Electrons Dynamics and Transport

P715

Electrons Dynamics and Transport

- Now that we understand band theory, we need to fill these bands with electrons! Ignore interactions (!), focus on Pauli exclusion $\longrightarrow$ Fermi sea (c.f. 1d example)
- Goals: Understand insulators vs metals, thermal and electric transport.

I Fermi surfaces (Metals vs insulators)

Reminder: Free e^-, no lattice. Box of size L.

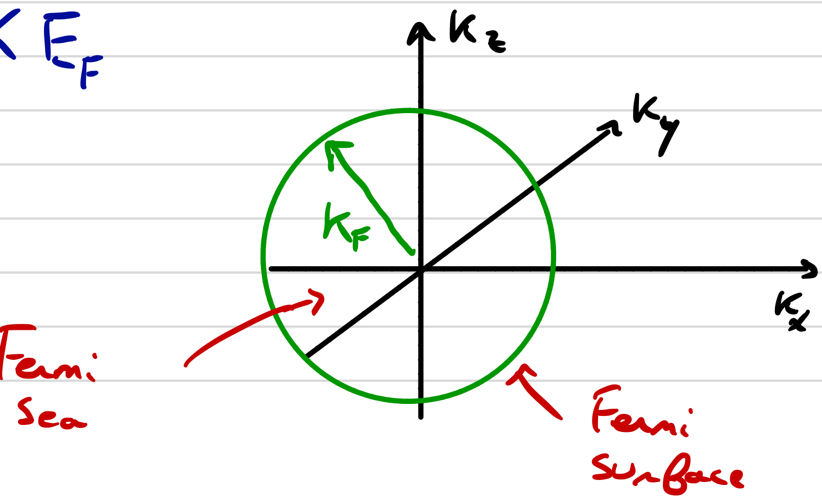
$$E_k = \frac{\hbar^2 \vec{k}^2}{2m}; \qquad k_i = \frac{2\pi}{L} n_i \text{ with } n_i \text{ integer}$$

$i = x, y, z$

$k = 0$ state can absorb $2\,e^-$ (spins $\uparrow$ and $\downarrow$)

then fill energy $E_k < E_F$

$$N = 2L^3 \int_{k<k_F} \frac{d^3k}{2\pi}$$



Recall: • $T_F = E_F / k_B \sim 10^4\,K$ (huge! $T \ll T_K$ always)

• low energy excitations near Fermi surface

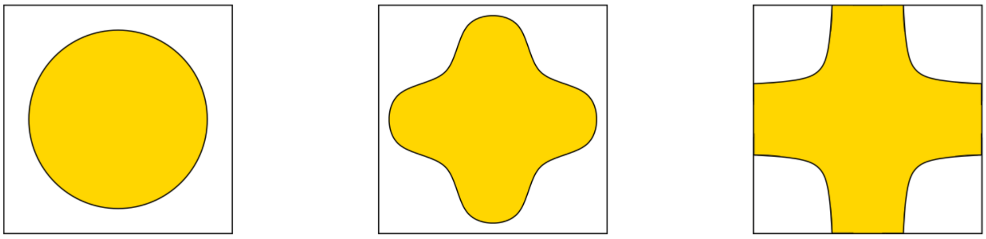
Also: • Energy spectrum given by bands.

N sites in Bravais lattice $\Rightarrow \underbrace{2}_{\text{spins}} N$ states in band

• Each atom on the lattice provides Z valence e^-

Z = 1 (Focus on 2d):

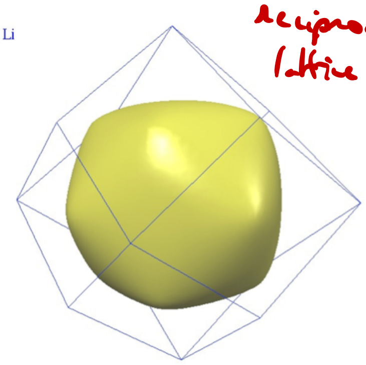
free e^- $\xrightarrow{\text{increase}}$ lattice effects



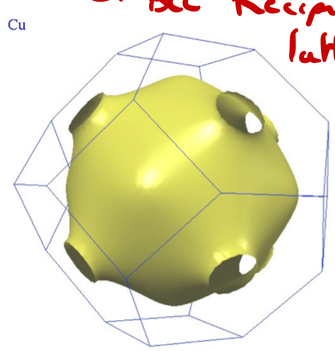
All e^- can easily fit inside the first BZ.

