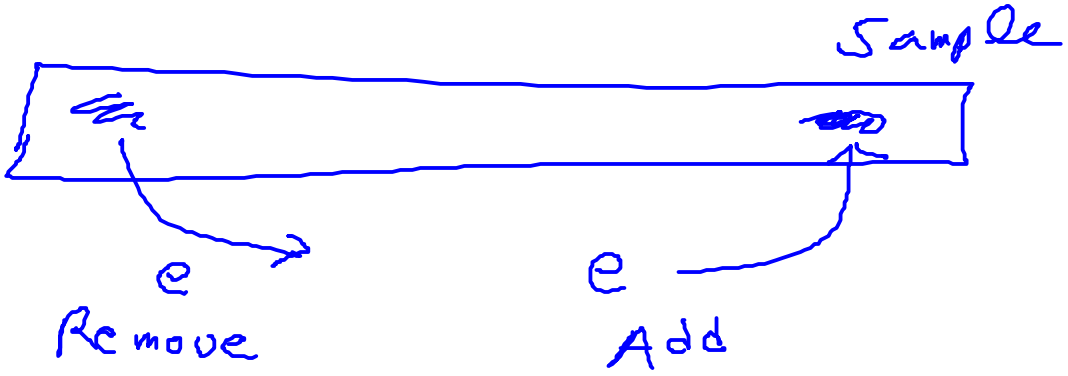
Lecture 15

Tuesday, February 22, 2011

How to distinguish metals and non-metals?

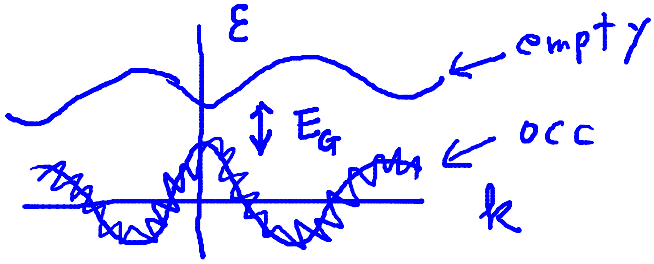
The defining characteristics of the metal and non-metal is the presence of an energy gap. What is the energy gap?



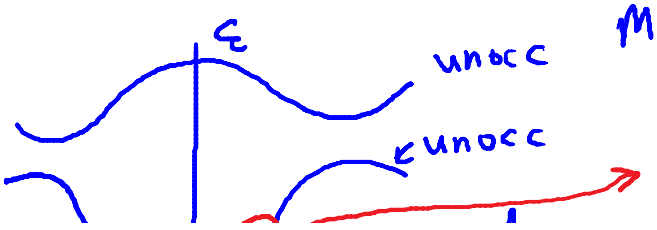
Consider the above procedure. You remove an electron from one part of the sample and then add it back to another part of the sample. Assume that these two parts are macroscopically separated so that they can be considered as two identical but separate samples. The energy gap is the minimum energy cost to accomplish this procedure.

This definition is very general, and applies to any materials, whether that material is described by the band theory (as we explored in last classes) or not.

(1) Within the band theory, the energy gap (E_G) is the energy separation between the top of the occupied state and the bottom of the un-occupied state.

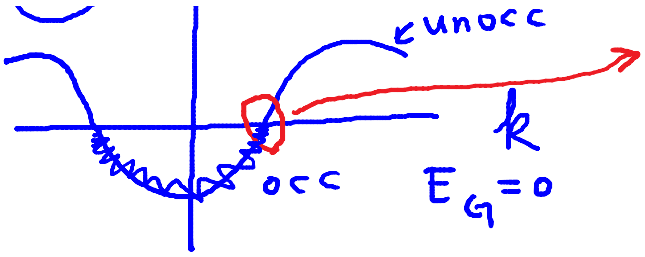


Insulator
Semiconductor



Metal

An unoccupied state is available right above the top of the occupied state. Thus, energy gap = 0



An unoccupied state is available right above the top of the occupied state. Thus, energy gap = 0.

