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

	SOMMERFELD	BLOCH
QUANTUM NUMBERS (EXCLUDING SPIN)	$\mathbf{k}$ ($\hbar\mathbf{k}$ is the momentum.)	$\mathbf{k}$, n ($\hbar\mathbf{k}$ is the crystal momentum and n is the band index.)
RANGE OF QUANTUM NUMBERS	$\mathbf{k}$ runs through all of k-space consistent with the Born-von Karman periodic boundary condition.	For each n, $\mathbf{k}$ 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	$\mathcal{E}(\mathbf{k}) = \dfrac{\hbar^2 k^2}{2m}$.	For a given band index n, $\mathcal{E}_n(\mathbf{k})$ has no simple explicit form. The only general property is periodicity in the reciprocal lattice: $\mathcal{E}_n(\mathbf{k} + \mathbf{K}) = \mathcal{E}_n(\mathbf{k})$.
VELOCITY	The mean velocity of an electron in a level with wave vector $\mathbf{k}$ is: $\mathbf{v} = \dfrac{\hbar\mathbf{k}}{m} = \dfrac{1}{\hbar}\dfrac{\partial\mathcal{E}}{\partial\mathbf{k}}$.	The mean velocity of an electron in a level with band index n and wave vector $\mathbf{k}$ is: $\mathbf{v}_n(\mathbf{k}) = \dfrac{1}{\hbar}\dfrac{\partial\mathcal{E}_n(\mathbf{k})}{\partial\mathbf{k}}$.
WAVE FUNCTION	The wave function of an electron with wave vector $\mathbf{k}$ is: $\psi_{\mathbf{k}}(\mathbf{r}) = \dfrac{e^{i\mathbf{k}\cdot\mathbf{r}}}{V^{1/2}}$.	The wave function of an electron with band index n and wave vector $\mathbf{k}$ is: $\psi_{n\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}u_{n\mathbf{k}}(\mathbf{r})$ where the function $u_{n\mathbf{k}}$ has no simple explicit form. The only general property is periodicity in the direct lattice: $u_{n\mathbf{k}}(\mathbf{r} + \mathbf{R}) = u_{n\mathbf{k}}(\mathbf{r})$.

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

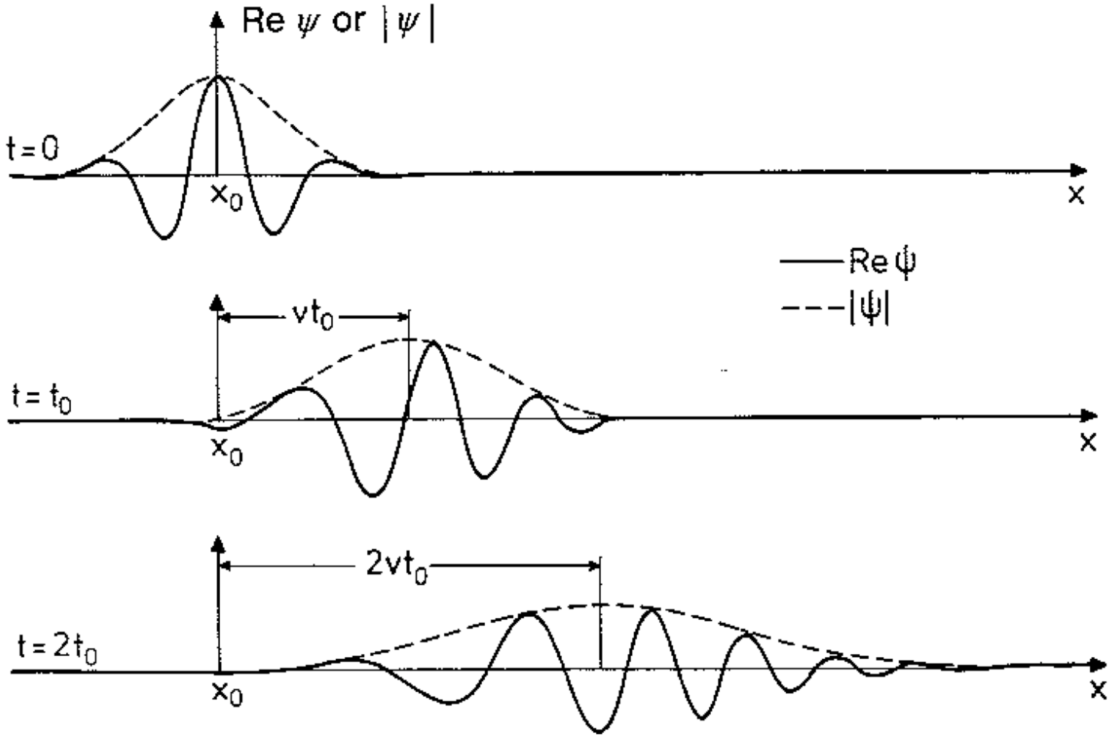
The Semiclassical Model of Electron Dynamics

- The electronic structure is described *quantum-mechanically*

- Electron dynamics is considered in a *classic way* – using classic equations of motion

goal

To relate the GIVEN band structure to the transport properties



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

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

Make E(r,t) and H(r,t) small, so to ignore the possibility of inter-band transitions

