# PHYS 551 Lecture 21A

Once again let us examine the electron dynamics.
An electron can be considered a wave packet

$$
\begin{aligned}
v_{group} &= d\omega/dk = \frac{1}{\hbar} dE/dk \\
\vec{v}_{group} &= \frac{1}{\hbar}\nabla_k E(k) \qquad \nabla_k = \frac{\partial}{\partial k_x}\hat{k}_x + \frac{\partial}{\partial k_y} + \frac{\partial}{\partial k_z}\hat{k}_z
\end{aligned}
$$

Clearly $\vec{v}_g$ is $\perp$ to a constant energy surface. If an applied electric field, $\varepsilon$

$$
\begin{aligned}
\Delta E = \text{change in energy} &= -e\,\varepsilon\, v_g \delta t \quad \text{where } \delta t \text{ represents an instant in time} \\
&= -e\,\varepsilon \frac{1}{\hbar}\frac{dE}{dk}\delta t
\end{aligned}
$$

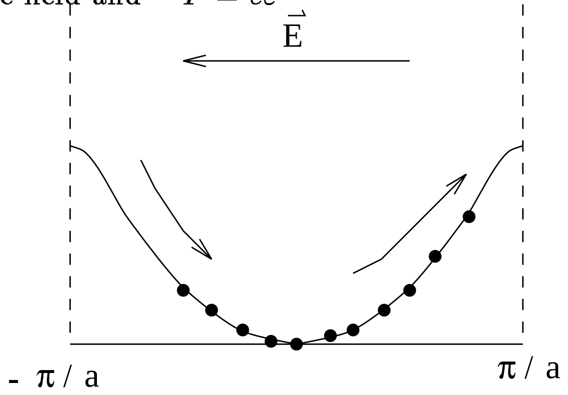
If there is a magnetic field:

$$
\begin{aligned}
\hbar\,\frac{d\vec{k}}{dt} &= -e(\vec{v}_g \times \vec{B}) \\
\frac{d\vec{k}}{dt} &= -\frac{e}{\hbar^2}(\nabla_k E \times \vec{B})
\end{aligned}
$$

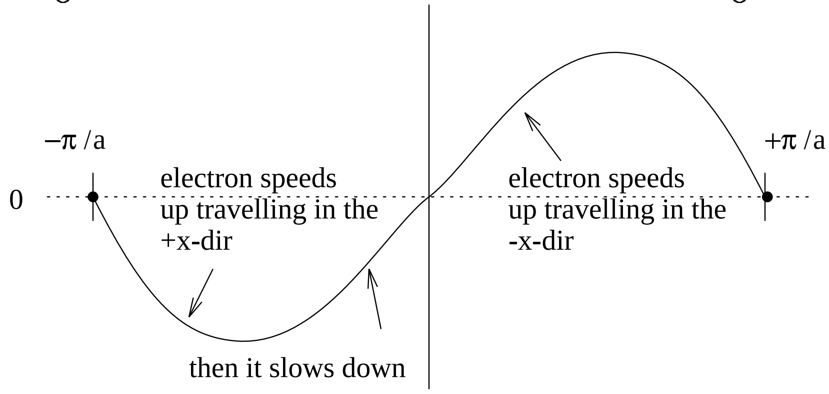
An electron moves in $k$-space normal to $\vec{B}$ and normal to $\nabla_k E$, (i.e., electron moves on a constant energy surface).

Transport - Let us examine a single electron constrained to move along a band in a one-dimensional crystal with no electron-electron, electron-phonon, or electron-impurity scattering.

