Electron Dynamics

-- using the semiclassical model
Recall:

- Drude: electrons collide with fixed ions.
- Sommerfeld: treat electrons as in the equilibrium case.
- Bloch: electrons are described by Bloch waves with wave vector $k$ -- provide stationary solutions.

Perfect conductivity in a perfect crystal (the relaxation time is infinite)
## COMPARISON OF SOMMERFELD AND BLOCH ONE-ELECTRON EQUILIBRIUM LEVELS

<table>
<thead>
<tr>
<th>QUANTUM NUMBERS (EXCLUDING SPIN)</th>
<th>SOMMERFELD</th>
<th>BLOCH</th>
</tr>
</thead>
<tbody>
<tr>
<td>k (h*k is the momentum.)</td>
<td></td>
<td>k, n (h*k is the crystal momentum and n is the band index.)</td>
</tr>
</tbody>
</table>

**RANGE OF QUANTUM NUMBERS**  
- k runs through all of k-space consistent with the Born-von Karman periodic boundary condition.
- For each n, k runs through all wave vectors in a single primitive cell of the reciprocal lattice consistent with the Born-von Karman periodic boundary condition; n runs through an infinite set of discrete values.

**ENERGY**  
\[ \varepsilon(k) = \frac{\hbar^2 k^2}{2m} \]
For a given band index n, \( \varepsilon_n(k) \) has no simple explicit form. The only general property is periodicity in the reciprocal lattice:
\[ \varepsilon_n(k + K) = \varepsilon_n(k). \]

**VELOCITY**  
- The mean velocity of an electron in a level with wave vector \( k \) is:
\[ v = \frac{\hbar k}{m} = \frac{1}{\hbar} \frac{\partial \varepsilon}{\partial k}. \]
- The mean velocity of an electron in a level with band index n and wave vector \( k \) is:
\[ v_n(k) = \frac{1}{h} \frac{\partial \varepsilon_n(k)}{\partial k}. \]

**WAVE FUNCTION**  
- The wave function of an electron with wave vector \( k \) is:
\[ \psi_k(r) = \frac{e^{i k \cdot r}}{\sqrt{V^{1/2}}}. \]
- The wave function of an electron with band index n and wave vector \( k \) is:
\[ \psi_{nk}(r) = e^{i k \cdot r} u_{nk}(r) \]
where the function \( u_{nk} \) has no simple explicit form. The only general property is periodicity in the direct lattice:
\[ u_{nk}(r + R) = u_{nk}(r). \]
In Reality

Even in a perfect crystal, ions will, at least, experience thermal vibration at $T \neq 0$ K – ions are not quite.

Deviations from Perfect Periodicity in potential
The Semiclassical Model of Electron Dynamics

The electronic structure is described \textit{quantum-mechanically}.

Electron dynamics is considered in a \textit{classic way} – using classic equations of motion.

To relate the \textit{GIVEN} band structure to the transport properties.
\[ \mathbf{v}_n(k) = \frac{d}{dt} \mathbf{r} = \frac{1}{\hbar} \frac{d\varepsilon_n(k)}{dk} \]

\[
F(r,t) = -e \left[ \mathbf{E}(r,t) + \frac{1}{c} \mathbf{v}_n(k) \times \mathbf{H}(r,t) \right] = \hbar \frac{d}{dt} \]
Make $E(r,t)$ and $H(r,t)$ small, so to ignore the possibility of inter-band transitions

$$e|E|a \ll \frac{\left[ \varepsilon_{\text{gap}}(k) \right]^2}{\varepsilon_F}$$

$$\hbar \omega_c = \hbar \left( \frac{eH}{mc} \right) \ll \frac{\left[ \varepsilon_{\text{gap}}(k) \right]^2}{\varepsilon_F}$$

$$\varepsilon_{\text{gap}}(k) = \varepsilon_n(k) - \varepsilon_n(k)$$
To relate the band structure to the transport properties:

Filled bands: \( (\hbar k, -\hbar k) \)

\[
J_{\text{filled-band}}^{\text{net}} = -ne \sum v = 0
\]

This results in a band insulator.

Partially filled bands:

\( J_{\text{net}} \neq 0 \)

This results in a band conductor.