$\Rightarrow$ metal! (gapless excitations)

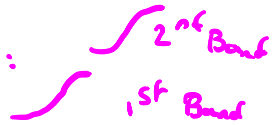
BCC lattice $\Rightarrow$ FCC reciprocal lattice



FCC lattice $\Rightarrow$ BCC Reciprocal lattice



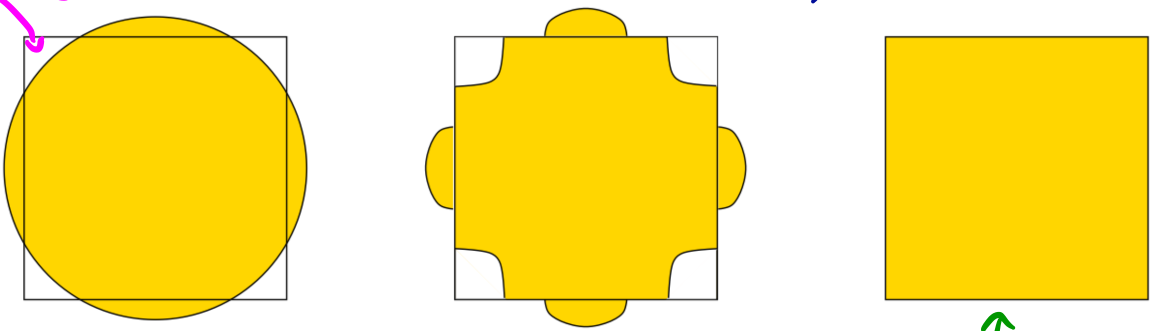
Recall 1d:



$Z=2$: enough e^- to fill the BZ entirely

holes in 1st band

increase lattice perturbation: lowers E of 1st BZ states, increases E of 2nd BZ/band states

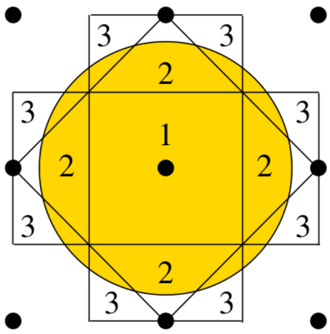


free e^-

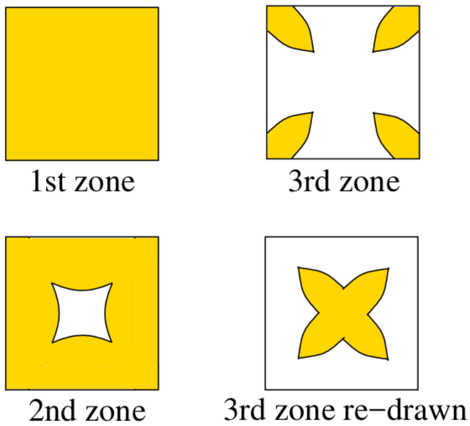
↳ partly fill 1st BZ and start filling 2nd one.

↑ insulator

$Z=3$:



filled "valence" band



Remarks :

- Some $Z=1$ materials are insulators:

  (Mott insulators, Anderson insulators ...)

  ↑ interactions ↑ disorder

- Insulators with band gap $\Delta \lesssim 2-4$ eV start to conduct as T is increased : Semiconductors (technically insulators at $T=0$) Si.

  resistivity ↓ as T ↗

II Dynamics of electrons in periodic potentials = "Bloch electrons"

Consider first a single e^- in a band (later we'll consider a "semiclassical wavepacket").

a) Group velocity

drop band index

We have $\vec{v} = \frac{1}{m} \langle \psi_{\vec{k}} | -i\hbar \vec{\nabla} | \psi_{\vec{k}} \rangle$

with $H|\psi_k\rangle = E_k |\psi_k\rangle$ and $\psi_k(\vec{x}) = e^{i\vec{k}.\vec{x}} u_{\vec{k}}(\vec{x})$

$$-\frac{\hbar^2 \nabla^2}{2m} \psi_k = -\frac{\hbar^2}{2m} \vec{\nabla} \cdot \left(i\vec{k} e^{i\vec{k}.\vec{x}} u_{\vec{k}}(\vec{x}) + e^{i\vec{k}.\vec{x}} \nabla u_k \right)$$

$$= -\frac{\hbar^2}{2m} \left(-k^2 u_k + 2i\vec{k}.\vec{\nabla} u_{\vec{k}} + \nabla^2 u_k \right) \times e^{i\vec{k}.\vec{x}}$$

$$= +\frac{\hbar^2}{2m} e^{i\vec{k}.\vec{x}} (\vec{k} - i\vec{\nabla})^2 u_{\vec{k}}$$

$$\Rightarrow \underbrace{\frac{\hbar^2}{2m} (\vec{k} - i\vec{\nabla})^2 u_{\vec{k}} + V u_{\vec{k}}}_{\hat{H}_{\vec{k}} u_{\vec{k}}} = E_k u_{\vec{k}}$$

