PHYS 551 Lecture #22

Title: Filled bands and empty bands - Semiconductors

At present we have seen how the introduction of a weak periodic potential due to the ion cores opens up a gap at each and every band crossing for which there is a *non-zero* Fourier component of the potential, $U(r)$. The presence of this gap allows an immediate and natural understanding to the question of why some elements are metals while others are insulators.

$\vec{E}$-field: With a partially filled electron energy surface, or band, the electrons can move, constrained to this surface, long enough to establish an equilibrium as a result of the characteristic relaxation time τ. Thus a net current exists.

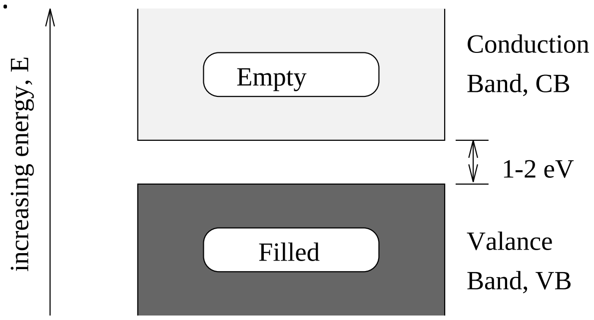
Insulator: With a filled band, the electrons <u>will</u> flow, once again constrained to the energy surface of allowed states, but regardless of how they flow there can be <u>no</u> net current.

Question: When can we observe all filled bands?

Answer: For a crystalline material which has an even number of electrons/unit cell such that the *highest* energy state of the highest occupied band lies lower in energy than the *lowest* energy state of the lowest unoccupied band!

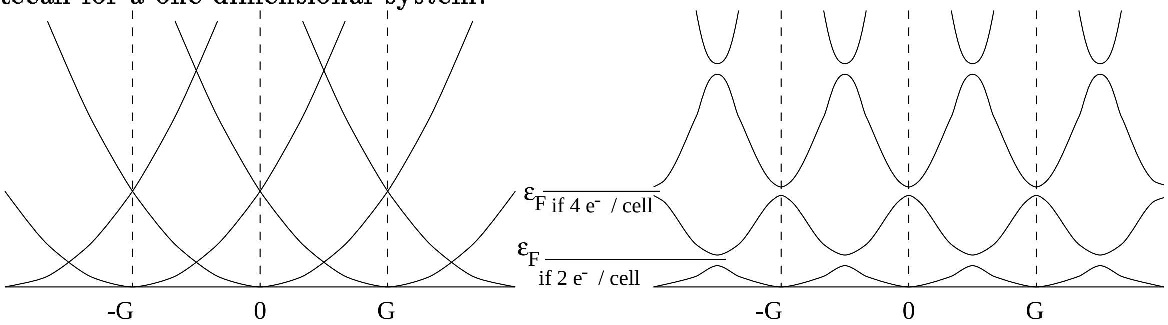
This is a situation that occurs for semi-conductors which are insulating if $T = 0°\text{K}$ (absolute zero). Without actually following the "shape" of the Fermi surface and the changes in the Density of Electron states, $\mathcal{D}(\varepsilon)$, it is expedient to examine the motion of electrons in a system which has a large bandgap ~1-2 eV between the highest filled band and the next band. These will be henceforth designated the VALANCE band and the CONDUCTION bands respectively.

In other words:

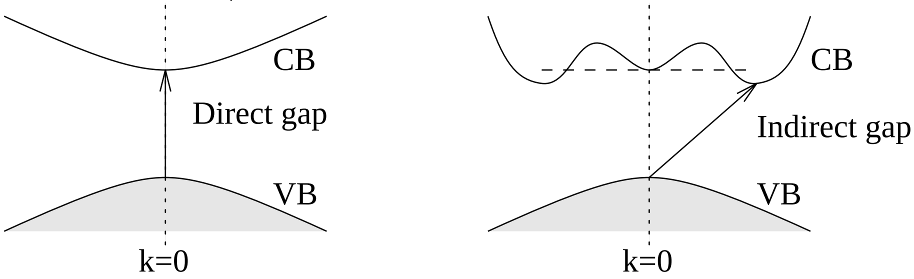


(Remember, an allowed state still exists even if it is unoccupied.)

Recall for a one-dimensional system:



For nearly free electron bands to have common energy eigenvalues it is necessary to have a two or three dimensional system. For Si and Ge which have 2 atoms/ primitive cell or 8 electrons/primitive cell, the GAP of interest lies near $\vec{k} = 0$. So,



Question: What type of processes will take an e^- from the VB and put it in the conduction band?