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

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

$$\varepsilon_{gap}\left(\mathbf{k}\right) = \varepsilon_{n'}\left(\mathbf{k}\right) - \varepsilon_n\left(\mathbf{k}\right)$$

To relate the <u>band structure</u> to the <u>transport properties</u>

Filled bands: $\left(\hbar\mathbf{k}, -\hbar\mathbf{k}\right)$

$$\mathbf{J}_{net}^{filled-band} = -ne\sum \mathbf{v} = 0$$

band insulator

Partially filled bands:

$$\mathbf{J}_{net} \neq 0$$

band conductor

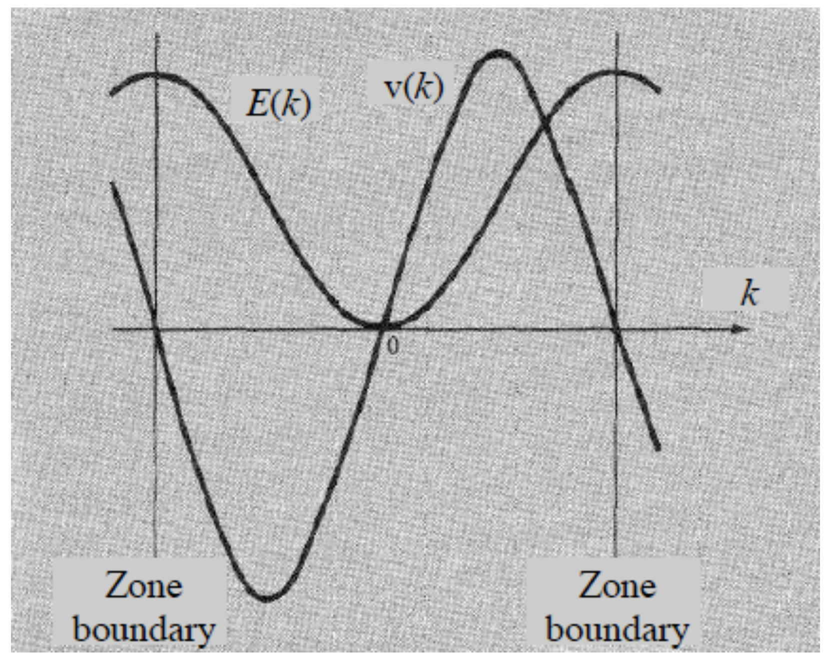
If **it is actually an insulator**
– the system is then called *Mott insulator*

In the case of $\mathbf{E}(\mathbf{r},t)=\mathbf{E}_0$, $\mathbf{H}=0$

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

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

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



The concept of holes

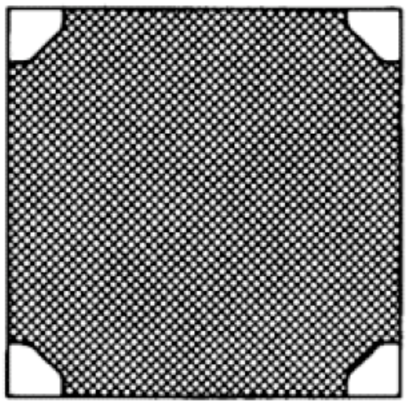
Since the current in a filled band is zero even if **E**≠0, this leads:

$$\mathbf{J}_{net}^{filled-band} = 0$$

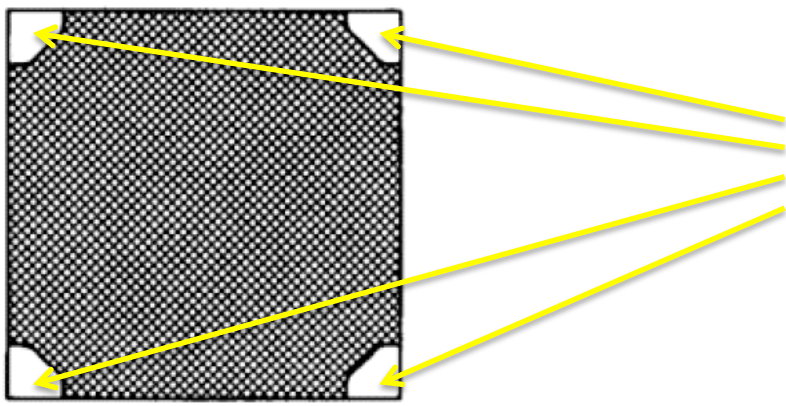
$$\Rightarrow (-e) \int_{zone} \frac{d\mathbf{k}}{4\pi^3} \mathbf{v}(\mathbf{k}) = 0$$

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

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



$$\mathbf{J} = (-e)\int_{occupied} \frac{d\mathbf{k}}{4\pi^3}\mathbf{v}(\mathbf{k}) = (+e)\int_{unoccupied} \frac{d\mathbf{k}}{4\pi^3}\mathbf{v}(\mathbf{k})$$