Now, consider: $\hat{H}_{\vec{k}+\vec{q}} = \hat{H}_{\vec{k}} + \frac{\partial H_{\vec{k}}}{\partial \vec{k}} \cdot \vec{q} + \dots$

for $\vec{q}$ small

New energy: $E_{\vec{k}+\vec{q}} = E_{\vec{k}} + \frac{\partial E}{\partial \vec{k}} \cdot \vec{q}$

Now use perturbation theory:

$$\Delta E = \underbrace{E_{\vec{k}+\vec{q}} - E_{\vec{k}}}_{\text{exact}} = \langle u_{\vec{k}} | \frac{\partial H}{\partial \vec{k}} \cdot \vec{q} | u_{\vec{k}} \rangle$$

$$= \frac{\partial E_{\vec{k}}}{\partial \vec{k}} \cdot \vec{q}$$

$$\Rightarrow \quad \underbrace{\langle u_{\vec{k}} | \frac{\partial H}{\partial \vec{k}} | u_{\vec{k}} \rangle}_{} = \frac{\partial E_k}{\partial \vec{k}}$$

$$\langle u_{\vec{k}} | \frac{\hbar^2}{m} (\vec{k} - i\vec{\nabla}) | u_{\vec{k}} \rangle = \frac{\hbar}{m} \langle \psi_{\vec{k}} | -i\hbar \vec{\nabla} | \psi_{\vec{k}} \rangle$$

$$= \hbar \vec{v}$$

Therefore: $$\boxed{\vec{v}_{\vec{k}} = \frac{1}{\hbar} \frac{\partial E_k}{\partial \vec{k}}}$$ (group velocity)

(b) Electric and Energy currents

Each e^- contributes a current: $\vec{j} = -e\vec{v}$

Total current density: $$\boxed{\vec{j} = -\frac{2e}{V} \sum_{\vec{k}} \vec{v}_{\vec{k}}} = -\frac{2e}{V} \sum_{\vec{k}} \vec{v}_k n_k$$

Fermi Dirac

spin

occupied states

Full band:

$$\vec{j} = -\frac{2e}{\hbar} \int_{BZ} \frac{d^3\vec{k}}{(2\pi)^3} \frac{\partial E_{\vec{k}}}{\partial \vec{k}} = 0$$

since integral of a total derivative, and $E_{\vec{k}}$ periodic in BZ.

$V = L^3$

Heat current: $\vec{j}_E = \vec{v}\, E$

$$\Rightarrow \boxed{\vec{j}_E = \frac{2}{V} \sum_{\vec{k}} \vec{v}_k\, E_k}$$

occupied modes only $\Rightarrow$ or include factor $n_k = \frac{1}{e^{\beta(E_k - \mu)} + 1}$

Again: filled band: $\vec{j}_E = \frac{2}{\hbar} \int \frac{d^3\vec{k}}{(2\pi)^3} \underbrace{\nabla_{\vec{k}} E_{\vec{k}} \times E_{\vec{k}}}_{\frac{1}{2}\vec{\nabla}_{\vec{k}}(E_k)^2}$

$= 0$

$\Rightarrow$ Filled bands do not carry any current, and can't contribute to transport $\leftarrow$ BUT see Topological bands

(c) Semiclassical equations of motion

Add external force $\vec{F} = -\vec{\nabla} U$: in principle, solve Schrödinger Equation again with potential $V + U$. However, in most cases of interest, where U is small (so band structure is unaffected) and slowly varying (vs lattice scale "a"):

Semiclassics:

$\Delta k \ll 1/a$

$\Delta x \gg a$

$U(\vec{x})$

Wavepacket of plane waves

Well defined $\vec{x}$ and $\hbar\vec{k}$

$\simeq 0$ if $|\vec{q} - \vec{k}| > \Delta k$

$$\phi(\vec{x}, \vec{k}, t) = \sum_{\vec{q}} C_{\vec{q},\vec{k}}\, \psi_{\vec{q}}(\vec{x})\, e^{-i/\hbar E_{\vec{q}} t}$$