$\vec{\varepsilon}$ is the field and $\vec{F} = e\vec{\varepsilon}$




This electron would oscillate in $k$-space (i.e., move at a constant rate $\frac{d\vec{k}}{dt} = -\frac{e\varepsilon}{\hbar}$). It must follow the band to the Zone Boundary $\pi/a$ at which point it would be Bragg reflected back to $-\pi/a$ at then again move towards $+k$ at a constant rate. Looking at the velocity gives:




Now look at the acceleration $a$:

$$a = \frac{d}{dt}(v_g) = \frac{d}{dt}\left(\frac{1}{\hbar}\frac{dE}{dk}\right) = \frac{dk}{dt}\frac{d}{dk}\left(\frac{1}{\hbar}\frac{d^2E}{dk^2}\right)$$

$$\vec{a} = \frac{1}{\hbar^2}(-e\vec{\varepsilon})\frac{d^2E}{dk^2}$$

And rearranging $$\left(\frac{\hbar^2}{\frac{d^2E}{dk^2}}\right)\vec{a} = -e\vec{\varepsilon}$$

The upshot $\longrightarrow$ the electron moves in an electric field as if it has an effective mass m$^*$

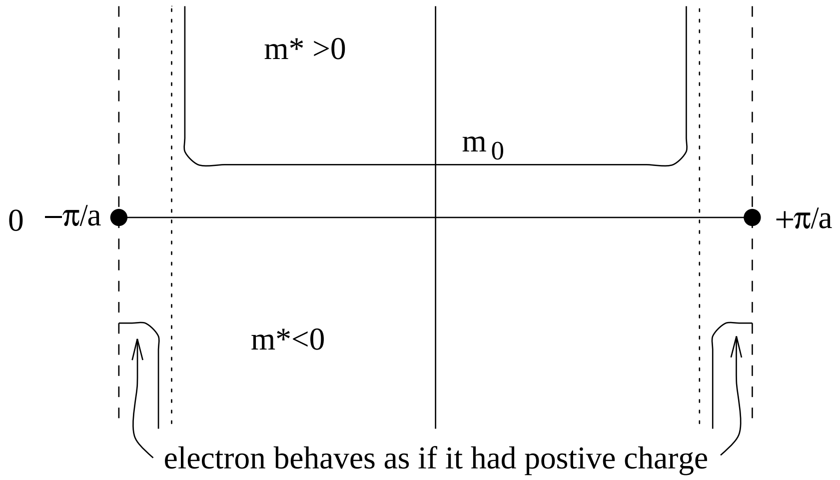
Nominally $m^* = \frac{1}{\frac{1}{\hbar^2}\frac{d^2E}{dk^2}}$ but we actually require a *tensor*: $m^*_{ij} = \frac{1}{\frac{1}{\hbar^2}\frac{\partial^2 E}{\partial k_i \partial k_j}}$

Check for free electron

$$E = \frac{\hbar^2k^2}{2m} \qquad \frac{d^2E}{dk^2} = \frac{2\hbar^2}{2m} \qquad m^* = m!$$

Notice that the slope of the band gives us the electron velocity.

Curvature gives us the effective electron mass! Basically, we can take into account all of the forces on the electron in the crystal by using this quantity m$^*$ in an appropriate equation of motion.



Insulators and Conductors:

Question: What is the difference between a conductor and an insulator?

Answer: An insulator has empty or full bands while a conductor has partially filled bands. Every band can accommodate just $2N$ electrons where $N \equiv \#$ of lattice sites.

If a band is full

$$\sum_{\substack{\text{all states}\\ \text{in band}}} \vec{v}_k = 0 \qquad \vec{j} = \sum_{\substack{\text{all states}\\ \text{occupied}}} -e\,\vec{v}_k = 0$$

For a net current there is a effective rigid shift of the Fermi surface.