unoccupied states
behave like +e charge
carriers - holes

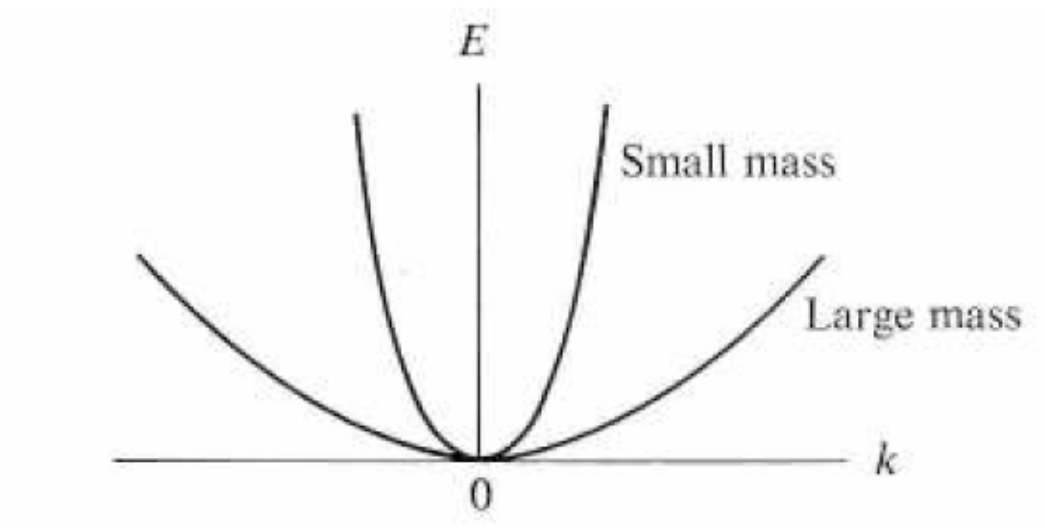
Warning:

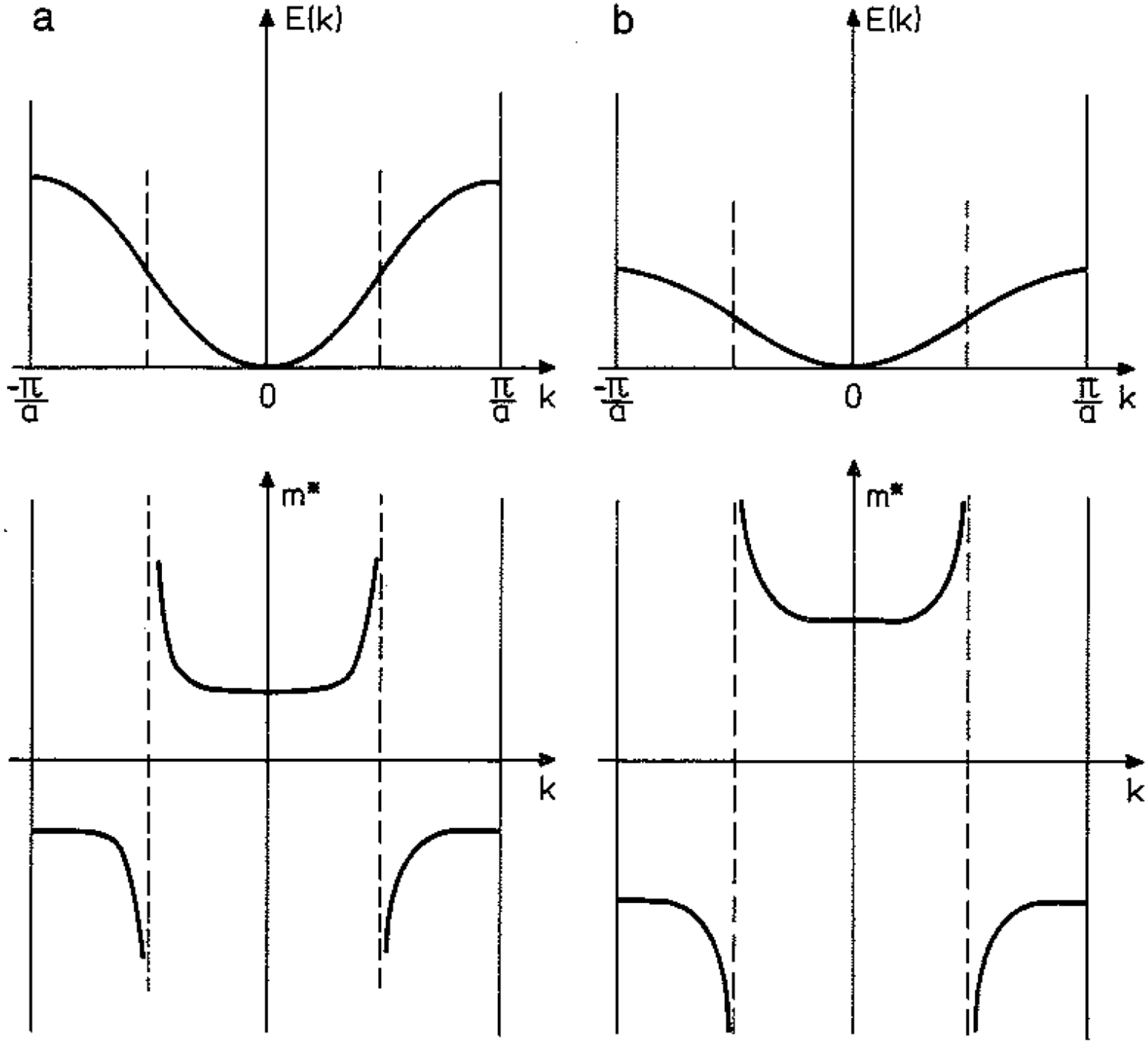
1. **Must not be double counted!!!**
2. **Unoccupied levels must lie sufficiently close to a highly symmetrical band maximum,** i.e., $\dot{\mathbf{k}}\cdot\mathbf{a} < 0$