Energy : $E_{\vec{k}} + U(\vec{x})$ with $\vec{k}(t)$ and $\vec{x}(t)$

$$\Rightarrow \frac{d}{dt}\left(E_{\vec{k}} + U(\vec{x})\right) = \dot{\vec{k}} \cdot \frac{\partial E}{\partial \vec{k}} + \dot{\vec{x}} \cdot \vec{\nabla} U$$

$$= \vec{v}_{\vec{k}} \cdot \left(\hbar \dot{\vec{k}} + \vec{\nabla} U\right) = 0$$

$$\Rightarrow \boxed{\begin{aligned} \hbar \dot{\vec{k}} &= -\vec{\nabla} U \\ \dot{\vec{x}} &= \frac{1}{\hbar} \vec{\nabla}_{\vec{k}} E_{\vec{k}} \end{aligned}}$$

Semi classical Equations of motion

We have : $\frac{d\vec{v}}{dt} = \frac{1}{\hbar} \frac{d}{dt} \frac{\partial}{\partial \vec{k}} E_{\vec{k}} = \frac{1}{\hbar}\left(\dot{\vec{k}} \cdot \frac{\partial}{\partial \vec{k}}\right) \frac{\partial E}{\partial \vec{k}}$

$\vec{v} = \dot{\vec{x}}$

$$\Rightarrow \ddot{x}_i = \frac{1}{\hbar} \sum_j \frac{\partial^2 E}{\partial k_i \partial k_j} \dot{k}_j$$

Let $$\boxed{\left(\hat{m}_*^{-1}\right)_{ij} = \frac{1}{\hbar^2} \frac{\partial^2 E}{\partial k_i \partial k_j}}$$

$\hat{m}_*$: Effective mass matrix

$= $ inverse of $\frac{1}{\hbar^2} \frac{\partial^2 E}{\partial k_i \partial k_j}$

$$\Rightarrow \ddot{\vec{x}} = \hbar\, \hat{m}_*^{-1} \dot{\vec{k}} \Rightarrow \hat{m}_* \ddot{\vec{x}} = \hbar \dot{\vec{k}} = -\vec{\nabla} U$$

$$\Rightarrow \boxed{\hat{m}_* \ddot{\vec{x}} = -\vec{\nabla} U}$$

"2^{nd} law"

effective mass

Effective Mass

. Isotropic crystal: $(m_*)_{ij} = m_* \delta_{ij}$

with $m_* = \frac{\hbar^2}{\partial_k^2 E_k}$ $\left(\text{if } E_k = \frac{\hbar^2 k^2}{2m} ,\ m_* = m \right)$

. Bottom of the band:

$$E_k = E_{min} + \underbrace{\frac{\partial_k^2 E_k |_{k_{min}}}{2}}_{\frac{\hbar^2}{2m_*}} (k - k_{min})^2 + \ldots$$

. Note that m_* can be infinite (near middle of a band), and can be negative near the top of a band!

→ we'll come back to this later.

m_* can be very ≠ from m_e!

Bloch oscillations : $\vec{E}$ field

$$\hbar \dot{\vec{k}} = -e\vec{E} \quad \Rightarrow \quad \vec{k}(t) = \vec{k}_0 - \frac{e\vec{E}}{\hbar} t$$

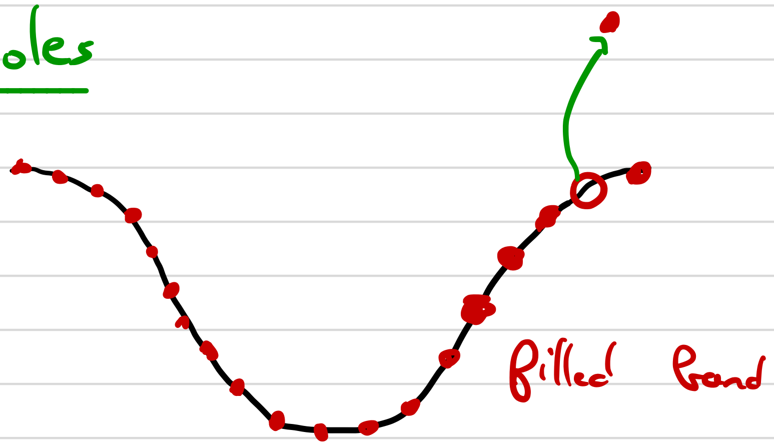
BUT: k periodic!

