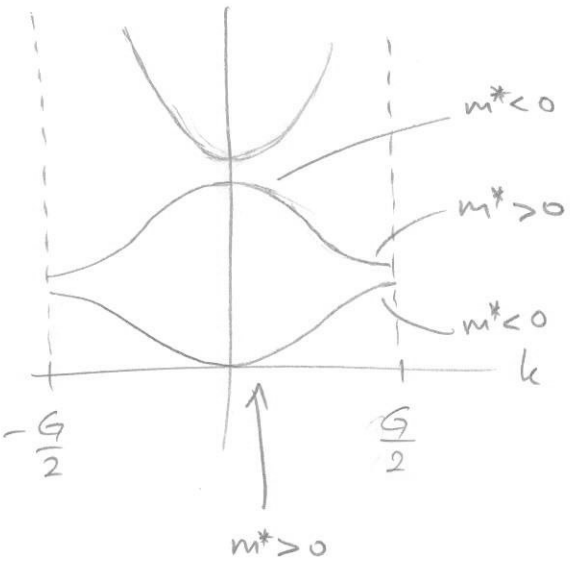
Holes (p. 225-228)

Effective mass



$$\frac{1}{m^*} = \frac{1}{\hbar^2}\frac{\partial^2 \mathcal{E}}{\partial k^2}$$

Define $m_h = -m^*$

$m_h > 0$

Alternative description of charge carriers

almost full electron bands.

Properties – Holes

① Charge $+e$

② $m_h > 0$

③ $\bar{k}_h = -\bar{k}_e$

④ $\mathcal{E}_h(\bar{k}_h) = -\mathcal{E}_e(\bar{k}_e)$

⑤ $\bar{v}_h = \bar{v}_e$

① Charge +e

Current produced by electrons in a set of levels is the same as the current produced if

a) the set of levels were unoccupied

b) all other levels in the band were occupied with particles of charge +e

$$\bar{j} = -ne\bar{v} = \underbrace{(-e)}_{V} \sum_{\bar{k}} \bar{v}_{\bar{k}}$$

Full band: $\underbrace{(-e)}_{V} \sum_{\text{all } \bar{k}} \bar{v}_{\bar{k}} = 0$ because every $\bar{v}_{\bar{k}}$ has $-\bar{v}_{\bar{k}}$

Assume one electron is missing at $\bar{k}'$:

$$\underbrace{(-e)}_{V} \sum_{\substack{\text{all } \bar{k} \\ \text{but } \bar{k}'}} \bar{v}_{\bar{k}} = \underbrace{\underbrace{(-e)}_{V} \sum_{\text{all } \bar{k}} \bar{v}_{\bar{k}}}_{=0} - \underbrace{(-e)}_{V} \bar{v}_{\bar{k}'} = \underbrace{(+e)}_{V} \cdot \bar{v}_{\bar{k}'}$$

Similarly

$$\bar{j} = (-e) \int_{\text{occupied}} \bar{v}_{\bar{k}} \cdot \frac{d\bar{k}}{4\pi^3} \qquad \text{but} \qquad 0 = (-e) \int_{\substack{\text{all} \\ \text{zone}}} \bar{v}_{\bar{k}} \frac{d\bar{k}}{4\pi^3}$$

$$\Rightarrow \bar{j} = (+e) \int_{\text{unoccupied}} \bar{v}_{\bar{k}} \cdot \frac{d\bar{k}}{4\pi^3}$$

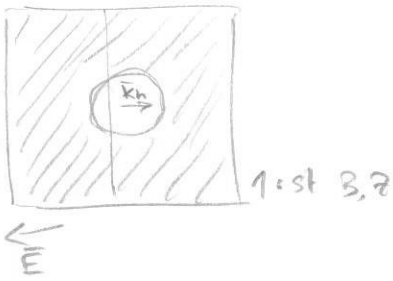
② $m_h > 0$

$$v = \frac{1}{\hbar} \frac{\partial E}{\partial k} \qquad \underbrace{\frac{dv}{dt}}_{a} = \frac{1}{\hbar} \frac{\partial^2 E}{\partial k^2} \frac{dk}{dt} = \underbrace{\frac{1}{\hbar^2} \frac{\partial^2 E}{\partial k^2}}_{(m^*)^{-1}} \cdot \underbrace{\frac{d(\hbar k)}{dt}}_{F}$$