Holes and effective masses

$$\mathbf{a} = \frac{d\,\mathbf{v}}{dt} = \frac{1}{\hbar}\frac{d^2E}{d\,\mathbf{k}\,dt} = \frac{1}{\hbar}\frac{d^2E}{d\,\mathbf{k}^2}\frac{d\,\mathbf{k}}{dt} = \frac{1}{\hbar^2}\frac{d^2E}{d\,\mathbf{k}^2}\left(\hbar\frac{d\,\mathbf{k}}{dt}\right) = \frac{1}{\hbar^2}\frac{d^2E}{d\,\mathbf{k}^2}\mathbf{F}$$

Effective mass m*: $\frac{1}{m^*} = \frac{1}{\hbar^2}\frac{d^2E}{d\,\mathbf{k}^2}$





a
E(k)
-π/a
0
π/a
k
b
E(k)
-π/a
0
π/a
k
m*
k
m*
k

Holes and effective masses

$$\dot{\mathbf{k}}\cdot\mathbf{a} = \dot{\mathbf{k}}\cdot\frac{1}{\hbar}\frac{d^2E}{d\mathbf{k}\,dt} = \hbar\sum_{ij}\dot{k}_i\left(\frac{1}{\hbar^2}\frac{\partial^2E}{\partial k_i\partial k_j}\right)\dot{k}_j = \hbar\sum_{ij}\dot{k}_i\frac{1}{m^*_{ij}}\dot{k}_j$$

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

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

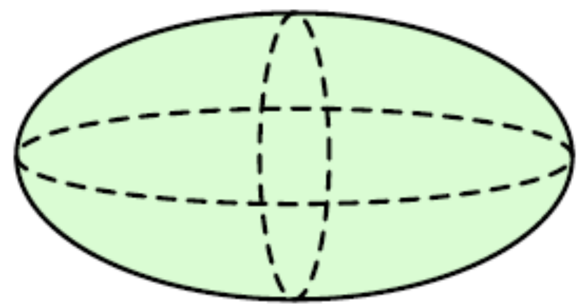
II

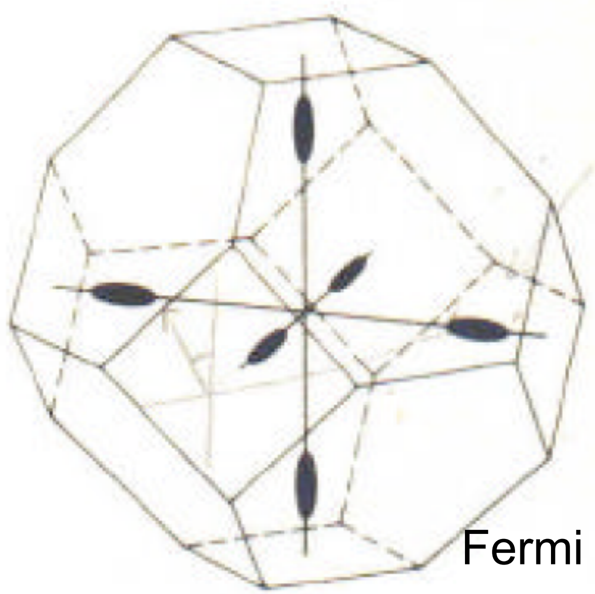
hole (+e) with positive mass ($|m^*| > 0$)

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

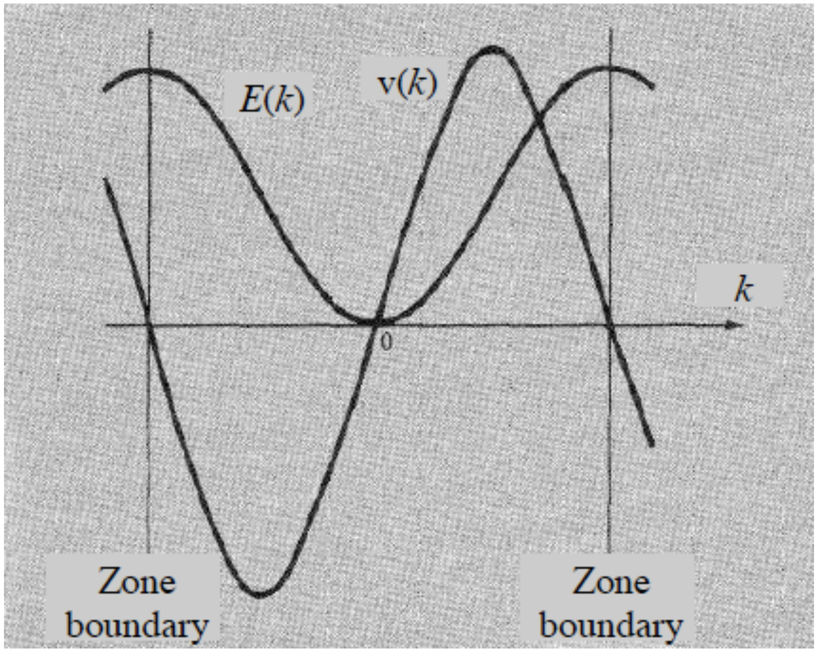
In the case of $\mathbf{E}(r,t)=\mathbf{E}_0$, $\mathbf{H}=0$