E.g.: 1d $E_k = -2t \cos ka \Rightarrow v_k = \frac{2ta}{\hbar} \sin ka$

$$v(t) = -\frac{2ta}{\hbar} \sin\left(\underbrace{\frac{eE}{\hbar} a}_{= \omega_{Bloch}} t \right)$$

Hard to observe in real materials, e^- scatter on impurities.

Holes



Near top of the band:

$$E_K = E_{max} + \frac{\hbar^2}{2m_*}|\vec{K}-\vec{K}_{max}|^2$$

with $m_* < 0$

Consider a hole: $\boxed{E_{hole} = -E_K}$ (low energy holes near top of band)

$$= -E_{max} + \frac{\hbar^2}{2m_{hole}}|\vec{K}-\vec{K}_{max}|^2 + \ldots$$

with $\boxed{m_{hole} = -m_*}$

we also take $\vec{K}_{hole} = -\vec{K}$, so $\vec{v}_{hole} = \vec{v}_{e^-} = \vec{v}_K$

If we have $m_* \frac{d\vec{v}}{dt} = -e\vec{E} \Rightarrow m_{hole}\frac{d\vec{v}_{hole}}{dt} = +e\vec{E}$

opposite charge!

Because a full band carries no current, we have:

$$\vec{j} = -2e\int_{\text{filled}} \frac{d^3\vec{K}}{(2\pi)^3} v_{\vec{K}} = +2e\int_{\text{unfilled}} \frac{d^3\vec{K}}{(2\pi)^3} \vec{v}_K$$

Drude model again : $m \to m_*$: $\sigma = \frac{e^2 \tau n}{m_*}$

But in some cases, dominant charge carriers are holes:
opposite sign of Hall coefficients $\left(\rho_{xy} = \frac{B}{ne} , R_H = \frac{\rho_{xy}}{B} = \frac{1}{ne} \right)$

(III) Motion of Bloch electrons in a magnetic field

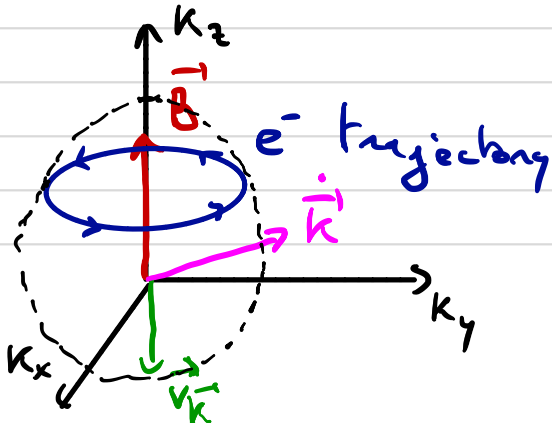
We have :
$$\boxed{\begin{aligned} \dot{\vec{x}} &= \vec{v}_k = \frac{1}{\hbar} \frac{\partial E_{\vec{k}}}{\partial \vec{k}} \\ \hbar \dot{\vec{k}} &= -e \, \vec{v}_k \times \vec{B} \end{aligned}}$$

Constants of motion:

$\vec{k} \cdot \vec{B}$: $\frac{d}{dt}(\vec{k} \cdot \vec{B}) = \dot{\vec{k}} \cdot \vec{B} = -e(\vec{v}_{\vec{k}} \times \vec{B}) \cdot \vec{B} = 0$

$E_{\vec{k}}$: $\frac{d}{dt} E_{\vec{k}} = \frac{\partial E_{\vec{k}}}{\partial \vec{k}} \cdot \dot{\vec{k}} = -e \, \vec{v}_{\vec{k}} \cdot (\vec{v}_{\vec{k}} \times \vec{B}) = 0$

$\vec{k}$ space e^- - orbits: intersection of constant energy surfaces with planes $\perp$ to $\vec{B}$: $\vec{B} = B \vec{e}_z \Rightarrow k_z = \text{constant}$



$\vec{v}_k = \frac{1}{\hbar} \frac{\partial E_{\vec{k}}}{\partial \vec{k}}$: points from low to high energies

e^- orbit the Fermi surface (constant energy)

$$\hat{B} = \frac{\vec{B}}{\|\vec{B}\|} = \vec{e_z}$$

<u>Real Space</u>: $\vec{x}_\perp = \vec{x} - (\hat{B}.\vec{x})\hat{B}$

$= \vec{x} - z\vec{e_z}$ (projection of $\vec{x}$ on plane $\perp$ to $\vec{B}$: (xy))

$$\Rightarrow \underbrace{\hat{B}}_{\vec{e_z}} \times \hbar\dot{\vec{k}} = -eB\,\hat{B}\times(\vec{v_k}\times\hat{B})$$