For electrons: $\underbrace{\frac{1}{\hbar^2} \frac{\partial^2 E}{\partial k^2}}_{\frac{1}{m^*}} \cdot \underbrace{(-eE)}_{F}$

For holes: $\underbrace{\left(-\frac{1}{\hbar^2} \frac{\partial^2 E}{\partial k^2}\right)}_{(m_h)^{-1} = -(m^*)^{-1}} \cdot (+eE)$

③ $\bar{k}_h = -\bar{k}_e$

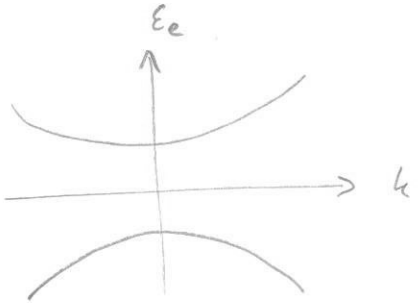


Full band: $\sum_{\text{all } k} \bar{k}_e = 0$

Assume missing electron at $\bar{k}'$

$$\bar{k}_h = \sum_{\substack{\text{all } k \\ \text{but } \bar{k}'}} \bar{k}_e = \underbrace{\left(\sum_{\text{all } k} \bar{k}_e\right)}_{=0} - \bar{k}_e' \quad \Rightarrow \quad \boxed{\bar{k}_h = -\bar{k}_e}$$

④ $\varepsilon_h(\bar{k}_h) = -\varepsilon_e(\bar{k}_e)$



⑤ $\bar{v}_e = \bar{v}_h$

Band velocities

$$\bar{v}_e = \frac{1}{\hbar}\nabla_{k_e}\varepsilon(k_e) = \frac{1}{\hbar}\left(-\nabla_{k_h}\right)\left(-\varepsilon(k_h)\right) = \frac{1}{\hbar}\nabla_{k_h}\varepsilon(k_h) = \bar{v}_h$$

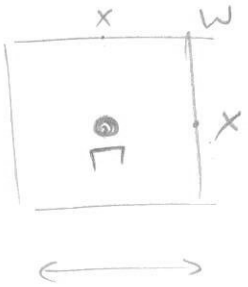
<u>But</u> drift velocities opposite directions

<u>Ohm's law</u>

$$j = \frac{n_h \cdot e^2 \tau}{m_h}\bar{E}$$

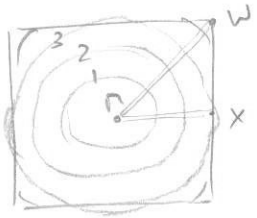
"positive charge carriers"

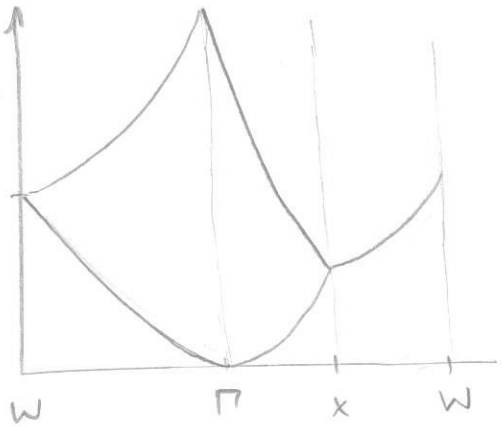
Bandstructures in 2D/3D



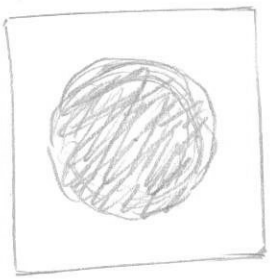
1:st BZ.