If it is actually an insulator – the system is then called *Mott insulator*.
In the case of $E(r,t) = E_0$, $H = 0$

$$F(r,t) = -e \left[ E(r,t) + \frac{1}{c} \mathbf{v}_n(k) \times H(r,t) \right] = \hbar \frac{d}{dt} \mathbf{k}$$

$$\hbar \frac{d}{dt} \mathbf{k} = -e \mathbf{E}$$

$$\mathbf{k}(t) = \mathbf{k}(0) - \frac{e}{\hbar} \mathbf{E} t$$
The concept of holes

Since the current in a filled band is zero even if $E \neq 0$, this leads:

\[ J_{\text{filled-band}}^\text{net} = 0 \]

\[ \Rightarrow (-e) \int_{\text{zone}} \frac{d\mathbf{k}}{4\pi^3} \mathbf{v}(\mathbf{k}) = 0 \]

\[ \Rightarrow \int_{\text{occupied}} \frac{d\mathbf{k}}{4\pi^3} \mathbf{v}(\mathbf{k}) + \int_{\text{unoccupied}} \frac{d\mathbf{k}}{4\pi^3} \mathbf{v}(\mathbf{k}) = 0 \]

\[ \Rightarrow J = (-e) \int_{\text{occupied}} \frac{d\mathbf{k}}{4\pi^3} \mathbf{v}(\mathbf{k}) = (+e) \int_{\text{unoccupied}} \frac{d\mathbf{k}}{4\pi^3} \mathbf{v}(\mathbf{k}) \]
\[ J = (-e) \int \frac{d\mathbf{k}}{4\pi^3} \mathbf{v}(\mathbf{k}) = (+e) \int \frac{d\mathbf{k}}{4\pi^3} \mathbf{v}(\mathbf{k}) \]

**Warning:**

1. Must not be double counted!!!
2. Unoccupied levels must lie sufficiently close to a highly symmetrical band maximum, i.e., \( \mathbf{k} \cdot \mathbf{a} < 0 \)

Unoccupied states behave like +e charge carriers - holes
Holes and effective masses

\[ a = \frac{dv}{dt} = \frac{1}{\hbar} \frac{d^2E}{dk dt} = \frac{1}{\hbar} \frac{d^2E}{dk^2} \frac{dk}{dt} = \frac{1}{\hbar^2} \frac{d^2E}{dk^2} \left( \frac{\hbar}{d} \frac{dk}{dt} \right) = \frac{1}{\hbar^2} \frac{d^2E}{dk^2} F \]

Effective mass \( m^* \):

\[ \frac{1}{m^*} = \frac{1}{\hbar^2} \frac{d^2E}{dk^2} \]
Holes and effective masses

\[ \dot{k} \cdot \mathbf{a} = k \cdot \frac{1}{\hbar} \frac{d^2E}{dk dt} = \hbar \sum_{ij} k_i \left( \frac{1}{\hbar^2} \frac{\partial^2 E}{\partial k_i \partial k_j} \right) k_j = \hbar \sum_{ij} k_i \frac{1}{m_{ij}^*} k_j \]

When \( E(k) \) is at a local extreme (e.g., at the zone boundary), \( m^* < 0 \) (i.e., \( \dot{k} \cdot \mathbf{a} < 0 \)).

Electron (-e) with negative mass (\( m^* < 0 \))

\[ \Pi \]

Hole (+e) with positive mass (\( |m^*| > 0 \))
Effective Mass Anisotropy

- For spherical Fermi surface, \( m_{ij}^* = m^* d_{ij} \)

- For ellipsoidal Fermi surface, there can be at most three different \( m^* \)s.

Fermi surface of Si
In the case of $E(r,t) = E_0$, $H=0$

$$F(r,t) = -e \left[ E(r,t) + \frac{1}{c} v_n(k) \times H(r,t) \right] = \hbar \frac{d k}{dt}$$

$$\hbar \frac{d k}{dt} = -e E$$

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

$$v(k) = \nabla_k \omega(k) = \frac{\nabla_k E(k)}{\hbar}$$
In a DC electric field (constant), electrons reverse its motion direction ($\mathbf{v}$ changes sign) at the B-zone boundary.