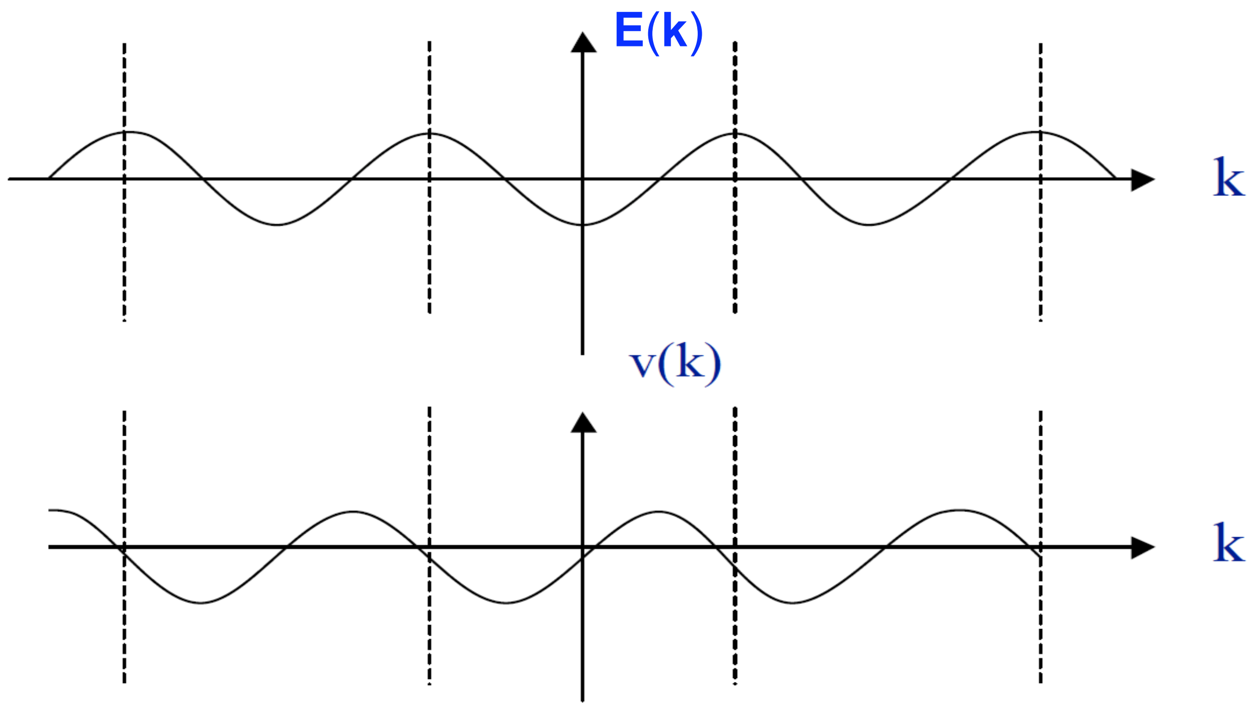
$$\mathbf{F}(\mathbf{r},t) = -e\left[\mathbf{E}(\mathbf{r},t) + \frac{1}{c}\mathbf{v}_n(\mathbf{k}) \times \mathbf{H}(\mathbf{r},t)\right] = \hbar \frac{d\,\mathbf{k}}{dt}$$

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

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

$$v(\mathbf{k}) = \nabla_k \omega(\mathbf{k}) = \frac{\nabla_k \mathbf{E}(k)}{\hbar}$$





In a DC electric field (constant), electrons reverse its motion direction (**v** changes sign) at the B-zone boundary

A DC electric field produces an AC current - **Bloch Oscillation**

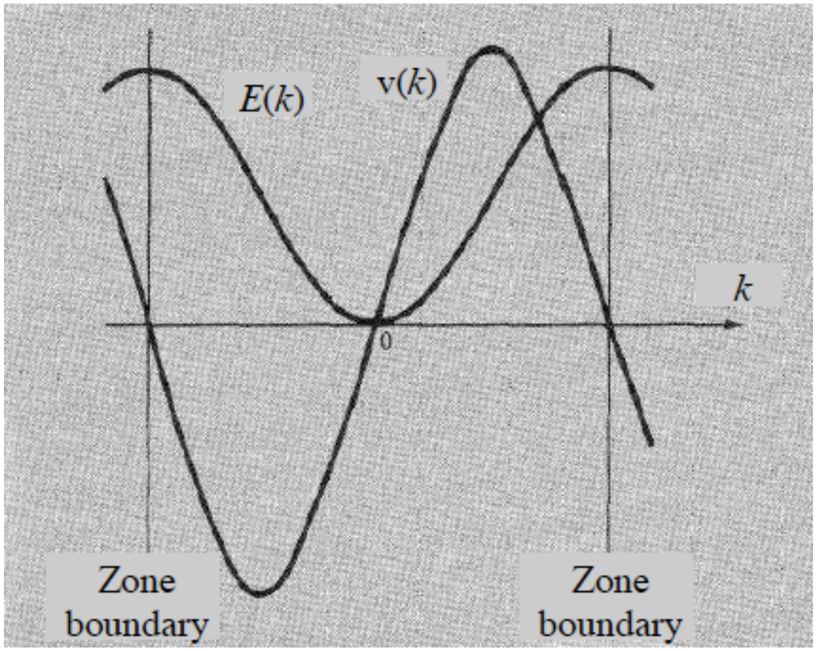
Can we observe Bloch oscillation in ordinary metals?