$$= -eB\left(\vec{v_k} - \hat{B}\,(\hat{B}.\vec{v_k})\right)$$

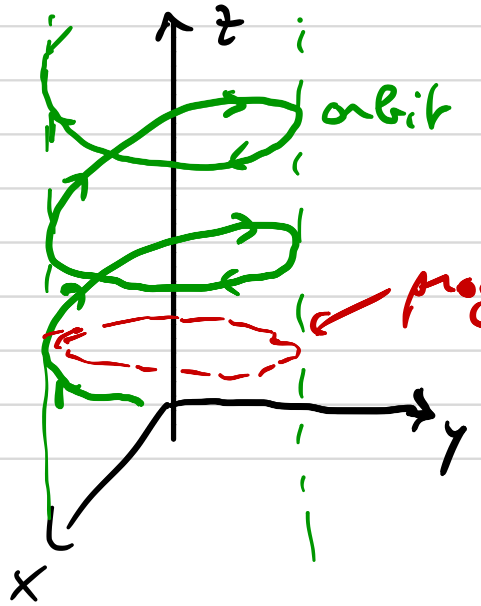
$$= -eB\,(\dot{\vec{x}} - \dot{z}\,\vec{e_z}) = -eB\,\dot{\vec{x}}_\perp$$

$$\Rightarrow \boxed{\vec{x}_\perp(t) - \vec{x}_\perp(0) = -\underbrace{\frac{\hbar}{eB}}_{\rho_B^2 = \text{magnetic length}}\vec{e_z}\times(\vec{k}(t) - \vec{k}(0))}$$

Real space orbit has projection of (xy) plane ($\perp$ to $\vec{B}$)

= $\vec{k}$ space orbit, rotated by 90° about $\vec{B}$, rescaled by ρ_B^2

For free e^-: recover helix (circles in xy plane)

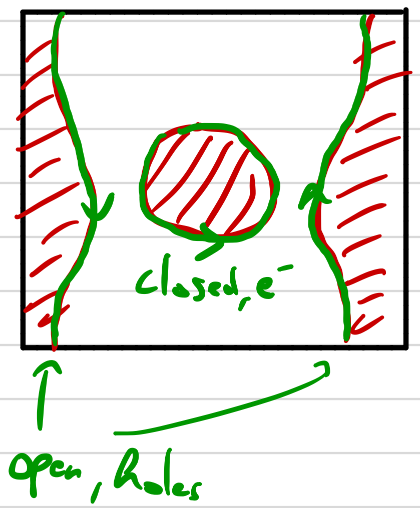


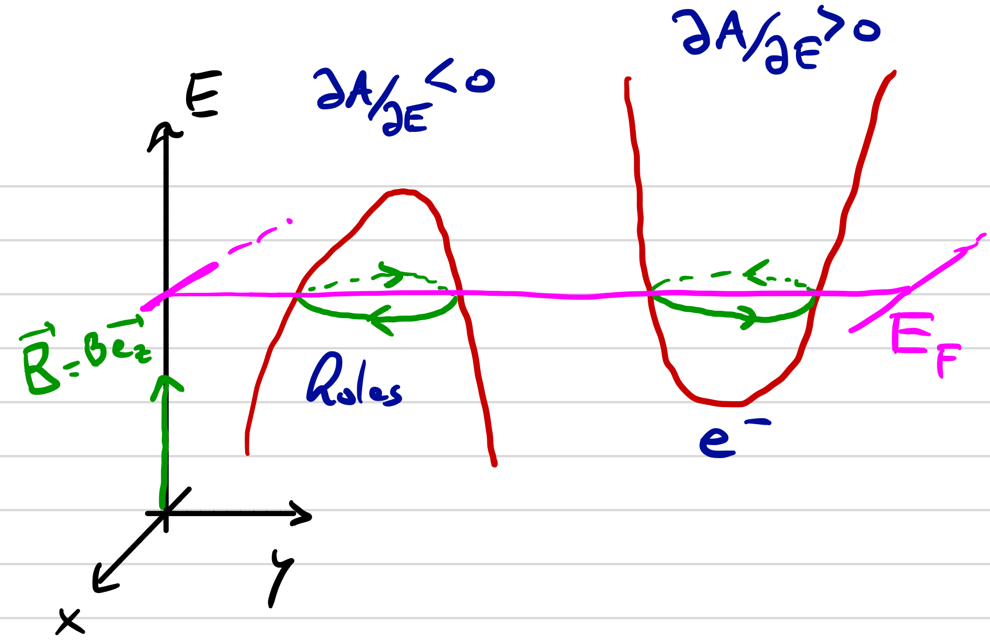
In general, not circles.