E(k)

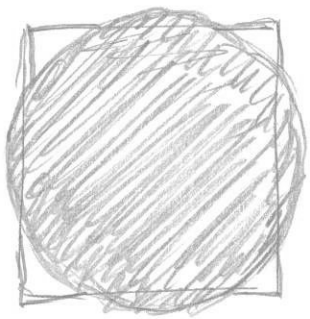




Fermi surface

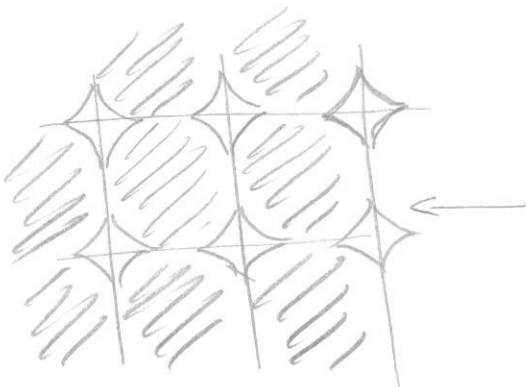


1 el/cell

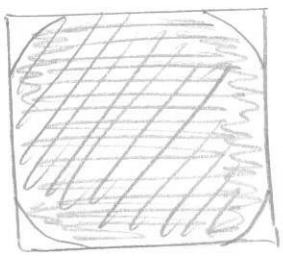


2 el/cell

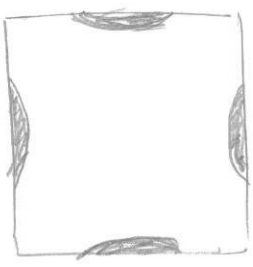
extended zone scheme



1:st band
periodic zone scheme
(shown in smaller scale)

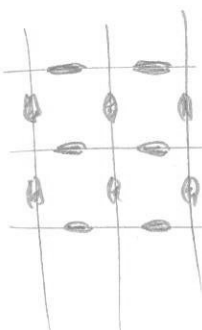


1:st band



2nd band

reduced zone scheme



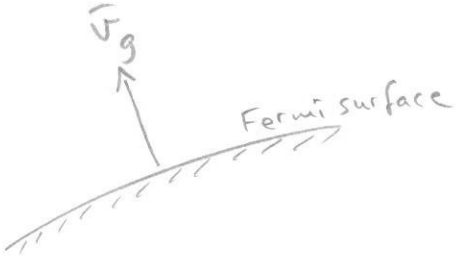
2nd band
periodic
z.s.

Motion of Bloch-electrons in magnetic field

Semiclassical approximation: neglect relaxation

$$\hbar \frac{d\bar{k}}{dt} = -e(\bar{v}_g \times \bar{B}) \qquad \bar{v}_g = \frac{1}{\hbar}\nabla_{\bar{k}}\mathcal{E}$$

$\Longrightarrow$ motion in $\bar{k}$-space is perpendicular to $\bar{B}$ and perpendicular to $\nabla_{\bar{k}}\mathcal{E}$



Ex Electron on Fermi surface

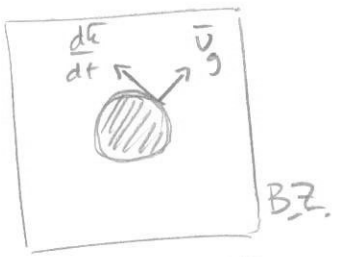
$\nabla_{\bar{k}}\mathcal{E}$ is perpendicular to the Fermi surface

$\Longrightarrow$ $\frac{d\bar{k}}{dt}$ is parallel with the Fermi surface

The electron moves along the Fermi surface, in a plane perpendicular to the magnetic field.

