

LECTURE 14

SEMICLASSICAL MODEL OF ELECTRON DYNAMICS & CONDUCTION

- The objective: Given the band theory, understand the effect of external electric & magnetic fields on electron motion in crystals.
- the fully quantum theory requires use of Green's functions; we will employ the semiclassical (WKB) model.
- Failures of Drude model
 - Drude model treats electrons as thermally diffusing CLASSICAL particles colliding with ions. It gives

$$\tau = \frac{n e^2}{m} \bar{\tau} \quad (1)$$

with scattering time $\bar{\tau} = \frac{e}{v} \leftarrow$ mean free path
 \leftarrow velocity

- From band theory we know, however, that
 - (i) $v = \frac{1}{\hbar} \left| \frac{\partial \epsilon(\vec{k})}{\partial \vec{k}} \right| \approx v_F$ (not thermal diffusion velocity)
 - (ii) individual ions DO NOT scatter electrons
 (only imperfections in the lattice do)

- WKB approximation describes electrons as wave-packets

$$\psi(\vec{r}, t) = \sum_{\vec{k}'} g(\vec{k}') \exp[i(\vec{k}' \cdot \vec{r} - \frac{\hbar k'^2}{2m} t)] \quad (2)$$

$g(\vec{k}') \approx 0 \text{ for } |\vec{k}' - \vec{k}| > \Delta k$

- Two key questions arise when discussing conduction by Bloch electrons:
 - (a) What is the nature of collisions?
 - (b) How do Bloch electrons move between them?

DESCRIPTION OF THE SEMICLASSICAL MODEL

1. The band index n is a constant of motion (ignore interband transitions.)
2. The time evolution of the position and wave vector are determined by the equations of motion:

$$\dot{\vec{r}} = \vec{v}_n(\vec{e}) = \frac{1}{\hbar} \frac{\partial E_n(\vec{e})}{\partial \vec{e}} \quad (3a)$$

$$\dot{\vec{k}} = -e \left[\vec{E}(\vec{r}, t) + \frac{1}{c} \vec{v}_n(\vec{e}) \times \vec{B}(\vec{r}, t) \right] \quad (3b)$$

3. The wave-vector \vec{k} is defined only to within an additive rec. lattice vector \vec{G} ; the labels (n, \vec{r}, \vec{e}) and $(n, \vec{r}, \vec{e} + \vec{G})$ are equivalent.
4. In thermal equilibrium the contribution to the electron density from the n -th band is given by the usual Fermi distribution

$$f(E_n(\vec{e})) \frac{d^3k}{4\pi^3} = \frac{d^3k / 4\pi^3}{e^{[E_n(\vec{e}) - \mu]/k_B T} + 1} \quad (4)$$

Limits of validity

- (i) To prevent interband transitions, there must be some minimum gap size $\Delta(\vec{e})$ at each \vec{e} :

$$eEA \ll \frac{\Delta(\vec{e})^2}{\epsilon_F} \quad \text{and} \quad \omega_c \ll \frac{\Delta(\vec{e})^2}{\epsilon_F} \quad (5)$$

where $\omega_c = eB/mc$ is the cyclotron freq. In practice the first condition almost never comes close to being violated in metals. The second can be violated at $B \approx \text{few Tesla}$; \rightarrow "magnetic breakdown".

(ii) The frequency of the applied fields must be small enough:

$$\omega \ll \min_{\vec{k}} \Delta(\vec{k}) \quad (6)$$

and the fields must vary slowly:

$$1 \gg a. \quad (7).$$

Consequences of semiclassical Eqs. of motion

- Filled bands are inert:

- The semiclassical Eqs. (3) implies that a filled band remains filled at all times, even in the presence of space- and time-dep. \vec{E} and \vec{B} fields.

- A filled band cannot carry current:

$$\text{electric: } \vec{j} = (-e) \int \frac{d^3 k}{4\pi^3} \frac{1}{t} \frac{\partial \epsilon}{\partial \vec{k}} \quad (8)$$

$$\text{heat: } \vec{j}_E = \int \frac{d^3 k}{4\pi^3} \epsilon(\vec{k}) \frac{1}{t} \frac{\partial \epsilon}{\partial \vec{k}} = \frac{1}{2} \int \frac{d^3 k}{4\pi^3} \frac{1}{t} \frac{\partial^2}{\partial \vec{k}^2} [\epsilon(\vec{k})]^2$$

Both integrals vanish because $\epsilon(\vec{k})$ is a periodic function of \vec{k} : $\epsilon(\vec{k} + \vec{G}) = \epsilon(\vec{k})$.