A DC electric field produces an AC current - Bloch Oscillation.
Can we observe Bloch oscillation in ordinary metals?

Require:

\[ |\mathbf{k}(t) - \mathbf{k}(0)| = \left| -\frac{eE}{\hbar} t \right| = \frac{2\pi}{a} \]

Travel time:

\[ t = \frac{\hbar}{aeE} \sim 10^{-10} \text{ sec} \]

for \( E \sim 10^4 \text{ V/cm} \)

In ordinary metals, electrons experience collisions every \( \sim 10^{-14} \text{ sec} \)

\( \Rightarrow \) Bloch electrons cannot reach the Zone boundary
How to obtain Bloch oscillation?

- Make super clean sample $\Rightarrow$ to reduce collisions
- Increase $E$ (only up to $10^6$ V/cm)
- Make superlattice structure $\Rightarrow$ to increase $a$

If observed: $t = \frac{h}{aeE} \sim 10^{-12} - 10^{-13}$ sec

$\Rightarrow$ frequency $f = 1/t \sim 10^{12}-10^{13}$ Hz

-- generate THz microwave
In the case of $E(r,t)=0$, $H=H_0$

$$F(r,t) = -e\left[ E(r,t) + \frac{1}{c} v_n(k) \times H(r,t) \right] = \hbar \frac{d k}{d t}$$

$$\hbar \frac{d k}{d t} = (-e) \frac{1}{c} v_n(k) \times H$$

$$v_n(k) = \frac{d r}{d t} = \frac{1}{\hbar} \frac{d \varepsilon_n(k)}{d k}$$
\[ \hbar \frac{d \mathbf{k}}{dt} = (-e) \frac{1}{c} \mathbf{v}_n(\mathbf{k}) \times \mathbf{H} \]

\[ \mathbf{v}_n(\mathbf{k}) = \frac{d \mathbf{r}}{dt} = \frac{1}{\hbar} \frac{d \varepsilon_n(\mathbf{k})}{d \mathbf{k}} \]

\[ \frac{d \mathbf{k}}{dt} \cdot \mathbf{H} = 0 \]

\[ \frac{d \mathbf{k}}{dt} \cdot \mathbf{v}_n(\mathbf{k}) = \frac{1}{\hbar} \frac{d \varepsilon_n(\mathbf{k})}{dt} = 0 \]

ически \ Change of \ \mathbf{k} \ is \ perpendicular \ to \ \mathbf{H} \n
\Rightarrow \ k_{/\mathbf{H}} = \text{constant} \n
\achuset \ E \ is \ constant \ of \ motion
Orientation of the orbit

Determined by right-hand rule
Cyclotron orbit in real space

\[ \hbar \frac{d\mathbf{k}}{dt} = (-e) \frac{1}{c} v_n(k) \times \mathbf{H} \quad \Rightarrow \quad \frac{d\mathbf{r}}{dt} = -\frac{\hbar c}{eH^2} \mathbf{H} \times \frac{d\mathbf{k}}{dt} \]

**r-orbit**

**k-orbit**

rotated by 90 degrees and scaled by \( \frac{\hbar c}{eH} = \lambda_B^2 \)
Period of the orbit
(if the orbit is a closed curve)

\[(k_1,t_1) \rightarrow (k_2,t_2)\]

\[t_2 - t_1 = \int_{t_1}^{t_2} dt = \int_{k_1}^{k_2} \frac{dk}{d\epsilon} \frac{\hbar^2 c}{eH} \int_{k_1}^{k_2} \frac{d\epsilon}{dk} \bigg|_{H} = \Delta \epsilon \Delta k(k)\]

\[t_2 - t_1 = \hbar^2 c \frac{1}{eH} \Delta \epsilon \int_{k_1}^{k_2} \Delta(k) dk = \frac{\hbar^2 c}{eH} \frac{\Delta A_{1,2}}{\Delta \epsilon}\]

To complete a circuit: \[T(\epsilon,k_z) = \frac{\hbar^2 c}{eH} \frac{\Delta A(\epsilon,k_z)}{\Delta \epsilon}\]
Compare \( T(\varepsilon, k_z) = \frac{\hbar^2 c}{eH} \frac{\Delta A(\varepsilon, k_z)}{\Delta \varepsilon} \)

