NOTES 13: Metal-Insulator Theorem

A great triumph of Bloch's theorem and band-structure theory is in predicting the electrical nature of solids as insulators or conductors. It is well known that solids offer a tremendous range in electrical conductivity ranging from values well over 10^7 S/m in the best conductors (e.g., copper) to values well under 10^{-10} S/m in the best insulators (e.g., quartz). This incredible range is fundamental to the success of solid-state electronics, because it allows semiconductor devices and circuits to be fabricated on substrates of much higher resistivity so there is little shunting of electrical current through the substrate. And it allows metallic interconnects to be fabricated between neighboring devices such that the resistive voltage drops in the interconnects is negligible compared to the drops in the devices themselves. Without both of these effects, integrated circuits would probably not be nearly as successful as they are today.

Electrical Current

In ECE215B we will discuss in more detail the "semi-classical" view of electrical current in a solid as the statistical average of the current operator over the entire band

$$J = e\frac{\int_{band} \vec{v}_g(\vec{k})\, f[U_n(\vec{k})]d\vec{k}}{4\pi^3} \tag{1}$$

where e is the electronic charge, $\vec{v}_g$ is the group velocity in state $\vec{k}$, f is the electron distribution function and $U_n(\vec{k})$ is the energy band function. At or near equilibrium, we can approximate f by the Fermi-Dirac function f_{FD}, which we know is symmetric (i.e., even) with respect to k since it depends only on $U_n(k)$ which itself is symmetric. Furthermore, $\vec{v}_g = \hbar^{-1}\vec{\nabla}_k U_n(\vec{k})$, which is antisymmetric (i.e., odd) with respect to $\vec{k}$. Hence at or near equilibrium, the electrical current integral contains a product of an even an odd function, which is always odd, making the integral vanish.

What happens if the given band is completely occupied with electrons and is isolated in energy from other bands by large gaps ? Under this condition, the distribution function will start out as unity for all space-spin states. And the application of an electric field, temperature gradient, or other external "force" will not change this distribution provided that the "force" is small enough to not elevate electrons to higher bands. There is simply no available states for any of the electrons to move into, and the distribution function over the band remains constant and symmetric, just as in thermal equilibrium. Hence, the electrical current integral of Eqn (1) remains zero, and we have an electrical insulator. This is yet another ramification of the Pauli exclusion principle.

What happens of the band is partially full rather than completely full in thermal equilibrium. In this case, the external "force" can and will create an asymmetry in the distribution function, breaking the perfect asymmetry of the integrand in Eqn (1) and creating a non-zero electrical current and a description of the solid as a "conductor." Partially full bands commonly occur in three different ways: (1) half filling of an isolated band, which is called a metal, (2) partial filling of a band owing to a small gap separating it from the next lower band, or from impurities (i.e. doping), which is called a semiconductor, and (3) a missing gap between two bands, creating overlap along the energy axis and partial occupancy of both, which is called a semi-metal. The procedure for deciding whether a given crystalline solid will be an insulator or conductor is described next.

Band-Filling Procedure

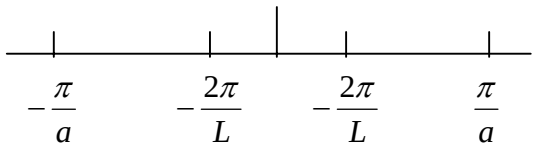
- Number states in each band =2×No. Primitive cells≡ $2 \cdot N_c$

spin

Insulator Theorem: If the highest band of a crystalline solid is full, then there must be an even number of electrons per primitive unit cell (e.g. Al→6) to fill all $2N_c$ levels. Converse is not true: (i.e. an even number of electrons per cell does not necessarily make an insulator because they can go in separate bands. E.g., some in valence band, others in conduction band).

Alternative proof of state number theorem:

Recall how wave vector are defined in 1-dimemsion



$k_{\max}$ (in 1st BZ)= $\frac{\pi}{a}$, $k_{\min} = \frac{2\pi}{L}$ (for sample of length L)

So number of K states $= 2 \times 2 \times \frac{\pi/a}{2\pi/L} = 2 \cdot L/a$

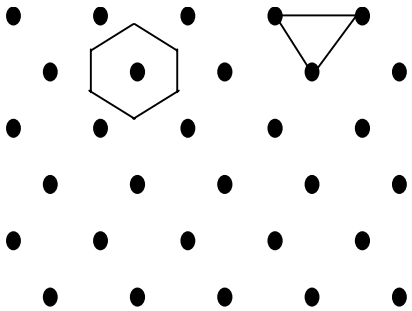
$= 2 \times N_{cells}$

Recapitulation on Primitive cell

Definition: The primitive cell is the volume that when translated through all the vectors in the Bravais lattice just fills space without overlapping or leaving voids.

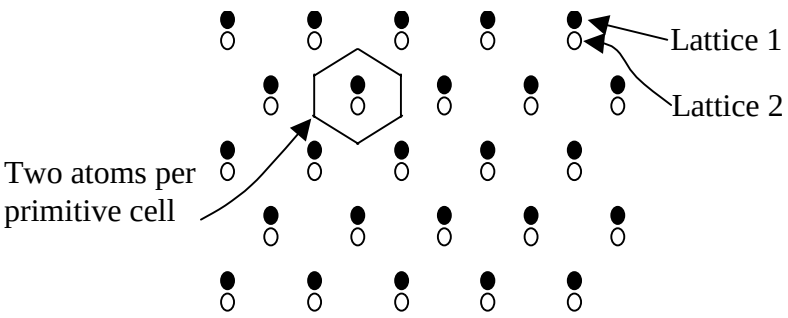
Most common primitive cell is Wigner-Seitz cell as discussed previously in the Course.

Easiest way to see primitive cells is in two dimensions, e.g., triangular lattice.



- According to insulator theorem, each primitive cell of Bravais Lattice must contribute two Bloch states to the highest energy band. So if there is one atom per primitive cell, each atom will have to contribute an even number of electrons, 2,4,6,… to fill all levels of one or more bands.
- However, there can be more than one atom per primitive cell! This is called a basis (e.g. Silicon) The over all crystal structure is called lattice with a basis.

For example: consider two interpenetrating triangular lattice.



With two atoms per primitive cell, now each atom only has to contribute on electron in order that each primitive cell fills all the given bands.

	Conductor	Insulator
#atoms/primitive cell	#electrons/atom/primitive cell	
Sc,fcc →1	1,3,5,…	2,4,6…
Dimand,Zineblende→2	No possibilities	1,2,3…
3	1/3,3/3,5/3,7/3	2/3,4/3,6/3…
4	¼,3/4,5/4…	2/4,4/4,6/4,8/4