$$\text{If } \vec{\varepsilon} = \varepsilon\hat{x} \qquad \delta\vec{k} = \frac{-e\vec{\varepsilon}}{\hbar}\tau \Longrightarrow \text{ relaxation time (small)}$$

$$j_x = (-e)v_{Fermi_x} \cdot \#\text{ unbalanced electron}$$

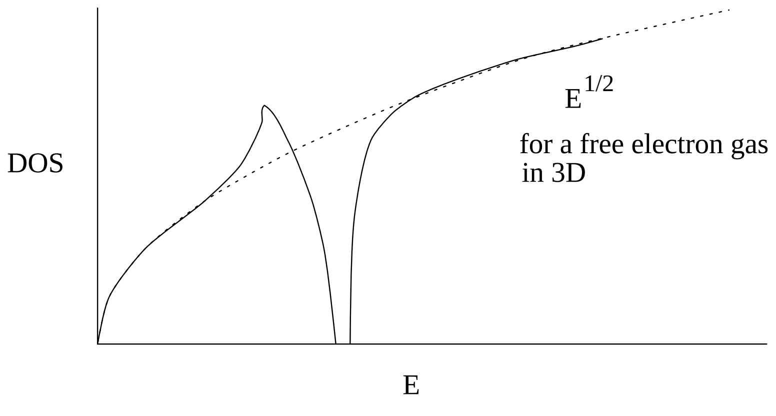
$$= -e\, v_{Fermi_x}\mathcal{D}(E)dE \text{ and } \Delta E = -e\varepsilon_x v_{F_x}\tau$$

$$= -e\, v_{F_x}\mathcal{D}(E)\frac{dE}{dk_x}\delta k = \mathcal{D}(E)(-e)^2(v_{F_x})^2\varepsilon_x\tau$$

$$j_x = \frac{e^2}{\hbar}\,\varepsilon_x(\overline{v}^2_{F_x})\mathcal{D}(E)\tau$$

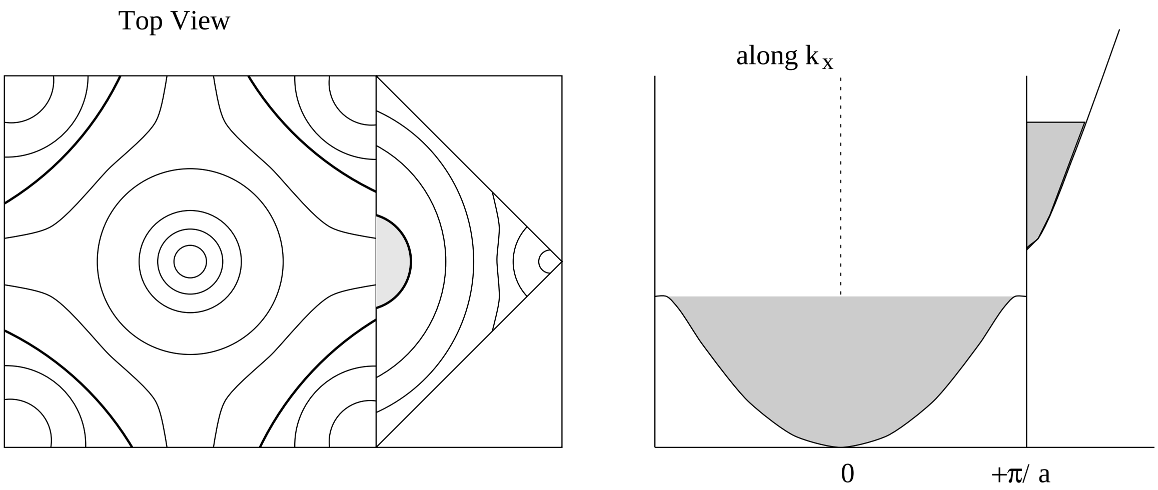
The conductivity is strongly dependent on the DOS (density of states) at $\varepsilon_F$, the Fermi velocity given by $v_{F_x}$ and on the relaxation time $\tau$ for electrons at the Fermi level.

A typical DOS's for a metal:




The cusp in $\mathcal{D}(E)$ comes as $k$ approaches Brillouin Zone boundary and $E(k)$ becomes flat and then decreases as the number of remaining states in the zone goes to zero.

A two-dimensional crystal with 2 electron per primitive unit cell:




If $E_{\text{corner}} - E_{\text{Face}} < E_{\text{gap}}$ *and* $E_{\text{gap}} = \text{constant}$, then the zone will fill completely and we now have an *insulator*.