Need not be closed!

"Open Fermi surfaces"

Orbits extend into other zones (wrap around first BZ)





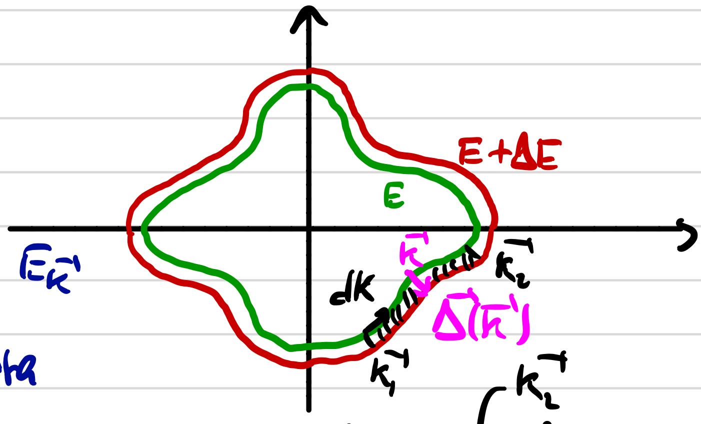
<u>Cyclotron frequency</u> : $t_2 - t_1 = \int_1^2 dt = \int_{\vec{k}_1}^{\vec{k}_2} \frac{d\vec{k}}{|\dot{\vec{k}}|}$ (time to go from 1 → 2)

$$|\dot{\vec{k}}| = \left| -\frac{e}{\hbar^2} \frac{\partial E_{\vec{k}}}{\partial \vec{k}} \times \vec{B} \right| = \frac{eB}{\hbar^2} \left| \frac{\partial E_{\vec{k}}}{\partial \vec{k}} \right|_{\perp}$$

(xy), $\perp$ to $\vec{B}$

$$\Rightarrow \Delta t = t_2 - t_1 = \frac{\hbar^2}{eB} \int_{\vec{k}_1}^{\vec{k}_2} \frac{d\vec{k}}{\left|\frac{\partial E}{\partial \vec{k}}\right|_{\perp}}$$

Geometric interpretation :



$\vec{\Delta}(\vec{k})$: Normal to orbit with energy $E_{\vec{k}}$ connecting it to orbit with energy $E_{\vec{k}} + \Delta E$

$$A_{12} = \int_{\vec{k}_1}^{\vec{k}_2} \Delta(k)\, dk$$

$$\Delta E = \left(\frac{\partial E}{\partial \vec{k}}\right)_{\perp} \cdot \vec{\Delta}(\vec{k})$$

parallel to $\vec{\Delta}(\vec{k})$

$\perp$ to constant energy surfaces, so $\perp$ to orbits

$$\Rightarrow \quad \Delta E = \left|\frac{\partial E}{\partial \vec{k}}\right|_{\perp} \Delta(\vec{k})$$

$A_{1,2}$: area of strip that separates the two orbits

So we find: $$t_2 - t_1 = \frac{\hbar^2}{eB}\,\frac{1}{\Delta E}\int_{\vec{k}_1}^{\vec{k}_2} \Delta(\vec{k})\,dk$$

as $\Delta E \to 0$:

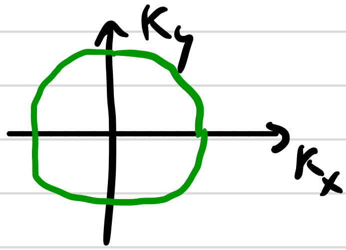
$$\boxed{t_2 - t_1 = \frac{\hbar^2}{eB}\,\frac{\partial A_{1,2}}{\partial E}} \quad \xrightarrow[\text{orbit}]{\text{closed}} \quad \boxed{T = \frac{\hbar^2}{eB}\,\frac{\partial A}{\partial E}}$$

area enclosed by orbit, depends on E, k_z

cyclotron frequency: $\omega_c = \frac{2\pi}{T}$. Free e^-: $E = \frac{\hbar^2 k^2}{2m}$

$$\vec{v}_k = \frac{1}{m}\vec{k}$$

Fermi surface: $E_F = \frac{\hbar^2 k_F^2}{2m}$



orbit: circle of radius:

$$E = E_F = \frac{\hbar^2}{2m}\left(R^2 + \underbrace{k_z^2}_{\text{fixed}}\right)$$

$$A = \pi R^2 = \frac{2\pi m E}{\hbar^2} - \pi k_z^2 \quad \Rightarrow \quad \frac{\partial A}{\partial E} = \frac{2\pi m}{\hbar^2}$$

$$\Rightarrow T = \frac{2\pi m}{eB} \Rightarrow \boxed{\omega_c = \frac{eB}{m}}$$

