Transport of Band Electrons

- Introduce nonequilibrium distribution function for each band $g_n(\vec{r}, \vec{k}, t)$.

g_n ↑ band index; $\vec{k}$ ← crystal momentum ($\vec{k} \in$ Brillouin Zone)

- Assuming no interband transitions, either due to applied fields, or due to scattering, write Boltzmann equation for <u>each</u> band:

$$\frac{\partial g_n}{\partial t} + \dot{\vec{r}} \cdot \frac{\partial g_n}{\partial \vec{r}} + \dot{\vec{k}} \cdot \frac{\partial g_n}{\partial \vec{k}} = \left(\frac{\partial g_n}{\partial t} \right)_{coll}$$

<u>Here</u>: $$\dot{\vec{r}} = \vec{V}_n(\vec{k}) = \frac{1}{\hbar} \frac{\partial \varepsilon_n(\vec{k})}{\partial \vec{k}}$$

$$\dot{\vec{k}} = \frac{-e}{\hbar} \left[\vec{E} + \frac{1}{c} \vec{V}_n(\vec{k}) \times \vec{B} \right]$$

<u>NB</u>: In general we <u>should</u> allow interband scattering, since this is needed to relax a general configuration to equilibrium. But, not important for 1-band examples.

Have currents:

$$\vec{J} = \sum_n \vec{J}_n \; ; \quad \vec{J}_n = -e \int_{\vec{k}\in B.Z.} \frac{d^3\vec{k}}{4\pi^3} \vec{V}_n(\vec{k})\, g_n(\vec{r},\vec{k},t)$$

$$\vec{J}_\varepsilon = \sum_n \vec{J}_{\varepsilon,n} \; ; \quad \vec{J}_{\varepsilon,n} = \int \frac{d^3\vec{k}}{4\pi^3} \varepsilon_n(\vec{k}) \vec{V}_n(\vec{k})\, g_n(\vec{r},\vec{k},t)$$

↑ energy current. ⟶ (Recall, $\vec{J}_Q = \vec{J}_\varepsilon + \frac{\mu}{e}\vec{J}$
$= \vec{J}_\varepsilon - \mu \vec{J}_N$ ← number current.)

Goals: (1) Understand insulating behavior
(2) Notion of electrons & holes
(3) Transport in $\vec{B}$-field: explain $R_H > 0$.

Insulators

Claim: System where every band is completely full (or completely empty), and bands are separated by an energy gap Δ, has $\sigma = 0$ at $T = 0$.

- In such a system, at $T=0$, $g_n = \begin{cases} 1, & \text{full bands} \\ 0, & \text{empty bands.} \end{cases}$

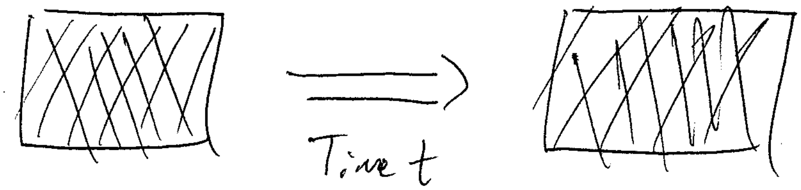
$$\Rightarrow \vec{J} = -e \sum_{n \text{ occupied}} \underbrace{\int \frac{d^3\vec{k}}{4\pi^3} \frac{\partial \mathcal{E}_n}{\partial \vec{k}}}_{\text{integrate gradient of periodic function } (\mathcal{E}_n(k)) \to 0.} = 0 \to \underline{\text{No current.}}$$

(Similarly, $\vec{J}_\varepsilon = 0$, since $\mathcal{E}_n(\vec{k}) V_n(\vec{k}) = \frac{1}{2} \frac{\partial}{\partial \vec{k}} [\mathcal{E}_n(\vec{k})]^2$.)

- Even for applied E-field, $g_n = \begin{cases} 1, & \text{full} \\ 0, & \text{empty} \end{cases}$

still solves Boltzmann equation (since $\frac{\partial g_n^{(0)}}{\partial \vec{k}} = 0$).