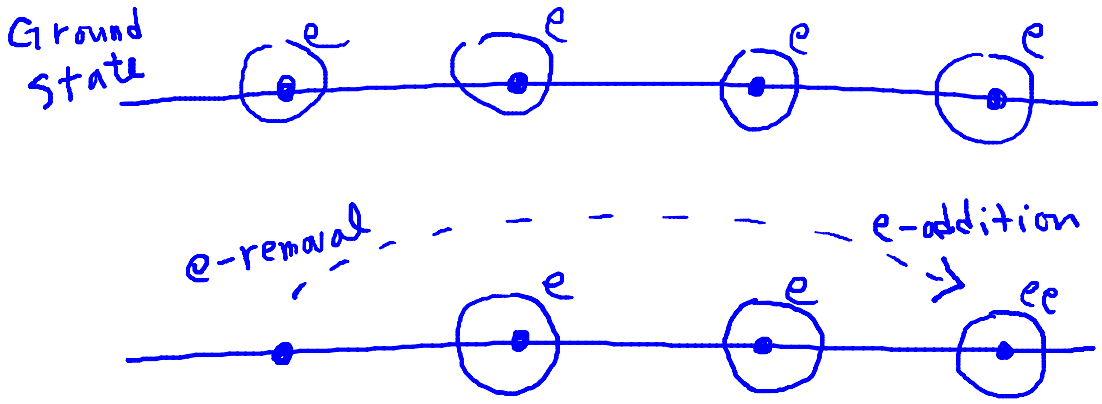
In the semiconductor field, the completely filled band above is called the **valence band**, while the completely empty band above it is called the **conduction band**.

(2) Now, as a different example, consider a H crystal. A 1D crystal. This is a hypothetical 1D crystal, but it is nevertheless a good example to consider. According to the band theory, this must be a metal, due to Wilson's rule. One electron per unit cell (per H), and thus we will necessarily be left with some partially filled band. Within the tight-binding theory that we did, the lowest lying 1s band is half filled, and all other bands (that we did not consider since they lie at high energies) are completely empty. And yet, the real H crystal that one makes in a lab (under moderate pressure) is an insulator. Why? It turns out that the electron-electron interaction energy that one ignores in the band theory is of more importance in this case. So, it is not correct to think of these electrons occupying a band. Instead it is correct to think of the ground state of a H crystal as something dramatically different -- a simple collection of H atoms! Each electron is bound to a proton, and there is no hopping of that electron to a neighboring site.

In order to realize that such a state must be a physical state can be realized from this reasoning. Consider any crystal, and imagine that you are free to expand the crystal so that the lattice constant can become arbitrarily large. When the lattice constant is very large (say 1 meter!), it is obvious that the physically correct picture is a simple collection of atoms, rather than electrons delocalized between atoms as in the band theory. So, any band theory will fail in the limit of large lattice constant. In the limit of large lattice constant, Coulomb interactions between electrons are much more important than band theory energy scale (hopping energy scale "t" which becomes very small).

Under natural conditions, some materials are in the regime where the band theory is a good description, while some other materials are in the regime where the band theory is not a good description. The H crystal above is an example of the latter. Materials such as MnO, CuO, MnF2, NiO, CeSi2, … (pretty much any material that involves 3d transition metal element or 4f rare earth element) are also examples of the latter, which can be called the "**strongly correlated electron materials**."

Back to the H crystal. The energy gap here is the so-called U, electron-electron repulsion. This is the concept of the **Mott insulator**.



The only difference between the ground state and the excited state (created by removing an electron and adding it to a different site) is the Coulomb interaction between two electrons on the same site, which we call "**Hubbard** U".

How to distinguish metals and non-metals (2)?