Require:

$$\left|\mathbf{k}(t)-\mathbf{k}(0)\right| = \left|-\frac{e\,\mathbf{E}}{\hbar}t\right| = \frac{2\pi}{a}$$

Travel time: $t = \dfrac{h}{aeE} \sim 10^{-10}\ \textbf{sec}$

for E ~ 10^4 V/cm



In ordinary metals, electrons experience collisions every ~ 10^{-14} sec

⇒ Bloch electrons cannot reach the Zone boundary

How to obtain Bloch oscillation?

- Make super clean sample ⇒ to reduce collisions

- Increase E (only up to 10^6 V/cm)

- Make superlattice structure ⇒ to increase *a*

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

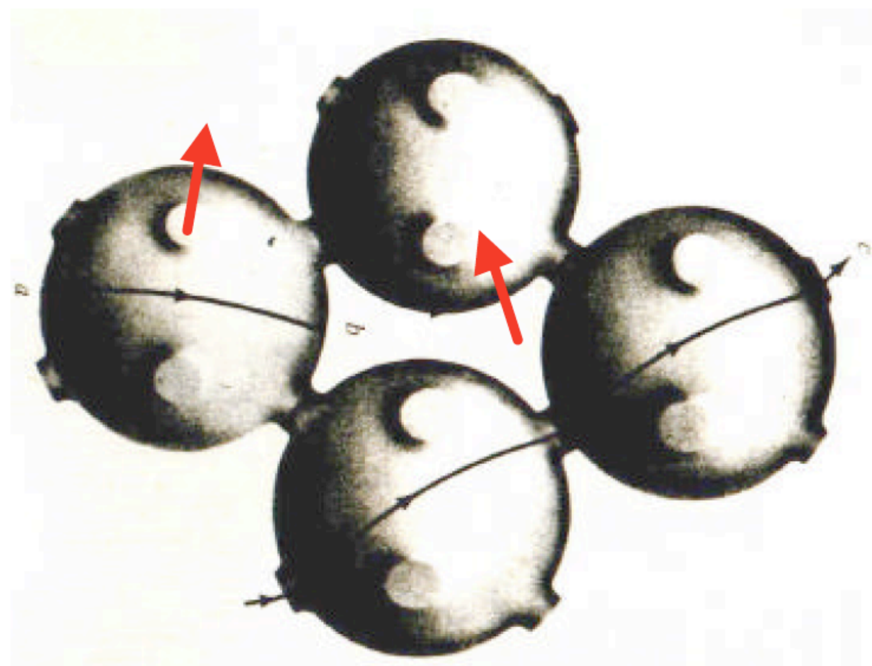
⇒frequency f = 1/t ~ 10^{12}-10^{13} Hz
-- generate THz microwave

In the case of **E**(r,t)=0, **H**=H_0

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

$$\hbar\frac{d\,\mathbf{k}}{dt} = (-e)\frac{1}{c}\mathbf{v}_n(\mathbf{k}) \times \mathbf{H}$$

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



$$\hbar \frac{d\,\mathbf{k}}{dt} = (-e)\frac{1}{c}\mathbf{v}_n(\mathbf{k}) \times \mathbf{H}$$

