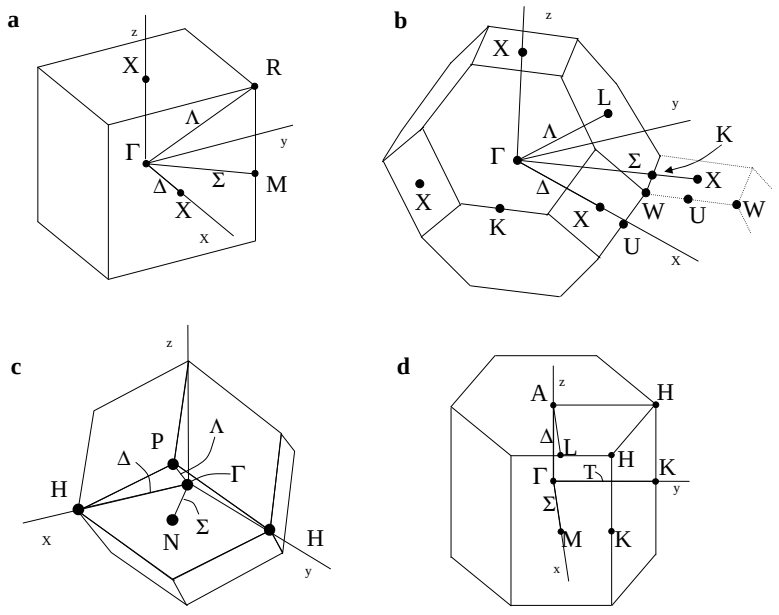

Figure 2: Free electron bands in an fcc crystal plotted as a function of wavevector **k** in the BZ.

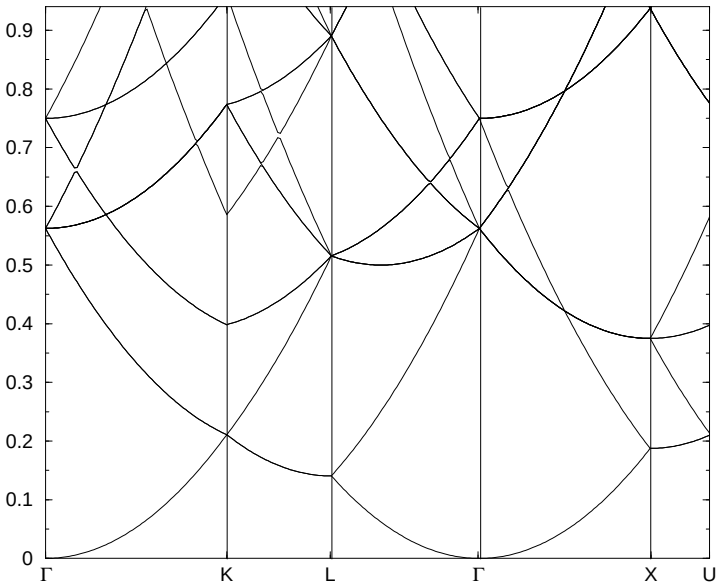

Figure 3: Electron bands in fcc Al compared to free electron bands (dashed lines) as calculated Segall

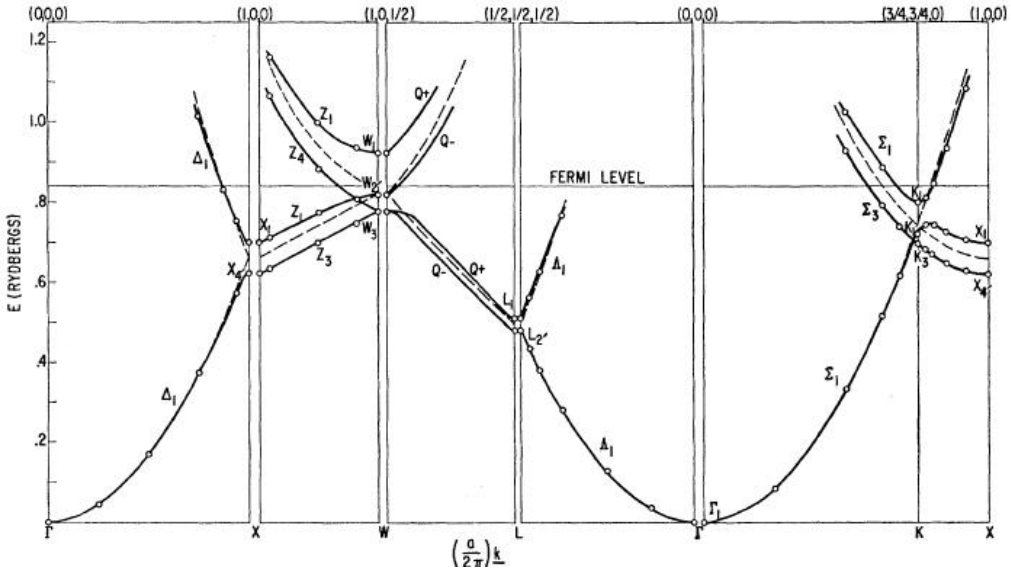

Figure 4: Free electron bands in GaAs which has the zinc blende structure, fcc with 2 atoms per primitive cell. The bands are plotted as a function of wavevector **k** in the BZ and compared with experimental date (from T. C. Chiang of UIUC). (The BZ is exactly the same as for any fcc crystal - only the scale $2\pi/a$ depends on the crystal which has lattice constant a.) GaAs is a semiconductor beacuse the lowest four bands are full and separated by a gap from the empty bands - more later.