1. Thermal effects–

$$f(\varepsilon) \;=\; \frac{1}{\exp\left(\frac{\varepsilon-\mu}{k_B T}\right)+1} \neq 0 \quad \text{for all } \varepsilon \text{ if } T > 0$$

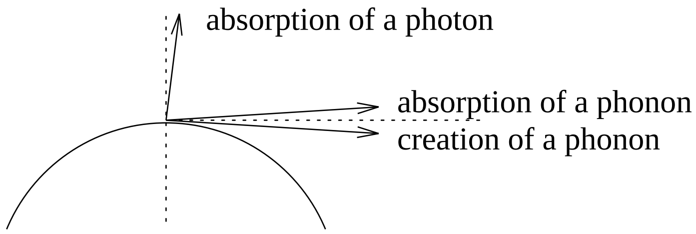
$\Longrightarrow$ Thus some electrons must be present in the CB.

2. Absorption of phonons or photons–

$\Longrightarrow$ An absorption of a phonon gives a modest change in $\vec{k}$ of the e^-, while only small changes in the energy of the electron

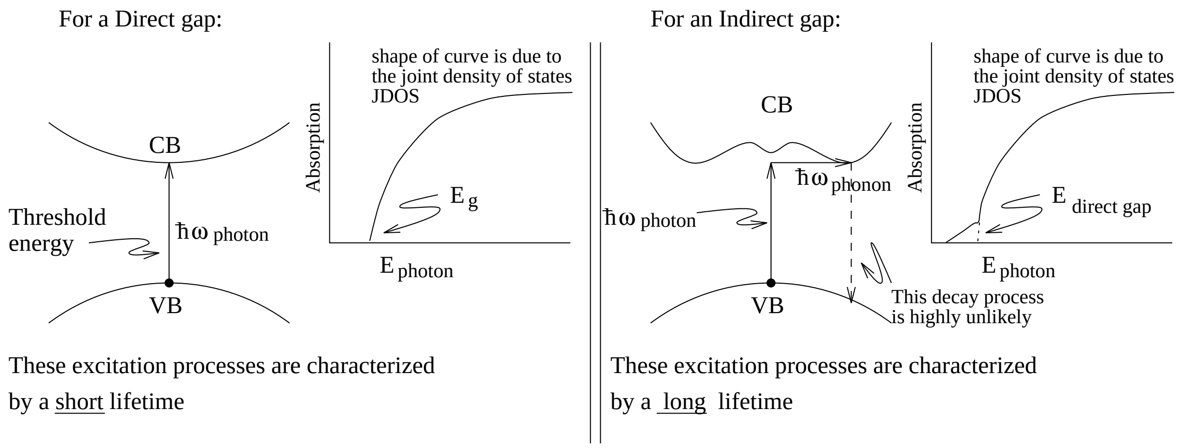
$\Longrightarrow$ An absorption of a photon gives only small changes in the $\vec{k}$ of the e^- while substantial changes in the electron energy.

Thus pictorially we get



Thus processes must still conserve energy and crystal momentum.

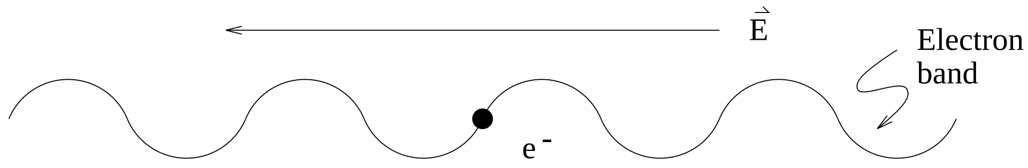
The *threshold energy* is the minimum energy required to take an electron from the VB and excite it to the CB.



So now that we have found a mechanism that will leave unoccupied states in the VB, how will the electrons evolve due to an applied $\vec{E}$-field or an applied $\vec{B}$-field?

$\Rightarrow$ Calculation of v_{group}, $\vec{v}_g = \nabla_k \omega = \hbar^{-1} \nabla_k \varepsilon(k)$

$$\text{and} \quad \vec{\nabla}_k = \frac{\partial}{\partial k_x}\hat{i} + \frac{\partial}{\partial k_y}\hat{j} + \frac{\partial}{\partial k_z}\hat{k}$$



Let $\vec{F} = q\vec{E}$ and $\vec{B} = 0$ which gives $WORK = \int \vec{F} \cdot d\vec{x} = \int -e\vec{E} \cdot d\vec{x}$

