Handout 16

Electrical Conduction in Energy Bands

In this lecture you will learn:

- The conductivity of electrons in energy bands
- The electron-hole transformation
- The conductivity tensor
- Examples
- Bloch oscillations

Inversion Symmetry of Energy Bands

Recall that because of time reversal symmetry:

$$\boxed{\psi^*_{n,-\vec{k}}(\vec{r}) = \psi_{n,\vec{k}}(\vec{r}) \qquad E_n(-\vec{k}) = E_n(\vec{k})}$$

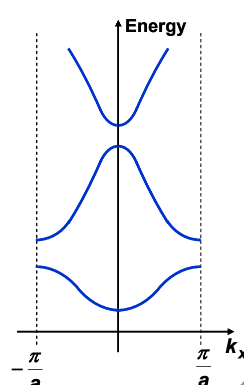
We know that:

$$\vec{v}_n(\vec{k}) = \frac{1}{\hbar}\nabla_{\vec{k}}\, E_n(\vec{k})$$

Now let $\vec{k}$ go to $-\vec{k}$ in the above equation:

$$\begin{aligned}
\vec{v}_n(-\vec{k}) &= \frac{1}{\hbar}\nabla_{-\vec{k}}\, E_n(-\vec{k}) \\
&= -\frac{1}{\hbar}\nabla_{\vec{k}}\, E_n(-\vec{k}) \\
&= -\frac{1}{\hbar}\nabla_{\vec{k}}\, E_n(\vec{k}) \\
&= -\vec{v}_n(\vec{k})
\end{aligned}$$

$$\boxed{\Rightarrow \vec{v}_n(-\vec{k}) = -\vec{v}_n(\vec{k})}$$



Current Density for Energy Bands

In Drude model, the electron current density was given as:

$$\vec{J} = n\,(-e)\,\vec{v}$$

For a free electron gas the current density was given as:

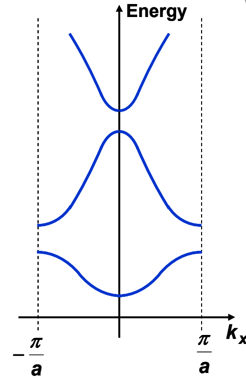
$$\vec{J} = (-e)\frac{2}{V}\times\sum_{\text{all }\vec{k}} f(\vec{k})\,\vec{v}(\vec{k}) = -2\,e\times\int\frac{d^3\vec{k}}{(2\pi)^3}\,f(\vec{k})\,\vec{v}(\vec{k})$$

Now we want to find the current density due to electrons in energy bands

The current density due to electrons in the *n*-th band can be written in a manner similar to the free-electron case:

$$\vec{J}_n = (-e)\frac{2}{V}\times\sum_{\vec{k}\text{ in FBZ}} f_n(\vec{k})\,\vec{v}_n(\vec{k})$$

$$= -2\,e\times\int_{\text{FBZ}}\frac{d^3\vec{k}}{(2\pi)^3}\,f_n(\vec{k})\,\vec{v}_n(\vec{k})$$



Current Density for a Completely Filled or Empty Bands

Consider a completely filled band for which $f_n(\vec{k}) = 1$ for all $\vec{k}$ in FBZ

Application of an external field will not change anything!

$$\vec{J}_n = -2\,e\times\int_{\text{FBZ}}\frac{d^3\vec{k}}{(2\pi)^3}\,f_n(\vec{k})\,\vec{v}_n(\vec{k}) = -2\,e\times\int_{\text{FBZ}}\frac{d^3\vec{k}}{(2\pi)^3}\,\vec{v}_n(\vec{k}) = 0$$

where I have used the fact:

$$\vec{v}_n(-\vec{k}) = -\vec{v}_n(\vec{k})$$

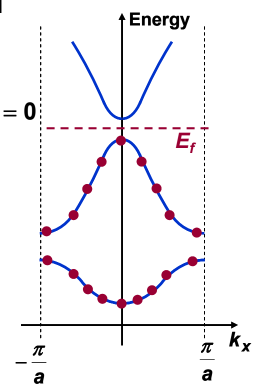
⇒ Completely filled bands do not contribute to electrical current or to electrical conductivity

Of course, if $f_n(\vec{k}) = 0$ for all $\vec{k}$ in FBZ:

$$\vec{J}_n = -2\,e\times\int_{\text{FBZ}}\frac{d^3\vec{k}}{(2\pi)^3}\,f_n(\vec{k})\,\vec{v}_n(\vec{k}) = 0$$

⇒ Completely empty bands do not contribute to electrical current or to electrical conductivity

Only partially filled bands contribute to electrical current and to electrical conductivity



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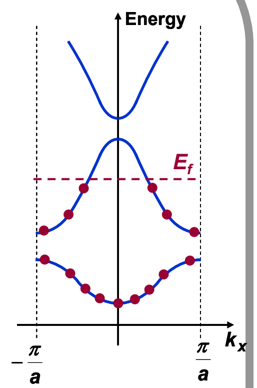
Current Density and Electron-Hole Transformation