- More physically:



Electrons follow semiclassical trajectories $\dot{\vec{k}} = -\frac{e}{\hbar}\vec{E}$ in $\vec{k}$-space. But a full band is still full after time t.

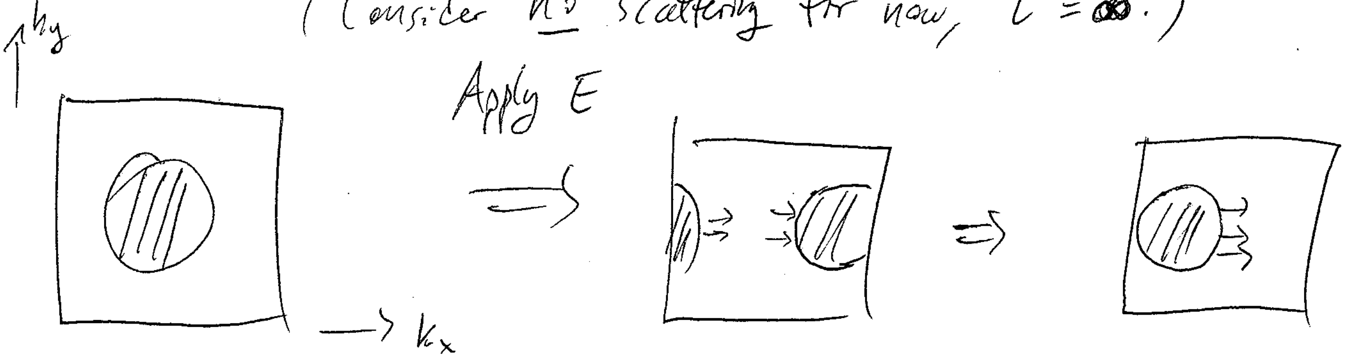
- Why does $\Delta \neq 0$ matter? If $\Delta = 0$ between empty & full band, can't neglect interband transitions. ~~(e.g. graphene)~~. Also have much more thermal excitation at low-T, etc.

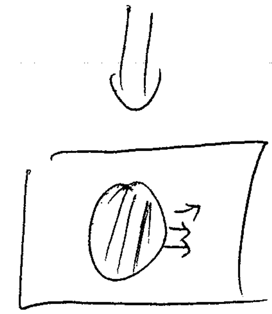
e.g. graphene

Metals:

- Consider a metal with a Fermi surface in just 1 band:

  (Consider no scattering for now, $\tau = \infty$.)





- Returns to initial position in $\vec{k}$-space!

$\Rightarrow$ $\vec{J}(t)$ is oscillatory, not $\vec{J} \propto t$, as for free electrons.

$\rightarrow$ "Bloch oscillations" $\rightarrow$ Unobservable in metals, since τ is too short.

Conductivity of a metal (just 1 band):

- Solve B.E. as before, get:

$$\vec{J} = e^2\tau \int \frac{d^3k}{4\pi^3}\left[-\frac{\partial f}{\partial \varepsilon}(\varepsilon(\vec{k}))\right] \vec{v}(\vec{k})\left(\vec{v}(\vec{k})\cdot\vec{E}\right)$$

$$\Rightarrow \sigma^{ij} = e^2\tau \int \frac{d^3k}{4\pi^3}\left[-f'(\varepsilon(\vec{k}))\right] v^i(\vec{k})\, v^j(\vec{k})$$

$\underline{T=0}$: $$\sigma^{ij} = e^2\tau \int \frac{d^3k}{4\pi^3}\, \delta(\varepsilon_F - \varepsilon(\vec{k}))\, v^i(\vec{k})\, v^j(\vec{k})$$

$$= e^2\tau\, D(\varepsilon_F)\, \frac{\int \frac{d^3k}{4\pi^3}\, \delta(\varepsilon_F - \varepsilon(\vec{k}))\, v^i(\vec{k})\, v^j(\vec{k})}{\underbrace{\int \frac{d^3k}{4\pi^3}\, \delta(\varepsilon_F - \varepsilon(\vec{k}))}_{= D(\varepsilon_F)}}$$