Instant in time, $\Delta\varepsilon = -e[E_x \Delta x + E_y \Delta y + E_z \Delta z]$ in Δt

$$\text{but } \Delta x = v_{g_x} \Delta t, \ \Delta y = v_{g_y} \Delta t, \ \Delta z = v_{g_z} \Delta t$$

$$\begin{aligned} \text{so} \quad \Delta\varepsilon &= -e[E_x v_{g_x} + E_y v_{g_y} + E_z v_{g_z}]\Delta t \\ \Delta\varepsilon &= -e(\vec{E} \cdot \vec{v}_g)\Delta t \approx \frac{d\varepsilon}{dk_x}\Delta k_x + \frac{d\varepsilon}{dk_y}\Delta k_y + \frac{d\varepsilon}{dk_z}\Delta k_z \\ &= \vec{\nabla}_k \varepsilon \cdot \Delta\vec{k} \\ -e(\vec{E} \cdot \vec{v}_g) &= \vec{\nabla}_k \varepsilon \cdot \frac{\Delta\vec{k}}{\Delta t} \end{aligned}$$

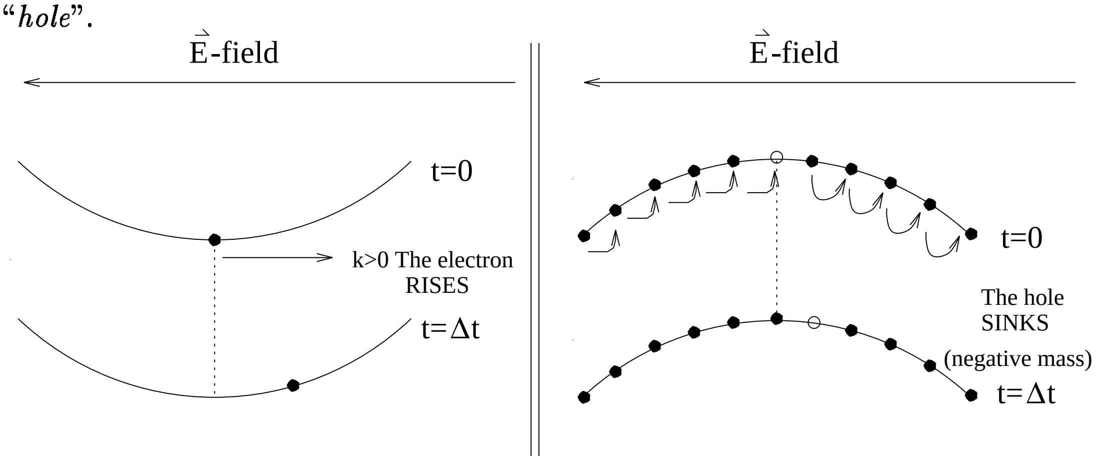
$$\text{or} \quad \frac{d\vec{k}}{dt} \cdot \vec{\nabla}_k \varepsilon(k) = -e(\vec{E} \cdot \vec{v}_g) \longrightarrow \hbar \frac{d\vec{k}}{dt} = -e\vec{E}$$

$$\text{or } \Delta\vec{k} = \frac{-e\vec{E}}{\hbar}\Delta t$$

NOTE: If B$\neq$ 0 and E = 0

$$\hbar\frac{d\vec{k}}{dt} = -\frac{e}{c}(\vec{v}_g \times \vec{B}) = -\frac{e}{c}(\vec{\nabla}_k\varepsilon \times \vec{B})$$

Notice that the $\vec{\nabla}_k\varepsilon$ is just the gradient of the energy "surface" with respect to the reciprocal space $\vec{k}$. This function is perpendicular to the energy contours. Thus $\vec{\nabla}_k \times \vec{B}$ is perpendicular to the perpendicular of the energy contours. The upshot: Electrons in $\vec{B}$-field move on a constant energy surface! Back to the case where $\vec{B} = 0$, $\vec{E} \neq 0$. The motion of the electrons in the CB is easy to follow. However, the effective motion of the electrons which remain in the VB is a bit more subtle. Rather than focus in on the whole of the electrons still remaining, we will examine the motion of the unoccupied electron state. This unoccupied state and its resulting motion is called a "*hole*".



Electron moves to the <u>right</u>

v_e is to the right

but $\vec{j}_e = nq\vec{v}_e$

$\vec{j} = \frac{ne^2\vec{E}\tau}{m^*}$

$\vec{j}_e$ is to the <u>left</u>

$\vec{j}_T = \vec{j}_e + \vec{j}_h = (n+p)\frac{e^2\vec{E}}{m^*}$

Hole moves to the <u>right</u>

As far as the electrons are concerned, there is just <u>one</u> more with $k<0$

k is to the left, k_h is to the left.

This electron has $|v_g|>0$.

v is to the right for the negative charge

v is the left for a positive charge

v_h is to the left, $\vec{j}_h = pq\vec{v}_h = \frac{pe^2\vec{E}\tau}{m^*}$

$\vec{j}_h$ is to the left