Consider the expression for the current density for a partially filled band:



$$\vec{J}_n = 2\,(-e)\times \int_{FBZ} \frac{d^3\vec{k}}{(2\pi)^3}\, f_n(\vec{k})\,\vec{v}_n(\vec{k}) \longrightarrow (1)$$

$$= 2\,(e)\times \int_{FBZ} \frac{d^3\vec{k}}{(2\pi)^3}\, \left[1 - f_n(\vec{k}) - 1\right]\vec{v}_n(\vec{k})$$

$$= -2\,e\times \cancelto{0}{\int_{FBZ} \frac{d^3\vec{k}}{(2\pi)^3}\,\vec{v}_n(\vec{k})} + 2\,e\times \int_{FBZ} \frac{d^3\vec{k}}{(2\pi)^3}\, \left[1 - f_n(\vec{k})\right]\vec{v}_n(\vec{k})$$

$$= 2\,(+e)\times \int_{FBZ} \frac{d^3\vec{k}}{(2\pi)^3}\, \left[1 - f_n(\vec{k})\right]\vec{v}_n(\vec{k}) \longrightarrow (2)$$

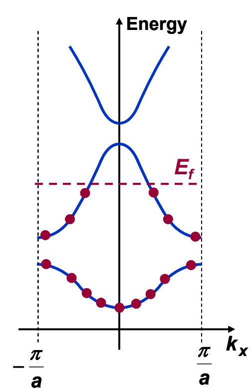
The final result implies that since the current density of a filled band is zero, the current density for any band can always be expressed in two equivalent ways:

a) As an integral over all the occupied states assuming negatively charged particles (as in (1) above)

a) As an integral over all the unoccupied states assuming positively charged particles (as in (2) above)

Current Density and Electron-Hole Transformation

One has two choices when calculating current from a partially filled band:



The Electron Choice:

The current density is given by:

$$\vec{J}_n = 2\,(-e)\times \int_{FBZ} \frac{d^3\vec{k}}{(2\pi)^3}\, f_n(\vec{k})\,\vec{v}_n(\vec{k})$$

- Current is understood to be due to negatively charged electrons
- This choice is better when the electron number is smaller than the hole number

The Hole Choice:

The current density is given by:

$$\vec{J}_n = 2\,(+e)\times \int_{FBZ} \frac{d^3\vec{k}}{(2\pi)^3}\, \left[1 - f_n(\vec{k})\right]\vec{v}_n(\vec{k})$$

- Current is understood to be due to positively charged fictitious particles called “holes”
- This choice is better when the hole number is smaller than the electron number

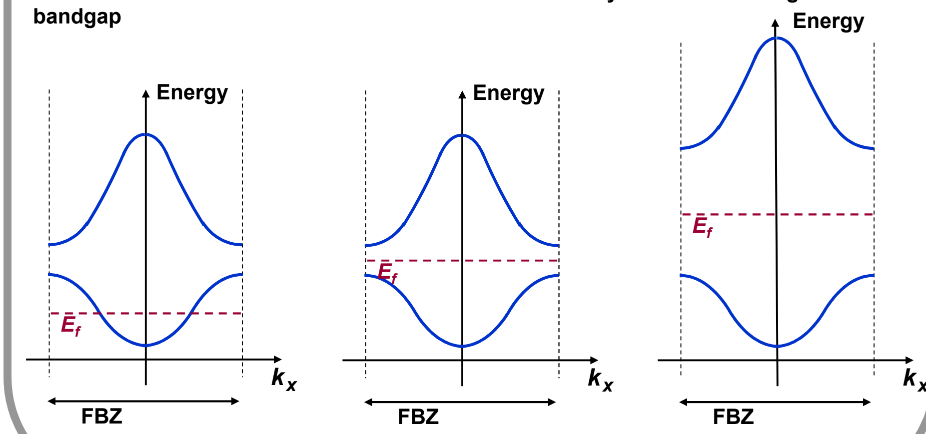
Metals, Semiconductors, and Insulators

Materials can be classified into three main categories w.r.t. their electrical properties:

Metals: In metals, the highest filled band is partially filled (usually half-filled)

Semiconductors: In semiconductors, the highest filled band is completely filled (at least at zero temperature)

Insulators: Insulators are like semiconductors but usually have a much larger bandgap



Metal | **Semiconductor** | **Insulator**

Inclusion of Scattering in the Dynamical Equation

In the presence of a uniform electric field the crystal momentum satisfies the dynamical equation:

$$\frac{d\,\hbar\vec{k}(t)}{dt} = -e\,\vec{E}$$

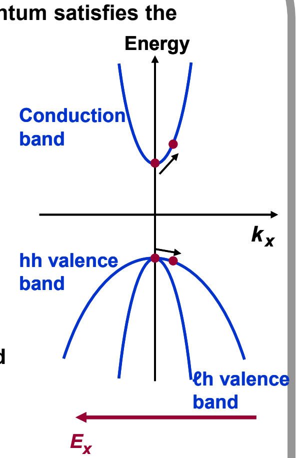
Now we need to add the effect of electron scattering. As in the free-electron case, we assume that scattering adds damping:

$$\frac{d\,\hbar\vec{k}(t)}{dt} = -e\,\vec{E} - \frac{\hbar\left[\vec{k}(t)-\vec{k}\right]}{\tau}$$