Note: In $\bar{k}$-space

$\odot\ \bar{B}$

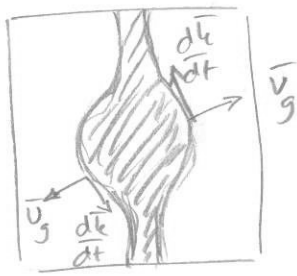


Electron orbit

"negative particles"

Hole orbit

"positive particles"



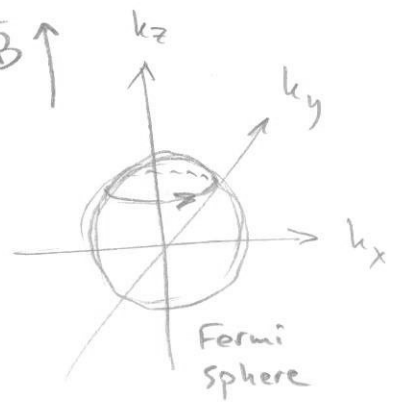
Open orbit

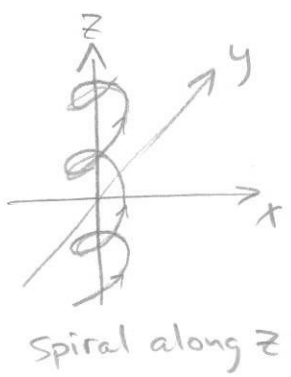
"changing signs"

Real space orbit

$$\frac{d\bar{r}}{dt} = \bar{v}_g(t)$$

Integrate $\bar{v}_g(t) = \frac{1}{\hbar}\nabla_{\bar{k}}\mathcal{E}(\bar{k}(t))$





de Haas - van Alphen effect ~1930

Exp: Measure $M(H)$ magnetization — de Haas - van Alphen

$\Longrightarrow$ Oscillations in M/H as a function of H.
— or better $\frac{\partial M}{\partial H}$

Onsager 1952: very useful!

Conductivity/resistivity shows similar oscillations:
Shubnikov - de Haas effect

Measurement

Pickup-coil around sample

Apply field with timedependence

$$\Rightarrow \underbrace{\frac{dM}{dt}}_{\text{measured}} = \underbrace{\frac{dM}{dH}}_{\text{wanted}} \underbrace{\frac{dH}{dt}}_{\text{applied}}$$

Onsager: (p. 268)

$$\Delta\left(\frac{1}{B}\right) = \frac{e}{\hbar} \cdot \frac{1}{A_e}$$

$\Delta\left(\frac{1}{B}\right)$: period

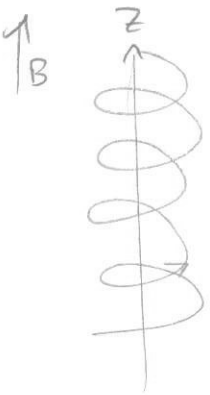
A_e: extremal cross-sectional area of Fermi surface in plane normal to magnetic field

$\Longrightarrow$ Fermi surface probe

Quantummechanical effect:

Bohr-van Leeuwen: No properties of a classical system in thermal equilibrium can depend in any way on the magnetic field

Free electrons, semiclassical motion



$$\hbar \frac{d\bar{k}}{dt} = -e(\bar{v} \times \bar{B})$$

$$\mathcal{E} = \left(n + \frac{1}{2}\right)\hbar\omega_c + \frac{\hbar^2 k_z^2}{2m}$$

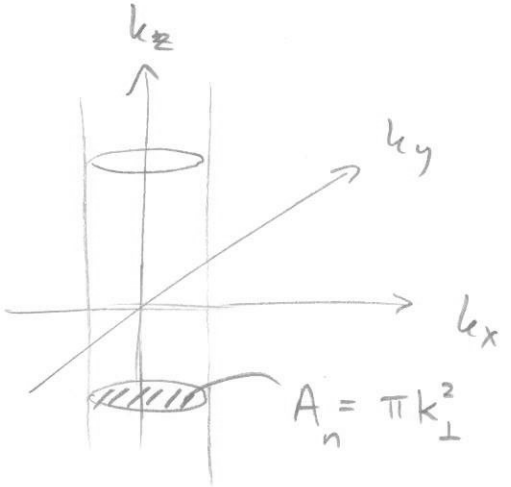
n: $0, 1, 2, \ldots$

$\omega_c = \frac{eB}{m}$ cyclotron frequency

$n \sim \frac{\mathcal{E}_F}{\hbar\omega_c} \sim 10^3 \longleftrightarrow$ well-defined "classical" orbits

$$\frac{\hbar^2 k_\perp^2}{2m} = \left(n + \frac{1}{2}\right)\hbar\omega_c$$

(orbit quantization)