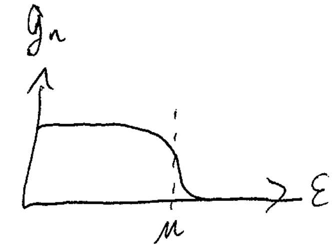
$$= e^2\tau\, D(\varepsilon_F) \left\langle v^i(\vec{k})\, v^j(\vec{k}) \right\rangle_{\text{F.S. average}}$$

- For a cubic crystal, $\sigma^{ij} = \sigma\,\delta_{ij}$

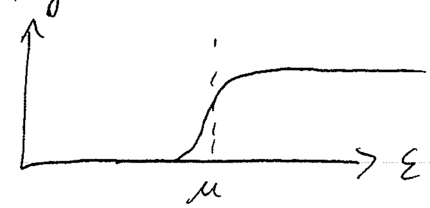
- <u>In general</u>, $\sigma \neq \frac{ne^2\tau}{m}$ density of electrons filling Fermi sea

Electrons & Holes

- Consider a single band n:



$$\vec{J}_n = -e \int \frac{d^3\vec{k}}{4\pi^3} \vec{V}_n(\vec{k})\, g_n$$

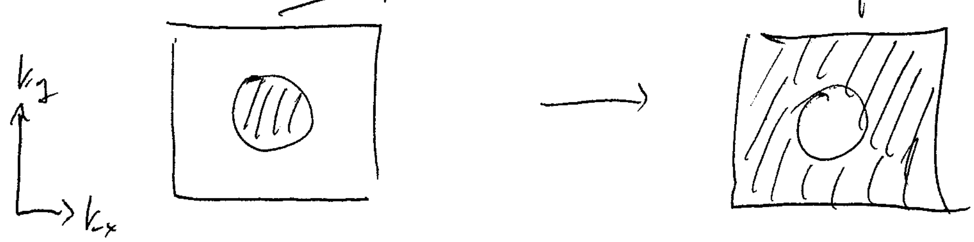


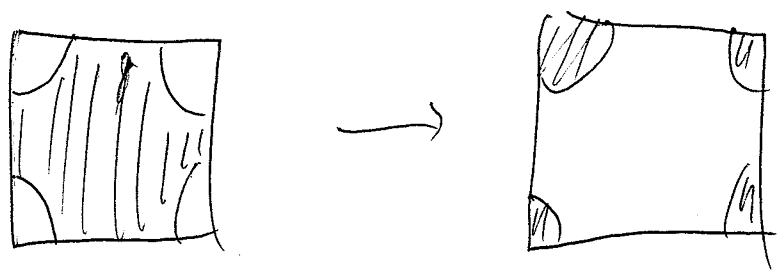
$$= +e \int \frac{d^3k}{4\pi^3} \vec{V}_n(\vec{k}) \left[1-g_n\right]$$

- $(1-g_n)$ is a distribution function for "holes," which are <u>empty</u> states (i.e. absence of an electron)

- Looks like holes can be viewed as positively charged particles... is it true??

electron picture — hole picture





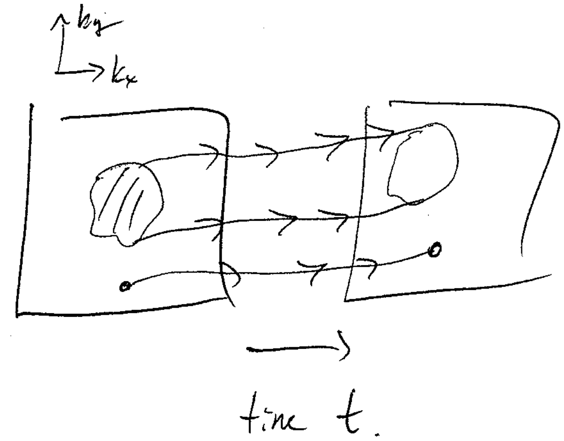
Hole picture most useful in cases like this (almost filled band)

<u>Observation</u>: Suppose state $\vec{k}$ is occupied/empty at time $t=0$.

Then state $\vec{k}(t)$ is occupied/empty at time t.