The boundary condition is that: $\vec{k}(t=0)=\vec{k}$

Note: the damping term ensures that when the field is turned off, the crystal momentum of the electron goes back to its original value

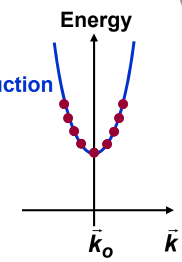
Steady State Solution: $\vec{k}(t=\infty)=\vec{k}-\frac{e\,\tau}{\hbar}\vec{E}$



In the presence of an electric field, the crystal momentum of every electron is shifted by an equal amount that is determined by the scattering time and the field strength

Electrical Conductivity: Conduction Band

Consider a solid in which the energy dispersion for conduction band near a band minimum is given by:



$$E_c(\vec{k}) = E_c(\vec{k}_o) + \frac{\hbar^2}{2}(\vec{k}-\vec{k}_o)^T \,.\, M^{-1} \,.\, (\vec{k}-\vec{k}_o)$$

The velocity of electrons is:

$$\vec{v}_c(\vec{k}) = M^{-1} \,.\, \hbar\,(\vec{k}-\vec{k}_o)$$

The current density is:

$$\vec{J}_c = -2\,e \times \int_{\text{near } \vec{k}_o} \frac{d^3\vec{k}}{(2\pi)^3}\, f_c(\vec{k})\,\vec{v}_c(\vec{k})$$

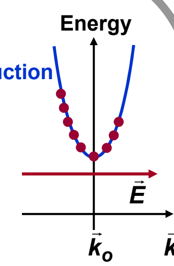
In equilibrium, for every state with crystal momentum $(\vec{k}-\vec{k}_o)$ that is occupied, the state $-(\vec{k}-\vec{k}_o)$ is also occupied and these two states have opposite velocities.

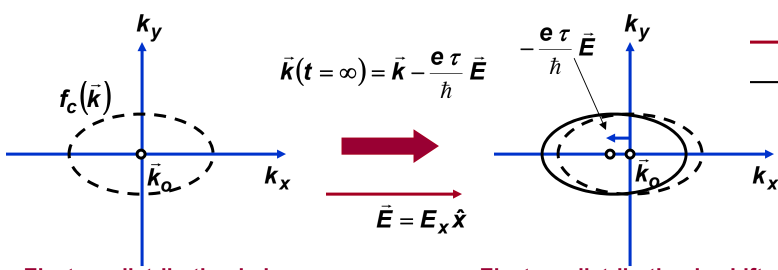
Therefore in equilibrium:

$$\vec{J}_c = -2\,e \times \int_{\text{near } \vec{k}_o} \frac{d^3\vec{k}}{(2\pi)^3}\, f_c(\vec{k})\,\vec{v}_c(\vec{k}) = 0$$

Electrical Conductivity: Conduction Band

Now assume that an electric field is present that shifts the crystal momentum of all electrons:





Electron distribution in k-space when E-field is zero

Distribution function: $f_c(\vec{k})$

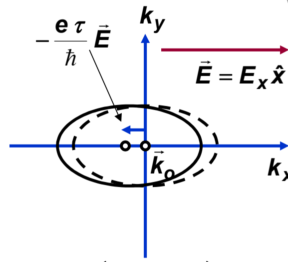
Electron distribution is shifted in k-space when E-field is not zero

Distribution function: $f_c\left(\vec{k} + \frac{e\,\tau}{\hbar}\vec{E}\right)$

Since the wavevector of each electron is shifted by the same amount in the presence of the E-field, the net effect in k-space is that the entire electron distribution is shifted as shown

Electrical Conductivity: Conduction Band

Current Density:



$f_c\left(\vec{k} + \frac{e\,\tau}{\hbar}\vec{E}\right)$

$$\vec{J}_c = -2\,e \times \int_{\text{near } \vec{k}_o} \frac{d^3\vec{k}}{(2\pi)^3}\, f_c\left(\vec{k} + \frac{e\tau}{\hbar}\vec{E}\right) \vec{v}_c\left(\vec{k}\right)$$

Do a shift in the integration variable:

$$\vec{J}_c = -2\,e \times \int_{\text{near } \vec{k}_o} \frac{d^3\vec{k}}{(2\pi)^3}\, f_c\left(\vec{k}\right) \vec{v}_c\left(\vec{k} - \frac{e\,\tau}{\hbar}\vec{E}\right)$$

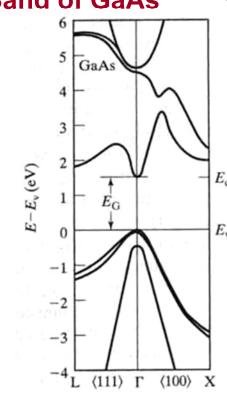
$$\vec{J}_c = -2\,e \times \int_{\text{near } \vec{k}_o} \frac{d^3\vec{k}}{(2\pi)^3}\, f_c\left(\vec{k}\right) M^{-1} . \hbar\left(\vec{k} - \vec{k}_o - \frac{e\,\tau}{\hbar}\vec{E}\right)$$

$$\vec{J}_c = e^2\tau \left[2 \times \int_{\text{near } \vec{k}_o} \frac{d^3\vec{k}}{(2\pi)^3}\, f_c\left(\vec{k}\right)\right] M^{-1} . \vec{E}$$

$$\vec{J}_c = n\,e^2\tau\, M^{-1} . \vec{E}$$
$$= \bar{\bar{\sigma}} . \vec{E}$$

Where the conductivity is now a tensor given by: $\bar{\bar{\sigma}} = n\,e^2\tau\, M^{-1}$

Electrical Conductivity Example: Conduction Band of GaAs



Consider the conduction band of GaAs near the Γ-point:

$$M^{-1} = \begin{bmatrix} 1/m_e & 0 & 0 \\ 0 & 1/m_e & 0 \\ 0 & 0 & 1/m_e \end{bmatrix}$$

Isotropic!