With free-electron-case: \( T = \frac{2\pi}{\omega_c} = \frac{2\pi mc}{eH} \)

Define:

**Cyclotron effective mass** \( m^* \):

\[
m^*_c(\varepsilon, k_z) = \frac{\hbar^2}{2\pi} \frac{\Delta A(\varepsilon, k_z)}{\Delta \varepsilon}
\]
In the case of $E(r,t)=E_0$, $H=H_0$

$$F(r,t) = -e \left[ E(r,t) + \frac{1}{c} v_n(k) \times H(r,t) \right] = \hbar \frac{d k}{d t}$$

$$\hbar \frac{d k}{d t} = -\frac{e}{c \hbar} \frac{\partial \varepsilon}{\partial k} \times H$$

with $\varepsilon(k) = \varepsilon(k) - \hbar k \cdot w$

The motion of electrons would be as if only the magnetic field were present, and if the band structure were given by $\bar{\varepsilon}(k)$ rather than $\varepsilon(k)$ ( $\hbar k \cdot w$ is usually small)
Real space orbit

\[ \hbar \frac{d}{dt} \left( \vec{k} + \frac{e}{\hbar} \vec{E}t \right) = -e \frac{\vec{r}}{c} \times \vec{H} \]

\[ \Rightarrow \quad \frac{d}{dt} \vec{r} = \lambda_B^2 \frac{d}{dt} \left( \vec{k} + \frac{e}{\hbar} \vec{E}t \right) \times \hat{H} \]

\[ \Rightarrow \quad \vec{r}(t) - \vec{r}(0) = \lambda_B^2 \left( \vec{k}(t) - \vec{k}(0) \right) \times \hat{H} + c \frac{E}{\hat{H}} \left( \vec{E} \times \hat{H} \right) t \]

A steady $\vec{E} \times \vec{H}$ drift

(drift velocity)
Conditions:

1. All occupied orbits are closed;

2. $\omega_c \tau >> 1$ (high-field to increase $\omega_c$ and long $\tau$)

$$\Rightarrow \mathbf{v} = -\frac{\hbar c}{eH} \mathbf{H} \times \frac{\mathbf{k}(\tau) - \mathbf{k}(0)}{\tau} + \mathbf{w} \sim \mathbf{w}$$

Occupied levels: $$\lim_{\tau/T \to \infty} J_\perp = -n_e e \langle \mathbf{v} \rangle \approx -n_e e \mathbf{w} = -\frac{n_e e c}{H} (\mathbf{E} \times \mathbf{H})$$

Unoccupied levels: $$\lim_{\tau/T \to \infty} J_\perp = n_h e \langle \mathbf{v} \rangle \approx n_h e \mathbf{w} = \frac{n_h e c}{H} (\mathbf{E} \times \mathbf{H})$$
Occupied levels: \( \lim_{\tau/T \to \infty} J_\perp = -n_e e \langle v \rangle \approx -n_e e w = -\frac{n_e ec}{H} (E \times H) \)

Unoccupied levels: \( \lim_{\tau/T \to \infty} J_\perp = n_h e \langle v \rangle \approx n_h e w = \frac{n_h ec}{H} (E \times H) \)

Hall coefficient: \( R_H^e = -\frac{1}{n_ee c} \quad R_H^h = \frac{1}{n_he c} \)

If both electrons and holes are present in a metal, then

\[
R_H = \frac{R_e \sigma_e^2 + R_h \sigma_h^2}{(\sigma_e + \sigma_h)^2}, \quad \sigma_{e,h} = \frac{n_{e,h} e^2 \tau_{e,h}}{m_{e,h}^*}
\]

Magneto-conductance
Electron Dynamics:

- DC electric field $\Rightarrow$ Bloch oscillation
- Magnetic field $\Rightarrow$ cyclotron motion
- Electric + magnetic field $\Rightarrow$ Hall effect, magnetoresistance
Homework
(due on 10/23/2009)

Problem 1 in p239
Problem 7 in p241