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

➔➔➔

$$\frac{d\,\mathbf{k}}{dt} \cdot \mathbf{H} = 0$$

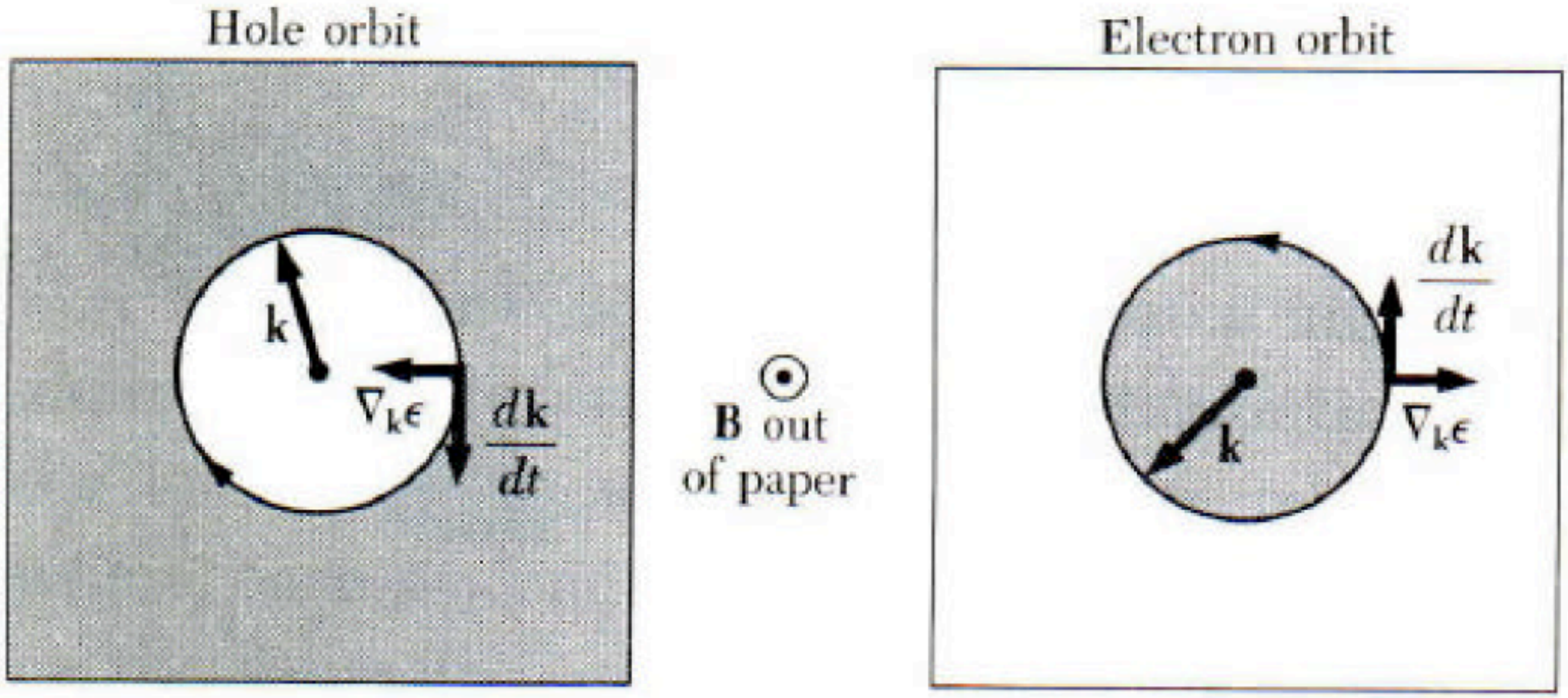
$$\frac{d\,\mathbf{k}}{dt} \cdot \mathbf{v}_n(\mathbf{k}) = \frac{1}{\hbar}\frac{d\varepsilon_n(\mathbf{k})}{dt} = 0$$

- Change of **k** is perpendicular to **H**

  ⇒ $k_{//H}$ = constant

- E is constant of motion

Orientation of the orbit



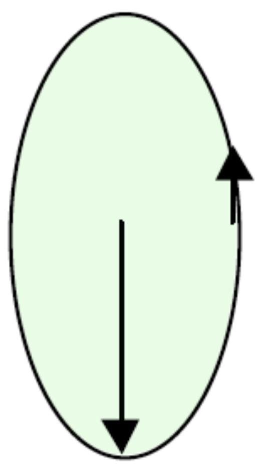
Determined by right-hand rule

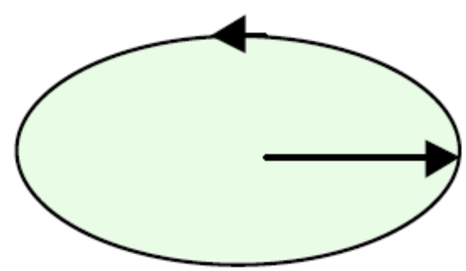
Cyclotron orbit in real space

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

r-orbit

k-orbit



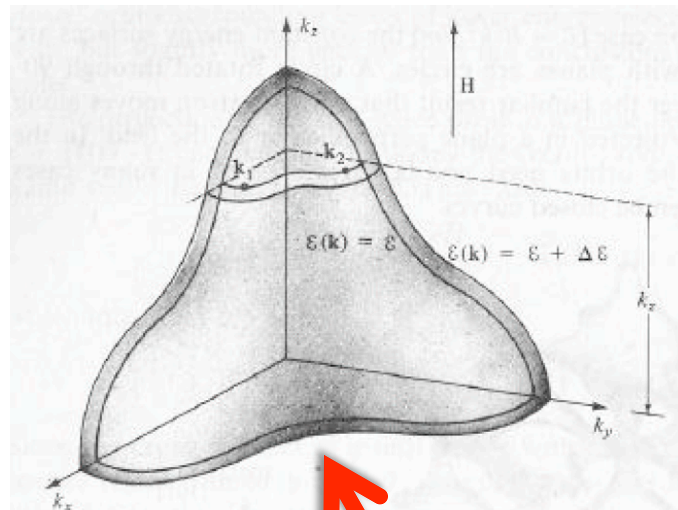


rotated by 90 degrees and scaled by $\hbar c/eH = \lambda_B^2$

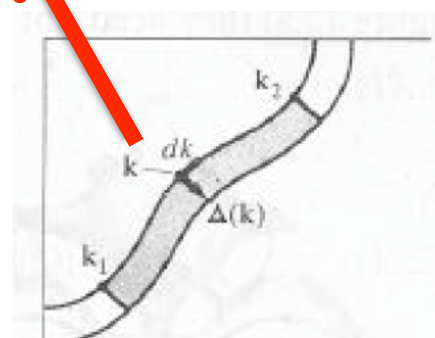
Period of the orbit (if the orbit is a closed curve)

$$(\mathbf{k}_1, t_1) \rightarrow (\mathbf{k}_2, t_2)$$

$$t_2 - t_1 = \int_{t_1}^{t_2} dt = \int_{k_1}^{k_2} \frac{dk}{\left|\frac{d\,\mathbf{k}}{dt}\right|} = \frac{\hbar^2 c}{eH} \int_{k_1}^{k_2} \frac{dk}{\left|\frac{\partial \varepsilon}{d\,\mathbf{k}}\right|_{\perp H}}$$



$$\left|\frac{\partial \varepsilon}{d\,\mathbf{k}}\right|_{\perp H} = \frac{\Delta \varepsilon}{\Delta(\mathbf{k})}$$



$$\Delta A_{1,2} = \int_{k_1}^{k_2} \Delta(\mathbf{k}) dk$$

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

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

Compare $$T(\varepsilon, k_z) = \frac{\hbar^2 c}{eH} \frac{\Delta A(\varepsilon, k_z)}{\Delta \varepsilon}$$