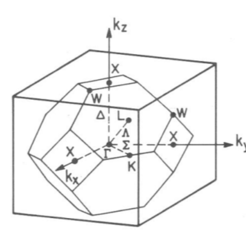
This implies:

$$\vec{J}_c = n\,e^2\tau\, M^{-1} . \vec{E}$$

$$\begin{bmatrix} J_{x,c} \\ J_{y,c} \\ J_{z,c} \end{bmatrix} = n\,e^2\tau \begin{bmatrix} 1/m_e & 0 & 0 \\ 0 & 1/m_e & 0 \\ 0 & 0 & 1/m_e \end{bmatrix} \begin{bmatrix} E_x \\ E_y \\ E_z \end{bmatrix}$$

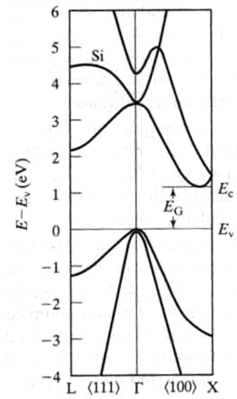
$$= \frac{n\,e^2\tau}{m_e} \begin{bmatrix} E_x \\ E_y \\ E_z \end{bmatrix} = \sigma\,\vec{E}$$

$$\Rightarrow \sigma = \frac{n\,e^2\tau}{m_e}$$



Electrical Conductivity Example: Conduction Band of Silicon

In Silicon there are six conduction band minima (valleys) that occur along the six Γ-X directions. For the one that occurs along the Γ-X(2π/a,0,0) direction:



$$\vec{k}_o = 0.85\left(\frac{2\pi}{a},0,0\right)$$

$$M^{-1} = \begin{bmatrix} 1/m_\ell & 0 & 0 \\ 0 & 1/m_t & 0 \\ 0 & 0 & 1/m_t \end{bmatrix}$$

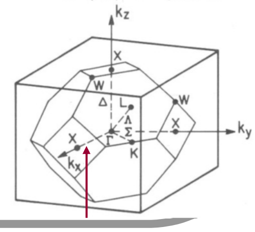
Not isotropic!

$m_\ell = 0.92\, m$
$m_t = 0.19\, m$

This implies that for this valley:

$$\vec{J}_c = \frac{n}{6} e^2 \tau\, M^{-1} . \vec{E}$$

$$\begin{bmatrix} J_{x,c} \\ J_{y,c} \\ J_{z,c} \end{bmatrix} = \frac{n}{6} e^2 \tau \begin{bmatrix} 1/m_\ell & 0 & 0 \\ 0 & 1/m_t & 0 \\ 0 & 0 & 1/m_t \end{bmatrix} \begin{bmatrix} E_x \\ E_y \\ E_z \end{bmatrix}$$



The factor of 6 is there because only 1/6th of the total conduction electron density in Silicon is in one valley

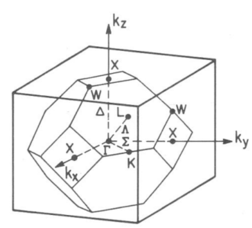
Electrical Conductivity Example: Conduction Band of Silicon

To find the conductivity tensor for Silicon one needs to sum over the current density contributions from all six valleys:

$$\begin{bmatrix} J_{x,c} \\ J_{y,c} \\ J_{z,c} \end{bmatrix} = \frac{n}{6} e^2 \tau \begin{bmatrix} 2/m_\ell + 4/m_t & 0 & 0 \\ 0 & 2/m_\ell + 4/m_t & 0 \\ 0 & 0 & 2/m_\ell + 4/m_t \end{bmatrix} \begin{bmatrix} E_x \\ E_y \\ E_z \end{bmatrix}$$

Isotropic!

$$= \frac{n\, e^2 \tau}{m_e} \begin{bmatrix} E_x \\ E_y \\ E_z \end{bmatrix} = \sigma\, \vec{E}$$

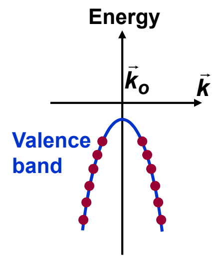


$$\frac{1}{m_e} = \frac{1}{3}\left(\frac{1}{m_\ell} + \frac{2}{m_t}\right) =$$ Conductivity effective mass

After adding the current density contributions from all six valleys, the resulting conductivity tensor in Silicon is isotropic and described by a conductivity effective mass