\Rightarrow Conduction (electrical or heat) is only due to PARTIALLY FILLED bands. Hence the distinction between METALS and INSULATORS.

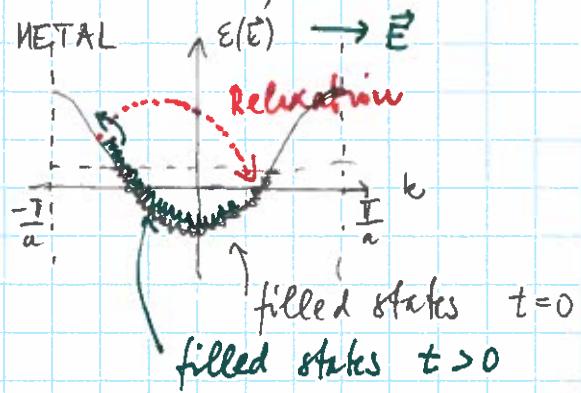
Semiclassical motion in DC electric field

According to Eq. (34) we have

$$\vec{k}(t) = \vec{k}(0) - \frac{e\vec{E}}{\hbar} t \quad (5)$$

Hence, every electron crystal momentum changes linearly in time t .

- for an insulator, filled band remains a filled band, no current is produced
- in a metal, in the ABSENCE OF RELAXATION, one obtains "Bloch oscillations" as occupied electron states traverse the BZ, giving OSCILLATORY CURRENT
- in REAL METALS disorder and scattering off phonons give rise to RELAXATION which brings about a NON-EQUILIBRIUM steady state with constant current $\vec{j} \sim \vec{E}$ described by Ohms law.



- ## Holes
- In some conductors measurements indicate that carriers have POSITIVE CHARGE, e.g. the Hall coefficient $R_H = -1/ne$. How is this possible?

$$\vec{j} = (-e) \int_{\text{occ}} \frac{d^3 k}{4\pi^3} \vec{v}(\epsilon), \quad \epsilon > 0 \quad (10)$$

$$0 = \int_{\text{BZ}} \frac{d^3 k}{4\pi^3} \vec{v}(\epsilon) = \int_{\text{occ}} \frac{d^3 k}{4\pi^3} \vec{v}(\epsilon) + \int_{\text{empty}} \frac{d^3 k}{4\pi^3} \vec{v}(\epsilon) \quad (11)$$

Eq. (II) is a re-statement of "filled bands are inert".

Combining (10) and (II) we may re-write the current

as

$$\vec{j} = (+e) \int_{\text{empty}} \frac{d^3 k}{4\pi^3} \vec{v}(\vec{k}) \quad (12)$$

\Rightarrow the current produced by electrons in the occupied states of a band can be equivalently attributed to fictitious carriers with **POSITIVE CHARGE** (holes) residing in empty states.

- Description in terms of holes is useful when describing empty space near the top of the band \vec{k}_0

$$\epsilon(\vec{k}) \approx \epsilon(\vec{k}_0) - A(\vec{k} - \vec{k}_0)^2, \quad A > 0 \quad (13)$$

Define effective mass

$$\frac{\hbar^2}{2m^*} = A \rightarrow \vec{v}(\vec{k}) = \frac{1}{\hbar} \frac{\partial \epsilon}{\partial \vec{k}} \approx - \frac{\hbar(\vec{k} - \vec{k}_0)}{m^*} \quad (14)$$

Hence the acceleration $\vec{a} = \frac{d}{dt} \vec{v}(\vec{k}) = - \frac{\hbar}{m^*} \dot{\vec{k}}$ is **OPPOSITE** to change in momentum $\dot{\vec{k}}$!

In the equation of motion

$$-m^* \vec{a} = (-e) (\vec{E} + \frac{1}{c} \vec{v} \times \vec{B}) \quad (15)$$

it is then useful to CANCEL the minus sign and think about the motion of a particle with positive charge ($+e$) and positive mass $+m^*$ \rightarrow **HOLE**.

• Effective mass tensor:

$$[\hat{M}^{-1}(\vec{k})]_{ij} = \underbrace{\frac{1}{\hbar} \frac{\partial^2 \epsilon(\vec{k})}{\partial k_i \partial k_j}}_{\substack{\text{electrons} \\ \text{holes}}} \quad (16)$$

$$\rightarrow \vec{a} = \frac{d\vec{r}}{dt} = \pm \hat{M}^{-1}(\vec{k}) \cdot \hbar \dot{\vec{k}}$$