$$A_n = \pi k_\perp^2 = \pi \cdot \frac{2m}{\hbar^2} \cdot \left(n + \frac{1}{2}\right) \cdot \hbar \cdot \frac{eB}{m} =$$

$$= \frac{2\pi \cdot e}{\hbar} \cdot B \cdot \left(n + \frac{1}{2}\right)$$

All levels of certain n are referred to as the nth Landau level

$$A_{n+1} - A_n = \frac{e}{\hbar} \cdot B$$

simplified description

× Level density has sharp peaks whenever $A_n \Longleftrightarrow$ extremal orbits

× Active electrons at Fermi surface

× High numbers n

$$\Delta\left(\frac{1}{B}\right) = \frac{e}{\hbar} \cdot \frac{1}{A_e}$$

A_e: extremal cross-section of Fermi surface

Band structure of selected metals

Alkali metals

[ ] s^1 → Free-electron like, spherical Fermi surface
Half-filled

[ ] = low-lying tight-binding bands (filled)

Noble metals

Cu, Ag: [ ] $d^{10}s^1$ ← additional electrons!

Au: [ ] $f^{14}d^{10}s^1$

[ ] = tightly bound inert core

5 narrow d-bands → d^{10}
filled, 2-5 eV below E_F

s-band → s^1
half-filled

see p. 289

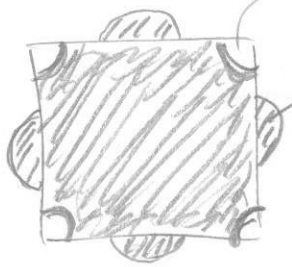
E_F far enough above the d-bands to give Fermi surface similar to free electron band, but close enough to give optical properties

Also: <111> directions touches the B.Z.

Divalent metals

Lower-lying d-bands, less active

Not strong enough potentials to fill 1:st B.Z. completely



Trivalent metals

Al : Fermi surface close to free electron fcc with 3 el/atom

4 zones used, 1:st zone completely filled
4:th basically empty
holes in 2:nd zone
el in 3:rd zone

Tetravalent metals

Sn, Pb

└ Even valence, similar to Al

4:th zone still depressed by potential

$$n_h^{II} = n_e^{III}$$

Semimetals

× Graphite — Almost no band overlap, small pockets Fermi surface

× Pentavalent — Rhombohedral, 2 atom basis

⟹ even number of el/cell

Transition metals

Partially filled d-shell

Properties dominated by d-electrons

d-bands extend through Fermi surface

Narrow d-bands, contain more levels than free el. bands

⟹ density of states much higher

Rare earths

Partially filled f-shell

More localized. 4f-levels not at Fermi surface

Independent el. model breakdown

Work function

Minimum energy required to remove electron from interior of solid to just outside

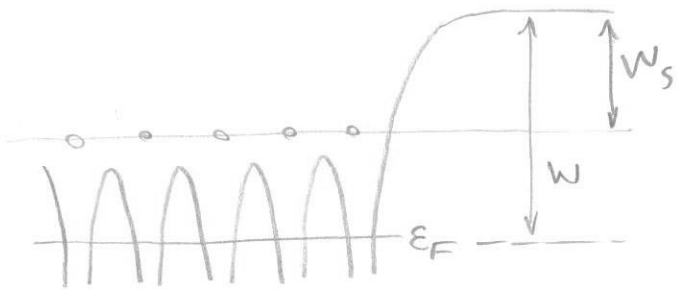
Surface effect

Charge distribution near surface of finite crystal different than in interior

- × Slight displacement of ions
- × Possible surface charge

$$W_s = \int e\bar{E}\cdot d\bar{\ell}$$

Work function $\quad W = -\mathcal{E}_F + W_s$



Metals in electrical contact $\longrightarrow$ el. redistribution $\longrightarrow$

$\longrightarrow$ surface charge so that $\mathcal{E}_F$ the same

(shift of all levels)

$\Longrightarrow$ Potential difference $\phi - \phi' = \frac{1}{e}(W - W')$