Electrical Conductivity: Valence Band

Consider a solid in which the energy dispersion for valence band near a band maximum is given by:



$$E_v(\vec{k}) = E_v(\vec{k}_o) + \frac{\hbar^2}{2}(\vec{k}-\vec{k}_o)^T \, . \, M^{-1} \, . \, (\vec{k}-\vec{k}_o)$$

The velocity of electrons is:

$$\vec{v}_v(\vec{k}) = M^{-1} \, . \, \hbar \, (\vec{k}-\vec{k}_o)$$

The current density is (using the electron-hole transformation):

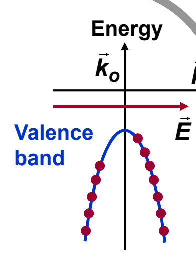
$$\vec{J}_v = -2\,e \times \int_{\text{near } \vec{k}_o} \frac{d^3\vec{k}}{(2\pi)^3} f_v(\vec{k})\,\vec{v}_v(\vec{k}) = 2\,e \times \int_{\text{near } \vec{k}_o} \frac{d^3\vec{k}}{(2\pi)^3} \left[1 - f_v(\vec{k})\right] \vec{v}_v(\vec{k})$$

In equilibrium, for every state with crystal momentum $(\vec{k}-\vec{k}_o)$ that is unoccupied, the state $-(\vec{k}-\vec{k}_o)$ is also unoccupied and these two states have opposite velocities.

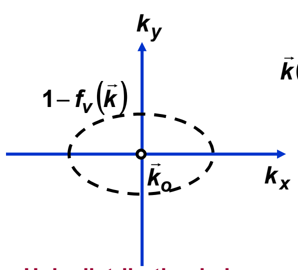
Therefore in equilibrium:

$$\vec{J}_v = 2\,e \times \int_{\text{near } \vec{k}_o} \frac{d^3\vec{k}}{(2\pi)^3} \left[1 - f_v(\vec{k})\right] \vec{v}_v(\vec{k}) = 0$$

Electrical Conductivity: Valence Band

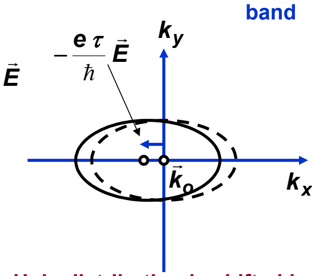


Now assume that an electric field is present that shifts the crystal momentum of all electrons in the valence band:



$$\vec{k}(t=\infty) = \vec{k} - \frac{e\,\tau}{\hbar}\vec{E}$$

$$\vec{E} = E_x \hat{x}$$



Hole distribution in k-space when E-field is zero

Distribution function: $1 - f_v(\vec{k})$

Hole distribution is shifted in k-space when E-field is not zero

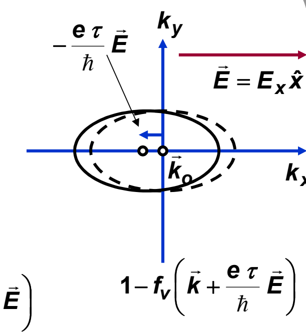
Distribution function: $1 - f_v\left(\vec{k} + \frac{e\,\tau}{\hbar}\vec{E}\right)$

Since the wavevector of each electron is shifted by the same amount in the presence of the E-field, the net effect in k-space is that the entire electron distribution (and hole distribution) is shifted as shown

Electrical Conductivity: Valence Band

Current Density:

$$\vec{J}_v = 2\,e \times \int_{\text{near } \vec{k}_o} \frac{d^3\vec{k}}{(2\pi)^3} \left[1 - f_v\left(\vec{k} + \frac{e\tau}{\hbar}\vec{E}\right)\right] \vec{v}_v\left(\vec{k}\right)$$



Do a shift in the integration variable:

$$\vec{J}_v = 2\,e \times \int_{\text{near } \vec{k}_o} \frac{d^3\vec{k}}{(2\pi)^3} \left[1 - f_v\left(\vec{k}\right)\right] \vec{v}_v\left(\vec{k} - \frac{e\,\tau}{\hbar}\vec{E}\right)$$

$$\vec{J}_v = 2\,e \times \int_{\text{near } \vec{k}_o} \frac{d^3\vec{k}}{(2\pi)^3} \left[1 - f_v\left(\vec{k}\right)\right] M^{-1}\,.\,\hbar\left(\vec{k} - \vec{k}_o - \frac{e\,\tau}{\hbar}\vec{E}\right)$$

$$\vec{J}_v = -e^2\tau\left[2 \times \int_{\text{near } \vec{k}_o} \frac{d^3\vec{k}}{(2\pi)^3} \left[1 - f_v\left(\vec{k}\right)\right]\right] M^{-1}\,.\,\vec{E}$$

$$\vec{J}_v = -p\,e^2\tau\,M^{-1}\,.\,\vec{E}$$

$$= \overline{\overline{\sigma}}\,.\,\vec{E}$$

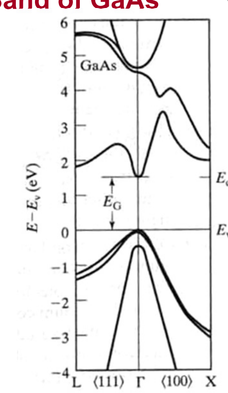
Where the conductivity is now a tensor given by: $\overline{\overline{\sigma}} = -p\,e^2\tau\,M^{-1}$

Electrical Conductivity Example: Heavy-Hole Band of GaAs

Consider the heavy-hole band of GaAs near the Γ-point:

$$M^{-1} = \begin{bmatrix} -1/m_{hh} & 0 & 0 \\ 0 & -1/m_{hh} & 0 \\ 0 & 0 & -1/m_{hh} \end{bmatrix}$$

Isotropic!