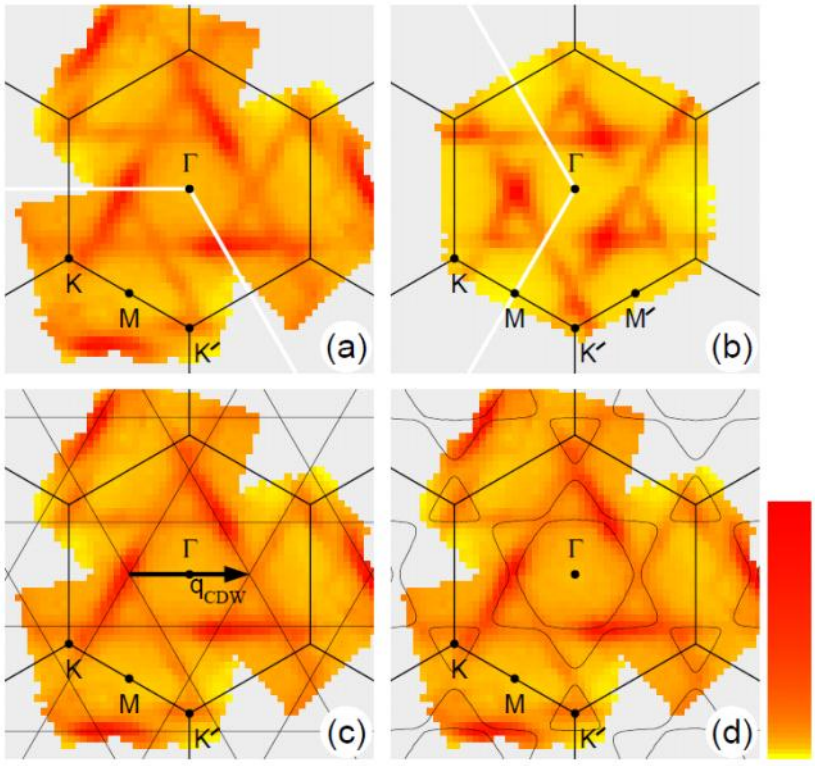
Related to the above general discussion, there is another method to distinguish metals from non-metals. **Metals have Fermi surface, while non-metals don't**. This statement is true for any materials, strongly correlated electron materials or not. It is however very easy to see this point for materials that are described well by the band theory, and so much discussion in the rest of this course (except magnetism and superconductivity) will focus on them.

Insulators and semi-conductors have no Fermi surface at zero temperature. Semi-metals do not have Fermi surface at zero temperature; instead they have Fermi "points", the limit of finite volume/area Fermi surfaces just before they disappear. In practice, if the Fermi surface is very small, then the material can be considered a semi-metal.

How do we know that the FS exists?

There is a rather direct way of observing a Fermi surface. This method is angle resolved photoelectron spectroscopy (ARPES), which is the method of choice for yours truly. This method uses the photoelectric effect, to excite electrons out of the specimen with high flux beams of ultraviolet light. The interpretation of the photoelectric effect (electron + photon → more energetic electron) mainly

involves only the energy conservation principle and the momentum conservation principle. Essentially, the electron that is taken out from the sample remembers the energy and the momentum it used to have inside the sample, and it is elementary for experimenters to compute them since the photon energy and the photon momentum involved in an ARPES experiment are very accurately known. The simplicity of the interpretation gives great power to the ARPES technique. From mid 90's, it has become quite routine to obtain "Fermi surface" maps, the intensity map at the chemical potential, where the high intensity region delineates the Fermi surface shape. The following is an example of such an early ARPES Fermi surface map, which was taken by yours truly for his Ph. D. thesis. The materials here are "Na/K purple bronzes" which have a strongly two dimensional electronic structure in a hexagonal unit cell. Shown here are the hexagonal BZ, ARPES maps, and theoretical predictions (c and d).



Other methods of probing the Fermi surface

ARPES works very well for layered materials with quasi-2D electronic structure. These are crystals that are built up by loosely coupled layers, and the electrons spend much of their time within the layer than hopping between layers. This class of materials include high temperature superconductors and graphene/graphite, and so ARPES continues to receive much attention.

However, the applicability of ARPES to more traditional 3D materials is weak.

What are other methods of probing the Fermi surface? Quantum oscillation measurements at high magnetic field is a very sharp measurement tool. Also, in recent days, the scanning tunneling spectroscopy has been used to infer the Fermi surface shape. Other effects such as Kohn anomaly (homework 4.5) can give information about the Fermi surface. None of these methods are as direct as ARPES in the sense that, while ARPES can give the shape of the Fermi surface without any band theory input, all these methods must use some prior knowledge from theory in order to interpret the results since they cannot obtain the absolute position of the Fermi surface and the exact shape of the Fermi surface. Nevertheless, these methods are very useful, and more advantageous to the ARPES technique in terms of applicability to 3D materials. Of these, we will review the quantum oscillation measurements below. Before doing that, though, we need to do establish some important facts about how the electron (or the hole) moves under an applied field.