↓

obtained by solving semiclassical equations



$\Rightarrow$ Holes follow the <u>same</u> semiclassical trajectories the electrons do, so always $\dot{\vec{k}} = -\frac{e}{\hbar}\left[\vec{E} + \frac{\vec{v}}{c}\times\vec{B}\right]$

(Doesn't mean holes behave like neg. charges though.)

Need to calculate <u>acceleration</u>:

$$\vec{a} = \frac{d\vec{v}}{dt} = \frac{d}{dt}\frac{1}{\hbar}\frac{\partial \varepsilon_n(\vec{k})}{\partial \vec{k}}$$

• Suppose we're near a band maximum/minimum at $\vec{k}=\vec{k}_0$,

then:
$$\underbrace{\varepsilon_n(\vec{k}) = \varepsilon_n(\vec{k}_0) \pm \frac{\hbar^2}{2m_*}(\vec{k}-\vec{k}_0)^2 + \cdots}_{\text{(Simplest case only)}}$$

m_* → "<u>effective mass</u>"

Then: $\vec{v} = \pm \frac{\hbar}{m^*}(\vec{k} - \vec{k}_0)$, and

$$\vec{a} = \pm \frac{\hbar}{m_*} \dot{\vec{k}}$$

→ Near minimum, $\vec{a}$ parallel to $\dot{\vec{k}}$

→ " maximum, " anti-parallel " " .

Near minimum: $m_* \vec{a} = -e\left[\vec{E} + \frac{1}{c}\vec{v}\times\vec{B}\right]$ (like −e charges)

Near maximum: $m_* \vec{a} = +e\left[\vec{E} + \frac{1}{c}\vec{v}\times\vec{B}\right]$ (like +e charges)

⇒

- Near band minimum, band electrons move like regular electrons (both current and $m_* \vec{a}$ have right form)

- Near band maximum, holes move like real charge +e particles.

- Away from maxima/minima, dynamics is more complicated
  → in particular, $\dot{\vec{k}}$ and $\vec{a}$ don't ~~point~~ lie on same axis.

Immediate consequence: Hall Coefficient

- Density n_e of electrons near band minimum:

~~Contribution to R_H → R_H~~

$$R_H = -\frac{1}{n_e e c}$$

- Density of n_h holes near band maximum:

$$R_H = +\frac{1}{n_h e c}$$

⇒ Explains why R_H is (sometimes) positive.

~~Multiple minima, maxima (say k minima, l maxima)~~

$$\cancel{R_H = \underbrace{\sum_{i=1}^{k}\left(-\frac{1}{n_i e c}\right)}_{\text{minima}} + \underbrace{\sum_{i=k+1}^{l+k}\left(+\frac{1}{n_i e c}\right)}_{\text{maxima}}}$$

~~⇒ R_H doesn't have to be simply related to density of carriers.~~

For a more general minimum / maximum:

$$\varepsilon_n(\vec{k}) = \varepsilon_n(\vec{k}_0) \pm \frac{\hbar^2}{2} \sum_{\mu,\nu} (k-k_0)_\mu (M^{-1})_{\mu\nu} (k-k_0)_\nu$$

$$M_{\mu\nu} = \left. \frac{\partial^2 \varepsilon_n(\vec{k})}{\partial k_\mu \partial k_\nu} \right|_{\vec{k}=\vec{k}_0}$$

↳ "effective mass tensor." By definition, symmetric & positive definite.

EOM:

$$\overleftrightarrow{M} \cdot \vec{a} = \mp e \left[\vec{E} + \frac{1}{c} \vec{v} \times \vec{B} \right]$$

- Note that $\overleftrightarrow{M}$ is diagonalized by choosing appropriate orthonormal axes, $(k_x, k_y, k_z) \to (k_1, k_2, k_3)$

$$\Rightarrow \varepsilon_n(\vec{k}) = \varepsilon_n(\vec{k}_0) \pm \sum_{\mu=1,2,3} \frac{\hbar^2 k_\mu^2}{2m_\mu^*}$$

- This description of band minima/maxima (and also holes & electron pictures) will be very important for semiconductors.