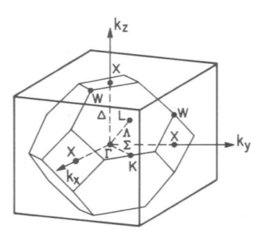
This implies:

$$\vec{J}_{hh} = -p_{hh}\,e^2\tau\,M^{-1}\,.\,\vec{E}$$

$$\begin{bmatrix} J_{x,hh} \\ J_{y,hh} \\ J_{z,hh} \end{bmatrix} = -p_{hh}\,e^2\tau \begin{bmatrix} -1/m_{hh} & 0 & 0 \\ 0 & -1/m_{hh} & 0 \\ 0 & 0 & -1/m_{hh} \end{bmatrix} \begin{bmatrix} E_x \\ E_y \\ E_z \end{bmatrix}$$

$$= \frac{p_{hh}\,e^2\tau}{m_{hh}} \begin{bmatrix} E_x \\ E_y \\ E_z \end{bmatrix} = \sigma\,\vec{E}$$

$$\Rightarrow \sigma = \frac{p_{hh}\,e^2\tau}{m_{hh}}$$

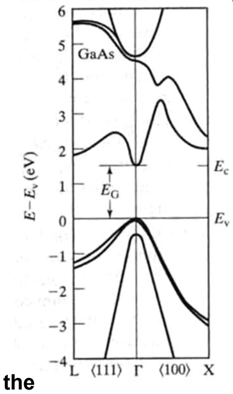


Electrical Conductivity Example: Light-Hole Band of GaAs

Consider the light-hole band of GaAs near the Γ-point:

$$M^{-1} = \begin{bmatrix} -1/m_{\ell h} & 0 & 0 \\ 0 & -1/m_{\ell h} & 0 \\ 0 & 0 & -1/m_{\ell h} \end{bmatrix}$$

Isotropic!



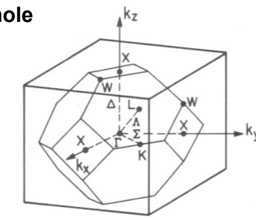
This implies:

$$\vec{J}_{\ell h} = -p_{\ell h}\, e^2 \tau\, M^{-1} . \vec{E} = \sigma\, \vec{E}$$

$$\Rightarrow \sigma = \frac{p_{\ell h}\, e^2 \tau}{m_{\ell h}}$$

The total valence band conductivity of GaAs can be written as the sum of the contributions from the heavy-hole and the light-hole bands:

$$\sigma = \frac{p_{hh}\, e^2 \tau}{m_{hh}} + \frac{p_{\ell h}\, e^2 \tau}{m_{\ell h}}$$



The Phenomenology Of Transport

The presence of external fields, and scattering, the following relations work for electrons in any energy band near the band edge (assuming parabolic bands):

$$\frac{d\;\hbar \vec{k}(t)}{dt} = -e\,\vec{E} - \frac{\hbar\left[\vec{k}(t) - \vec{k}\right]}{\tau}$$

$$\vec{v}_n\left(\vec{k}(t)\right) = M^{-1} . \hbar\left(\vec{k}(t) - \vec{k}_o\right)$$

$$\vec{J}_n(t) = -2\,e \times \int_{FBZ} \frac{d^3\vec{k}}{(2\pi)^3}\, f_n\left(\vec{k}\right) \vec{v}_n\left(\vec{k}(t)\right) = +2\,e \times \int_{FBZ} \frac{d^3\vec{k}}{(2\pi)^3} \left[1 - f_n\left(\vec{k}\right)\right] \vec{v}_n\left(\vec{k}(t)\right)$$

The first two can also be written as:

$$M . \frac{d\left[\vec{v}_n\left(\vec{k}(t)\right) - \vec{v}_n\left(\vec{k}\right)\right]}{dt} = -e\,\vec{E} - \frac{M . \left[\vec{v}_n\left(\vec{k}(t)\right) - \vec{v}_n\left(\vec{k}\right)\right]}{\tau}$$

Problem: One needs simple models for current transport so that non-specialists, like circuit designers, can understand devices and circuits without having to understand energy bands

Drift Velocity and Mobility for Electrons

We define the drift velocity for the electrons in the conduction band (for parabolic bands) as:

$$\vec{v}_e(t) = \vec{v}_c\left(\vec{k}(t)\right) - \vec{v}_c\left(\vec{k}\right)$$

The drift velocity is independent of wavevector for parabolic bands and satisfies:

$$M \cdot \frac{d\,\vec{v}_e(t)}{dt} = -e\,\vec{E} - \frac{M \cdot \vec{v}_e(t)}{\tau} \qquad \longrightarrow (1)$$