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

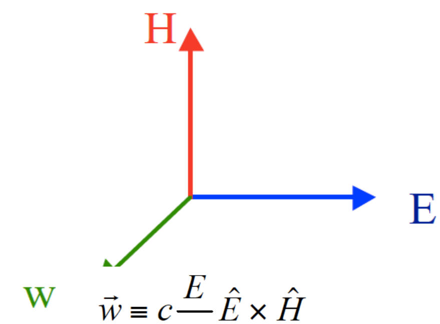
Define:

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 $\mathbf{E}(\mathbf{r},t)=\mathbf{E}_0$, $\mathbf{H}=\mathbf{H}_0$

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



$$\vec{w} \equiv c\frac{E}{H}\hat{E} \times \hat{H}$$

$$\hbar \frac{d\,\mathbf{k}}{dt} = -\frac{e}{c\hbar}\frac{\partial \bar{\varepsilon}}{\partial \mathbf{k}} \times \mathbf{H}$$

with $\bar{\varepsilon}(\mathbf{k}) = \varepsilon(\mathbf{k}) - \hbar\,\mathbf{k}\cdot\mathbf{w}$

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

Real space orbit

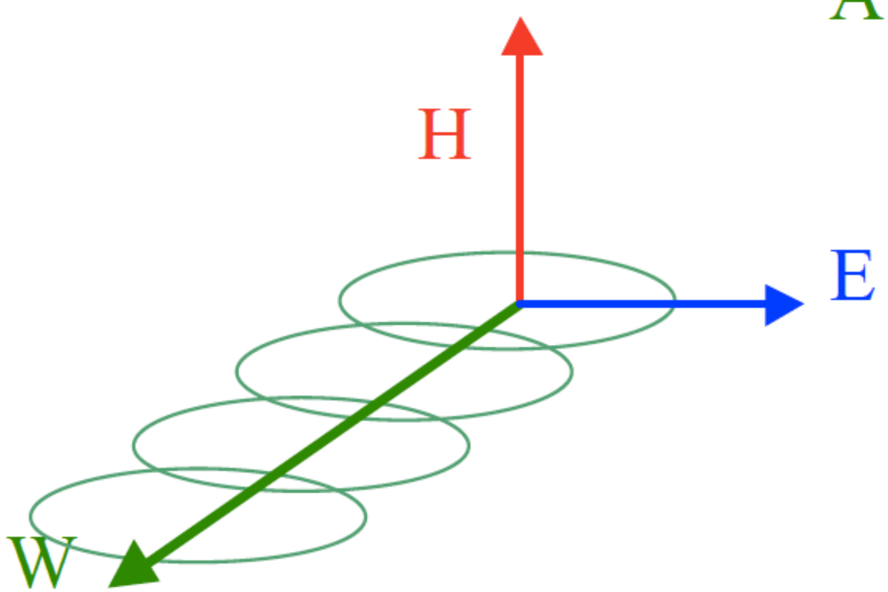
$$\hbar \frac{d}{dt}\left(\vec{k} + \frac{e}{\hbar}\vec{E}t\right) = -e\frac{\dot{\vec{r}}}{c} \times \vec{H}$$

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

$$\rightarrow \quad \vec{r}(t) - \vec{r}(0) = \lambda_B^2\left(\vec{k}(t) - \vec{k}(0)\right) \times \hat{H} + \underbrace{c\frac{E}{H}\left(\hat{E} \times \hat{H}\right)t}_{\text{A steady E×H drift}}$$

A steady E×H drift

(drift velocity)



Conditions:

1. **All occupied orbits are closed;**

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

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

$$\Downarrow$$

Occupied levels: $\lim\limits_{\tau/T\to\infty}\mathbf{J}_\perp = -n_e e\langle\mathbf{v}\rangle \approx -n_e e\,\mathbf{w} = -\frac{n_e ec}{H}(\mathbf{E}\times\mathbf{H})$

Unoccupied levels: $\lim\limits_{\tau/T\to\infty}\mathbf{J}_\perp = n_h e\langle\mathbf{v}\rangle \approx n_h e\,\mathbf{w} = \frac{n_h ec}{H}(\mathbf{E}\times\mathbf{H})$

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

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

Hall coefficient: $R_H^e = -\frac{1}{n_e ec}$ $\quad R_H^h = \frac{1}{n_h ec}$

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 ⇒ Bloch oscillation
- 👌 Magnetic field ⇒ cyclotron motion
- 👌 Electric + magnetic field ⇒ Hall effect, magnetoresistance

Homework
(due on 10/23/2009)

Problem 1 in p239

Problem 7 in p241