Semiclassical motion in uniform magnetic field

Eqs. of motion ($\vec{E} = 0$, $\vec{B} \neq 0$):

$$\dot{\vec{r}} = \vec{v}(\vec{e}) = \frac{1}{\hbar} \frac{\partial \epsilon(\vec{e})}{\partial \vec{e}} \quad (17)$$

$$i\hbar \dot{\vec{k}} = (-e) \vec{v}(\vec{e}) \times \vec{B}$$

- it is easy to see that \vec{k}_{\parallel} and $\epsilon(\vec{e})$ are constants of motion:

$$(i) \vec{k}_{\parallel}: \quad \vec{k}_{\parallel} = \hat{\vec{B}} (\vec{e} \cdot \hat{\vec{B}}) \quad \text{where} \quad \hat{\vec{B}} = \vec{B}/|\vec{B}| \quad (18)$$

then $\dot{\vec{e}} \cdot \hat{\vec{B}} = -\frac{e}{\hbar c} (\vec{v} \times \vec{B}) \cdot \hat{\vec{B}} = 0 \Rightarrow \underline{\dot{\vec{k}}_{\parallel} = 0} \quad \checkmark$

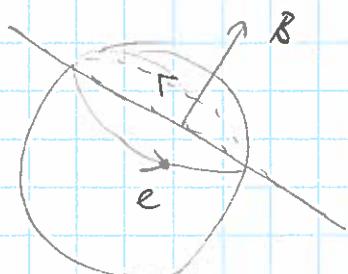
$$(ii) \frac{d\epsilon}{dt} = \frac{\partial \epsilon}{\partial \vec{e}} \cdot \frac{\partial \vec{e}}{\partial t} = \vec{v}(\vec{e}) \cdot \dot{\vec{e}} = -\frac{e}{\hbar c} \vec{v} \cdot (\vec{v} \times \vec{B}) = 0 \quad \checkmark \quad (19)$$

The implication is that electrons move along curves in k -space given by intersection of surfaces of constant energy with planes perpendicular to \vec{B}

Motion in real space:

define $\vec{r}_\perp = \vec{r} - \vec{r}_{\parallel} = \vec{r} - \hat{\vec{B}}(\hat{\vec{B}} \cdot \vec{r})$

↑ projection of \vec{r} onto plane perp. to \vec{B}



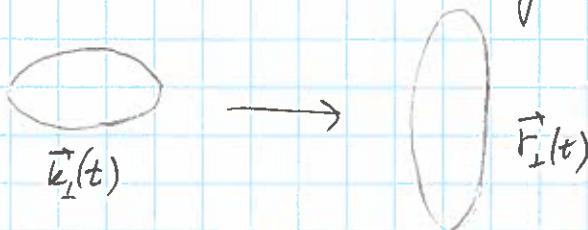
$$\hat{\vec{B}} \times \dot{\vec{r}} = -\frac{e}{\hbar c} \hat{\vec{B}} \times (\vec{v} \times \vec{B}) = -\frac{eB}{\hbar c} \hat{\vec{B}} \times (\vec{v} \times \hat{\vec{B}})$$

$$= -\frac{eB}{\hbar c} [(\hat{\vec{B}} \cdot \hat{\vec{B}}) \vec{r} - (\vec{r} \cdot \hat{\vec{B}}) \hat{\vec{B}}] = -\frac{eH}{\hbar c} \vec{r}_\perp \quad (20)$$

$$\dot{\vec{r}}_\perp = \vec{v}_\perp = -\frac{\hbar c}{eH} (\hat{\vec{B}} \times \dot{\vec{L}}) \quad \text{integrate } \int dt'$$

$$\Rightarrow \vec{r}_I(t) - \vec{r}_I(0) = - \frac{\hbar c}{eB} \hat{B} \times [\vec{k}(t) - \vec{k}(0)] \quad (21)$$

- The real-space orbit is the k -space orbit rotated by 90° and scaled by $-(\hbar c/eB)$:



- Parallel component:

$$\vec{r}_{||}(t) = \vec{r}_{||}(0) + \int_0^t dt' \vec{v}_{||}(t') dt'$$

→ if there is a velocity $\parallel \hat{B}$ then the motion in real space is a spiral along \hat{B} with cross section given by $\vec{r}_I(t)$ above.

- Hall effect

- analysis parallel to that in Drude model gives the Hall coefficient $R_H = j_y/E_x B$

Motion in perp.
 \vec{B} and \vec{E}
fields

as

$$R_H = \begin{cases} -\frac{1}{nec} & \text{electrons} \\ +\frac{1}{nec} & \text{holes} \end{cases}$$

- valid for closed orbits in high fields

- In a situation with many partially filled bands one obtains

$$R_H = -\frac{1}{n_{\text{eff}} e c} \quad \text{with } n_{\text{eff}} = n_c - n_h$$