In steady state:

$$\vec{v}_e(t\to\infty) = \vec{v}_c\left(\vec{k}(t\to\infty)\right) - \vec{v}_c\left(\vec{k}\right) = -e\tau\, M^{-1} \cdot \vec{E} = -\overline{\overline{\mu}}_e \cdot \vec{E} \qquad \overline{\overline{\mu}}_e = \text{mobility tensor}$$

Once the drift velocity is calculated, the electron current density is:

$$\vec{J}_e(t) = -2\,e \times \int_{FBZ} \frac{d^3\vec{k}}{(2\pi)^3} f_c\left(\vec{k}\right) \vec{v}_c\left(\vec{k}(t)\right) = -2\,e \times \int_{FBZ} \frac{d^3\vec{k}}{(2\pi)^3} f_c\left(\vec{k}\right)\left[\vec{v}_c\left(\vec{k}(t)\right) - \vec{v}_c\left(\vec{k}\right) + \underbrace{\cancel{\vec{v}_c\left(\vec{k}\right)}}_{0}\right]$$

$$= -2\,e \times \int_{FBZ} \frac{d^3\vec{k}}{(2\pi)^3} f_c\left(\vec{k}\right)\left[v_e(t)\right] = n\,(-e)\,v_e(t) \qquad \longrightarrow (2)$$

Electrons in the conduction band are to be thought of as negatively charged particles. In case of multiple electron pockets, current density contributions are calculated separately for each and added in the end.

Drift Velocity and Mobility for Holes

We define the drift velocity for the "holes" in the valence band (assuming parabolic bands) as:

$$\vec{v}_h(t) = \vec{v}_v\left(\vec{k}(t)\right) - \vec{v}_v\left(\vec{k}\right)$$

The drift velocity is independent of wavevector and satisfies the equation:

$$(-M) \cdot \frac{d\;\vec{v}_h(t)}{dt} = +e\,\vec{E} - \frac{(-M) \cdot \vec{v}_h(t)}{\tau} \qquad \longrightarrow (1)$$

Where realizing that the inverse effective mass tensor will have negative diagonal terms for valence band, I have multiplied throughout by a negative sign, with the result that the charge "-e" becomes "+e"

In steady state: $\vec{v}_h(t\to\infty) = -e\tau\, M^{-1} \cdot \vec{E} = \overline{\overline{\mu}}_h \cdot \vec{E}$ $\quad \overline{\overline{\mu}}_h$ = mobility tensor

Once the drift velocity is calculated, the hole current density is:

$$\vec{J}_h(t) = +2\,e \times \int_{FBZ} \frac{d^3\vec{k}}{(2\pi)^3} \left[1 - f_v\left(\vec{k}\right)\right] \vec{v}_v\left(\vec{k}(t)\right) = p\,(+e)\,v_h(t) \qquad \longrightarrow (2)$$

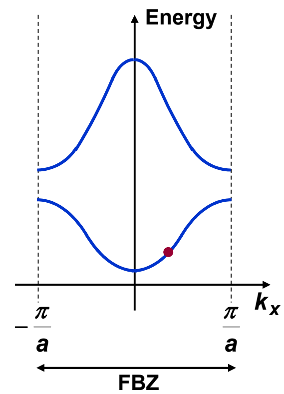
Holes in the valence band are to be thought of as positively charged particles. In case of degenerate valence band maxima, the heavy and light hole current density contributions are calculated separately and added in the end.

The Case of No Scattering: Bloch Oscillations

Consider an electron in a 1D crystal subjected to a uniform electric field. The energy band dispersion and velocity are:

$$E_n(k_x) = E_s - 2\,V_{ss\sigma}\cos(k_x a)$$

$$v_n(k_x) = \frac{1}{\hbar}\frac{dE_n(k_x)}{dk_x} = 2a\,V_{ss\sigma}\sin(k_x a)$$



In the absence of scattering, the crystal momentum satisfies the dynamical equation:

$$\frac{d\,\hbar k_x(t)}{dt} = eE_o$$

$$\Rightarrow k_x(t) = \frac{eE_o}{\hbar}t + k_x(t=0)$$

The time-dependent velocity of the electron is:

$$v_n(t) = 2a\,V_{ss\sigma}\sin(k_x(t)a)$$

$$= 2a\,V_{ss\sigma}\sin\left(\frac{e\,a\,E_o}{\hbar}t + k_x(t=0)a\right)$$

$\vec{E} = -E_o\hat{x}$

Periodic!

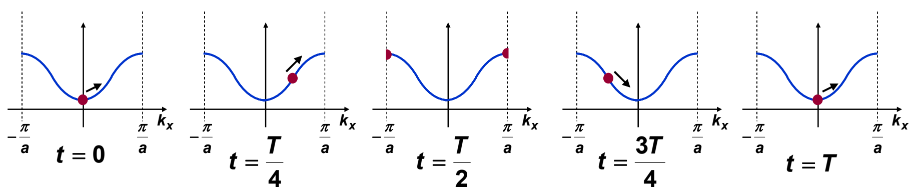
The Case of No Scattering: Bloch Oscillations

A periodic velocity means that the electron motion in real space is also periodic:

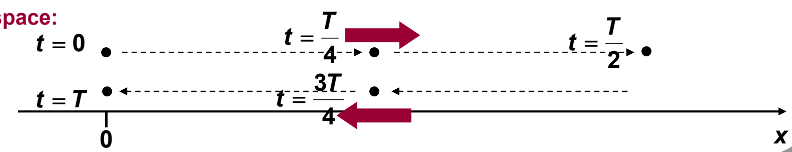
$$\frac{dx(t)}{dt} = v_n(t) = 2a\,V_{ss\sigma}\sin\left(\frac{e\,a\,E_o}{\hbar}t + k_x(t=0)a\right)$$

$$\Rightarrow \int_o^T \frac{dx(t)}{dt}dt = x(t=T) - x(t=0) = 0 \quad \text{where the period } T \text{ is:} \quad T = \frac{2\pi\,\hbar}{e\,a\,E_o}$$

Reciprocal space:



Real space:



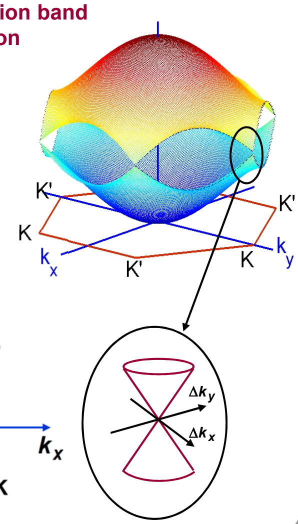
Conductivity of Electrons in Graphene

$$\vec{k}_o = \mathbf{K}$$

$$E_c(\vec{k}) \approx E_p + \hbar v \sqrt{(k_x - k_{ox})^2 + (k_y - k_{oy})^2} \quad \Big\} \text{ Conduction band dispersion}$$

$$\vec{v}_c(\vec{k}) = \frac{1}{\hbar}\nabla_{\vec{k}} E_c(\vec{k}) = v\,\frac{(k_x - k_{ox})\hat{x} + (k_y - k_{oy})\hat{y}}{\sqrt{(k_x - k_{ox})^2 + (k_y - k_{oy})^2}}$$

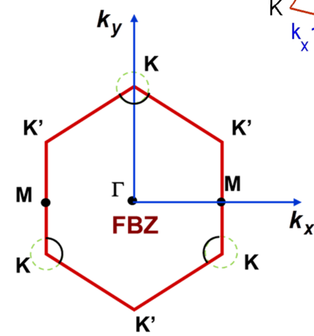
$$= v\,\frac{\vec{k} - \vec{k}_o}{\left|\vec{k} - \vec{k}_o\right|} = v\,\frac{\Delta\vec{k}}{\left|\Delta\vec{k}\right|}$$



The dynamical equation for the crystal momentum still works:

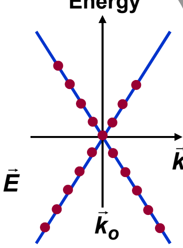
$$\frac{d\ \hbar\vec{k}(t)}{dt} = -e\,\vec{E} - \frac{\hbar\left[\vec{k}(t) - \vec{k}\right]}{\tau}$$

$$\Rightarrow \vec{k}(t=\infty) = \vec{k} - \frac{e\,\tau}{\hbar}\vec{E}$$

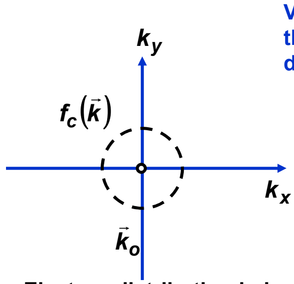


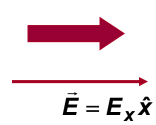
Conductivity of Electrons in Graphene

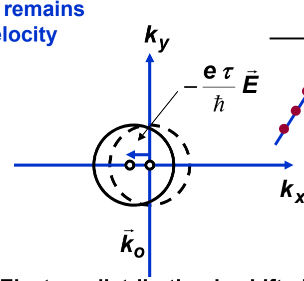
$$\vec{k}(t=\infty) = \vec{k} - \frac{e\,\tau}{\hbar}\vec{E} \quad \Rightarrow \quad \vec{v}_c\left(\vec{k}(t)\right) = v\,\frac{\vec{k} - e\tau\vec{E}/\hbar - \vec{k}_o}{\left|\vec{k} - e\tau\vec{E}/\hbar - \vec{k}_o\right|}$$



Velocity magnitude remains the same but the velocity direction changes







Electron distribution in k-space when E-field is zero

Distribution function: $f_c(\vec{k})$

Electron distribution is shifted in k-space when E-field is not zero

Distribution function: $f_c\left(\vec{k} + \frac{e\,\tau}{\hbar}\vec{E}\right)$

Current density can be obtained by the familiar expression:

$$\vec{J} = -e \times \underbrace{2}_{\text{2 pockets or valleys}} \times \underbrace{2}_{\text{2 spins}} \times \int_{\text{near } \vec{k}_o} \frac{d^2\vec{k}}{(2\pi)^2}\, f\left(\vec{k} + \frac{e\tau\,\vec{E}}{\hbar}\right)\vec{v}(\vec{k})$$