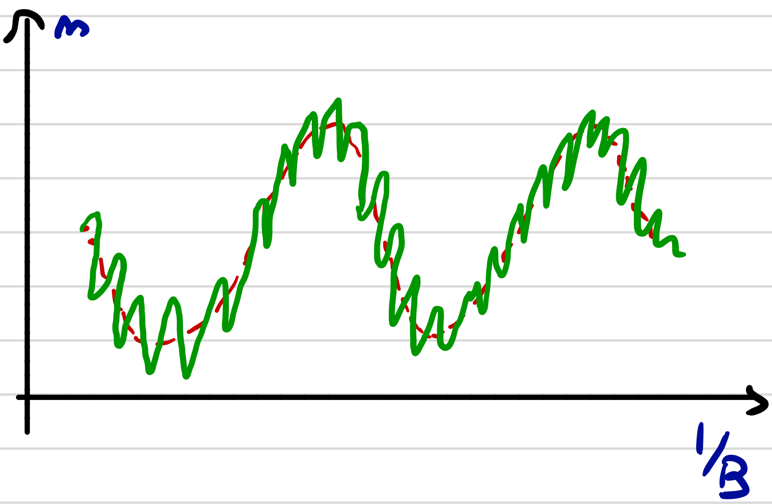
can be used to "map out" Fermi surfaces, see below!

Quantum Oscillations

How do we determine the shape of the Fermi surface (FS) of a metal? Apply B field, various quantities oscillate with B

$\Rightarrow$ can be used to map out the FS!

"de Haas - van Alphen effect": oscillations of magnetization vs applied field



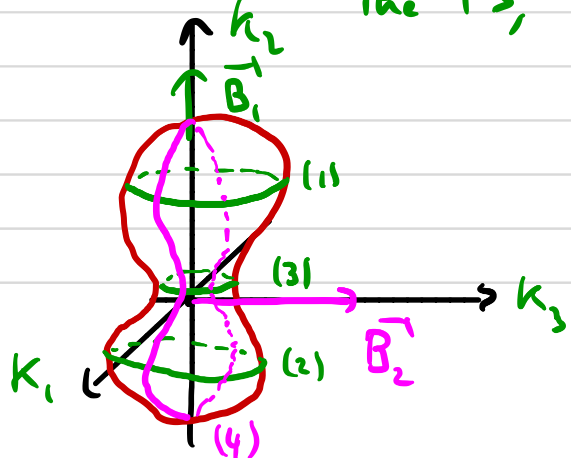
Shubnikov - de Haas effect: Similar oscillation in conductivity

$$\boxed{\Delta\left(\frac{1}{B}\right) = \frac{2\pi e}{\hbar}\,\frac{1}{A_e}}$$

← we'll show this below

period of oscillations

any extremal cross section area of the FS, in plane $\perp$ to $\vec{B}$



$\vec{B}_1$: (1), (2): maximal
(3): minimal

$\vec{B}_2$: (4): maximal

By changing the orientation of $\vec{B}$, we can map out the FS!

Why? Need QM: $\vec{B}$ field + e^- on a lattice

Landau levels (field) — bands (lattice)

free space: $E_n = \frac{\hbar^2}{2m} k_z^2 + \left(n+\frac{1}{2}\right)\hbar\omega_c$, $\omega_c = \frac{eB}{m}$

$L \times L \times L$ cube, $k_z = \frac{2\pi}{L} n_z$

. degeneracy: $\frac{2e}{\hbar} B L^2 \longrightarrow \sim 10^{10}$ states for $L \sim 1\,\text{cm}$, $B \sim 0.1\,\text{T}$

How is this modified by lattice? $\Rightarrow$ Onsager

(Approx only at semiclassical level: large n

OK: $E_F / \hbar\omega_c \sim 10^4$ for typical fields) $B \sim 1\text{T}$

Bohr's correspondence principle: $E_{n+1} - E_n = \frac{\hbar}{T(E_n, k_z)}$

quantization of semiclassical orbits

T: period of semiclassical orbits

$\Leftrightarrow \quad E_n \underset{n \gg 1}{\simeq} \hbar\omega_c n$, $\omega_c = 2\pi / T$

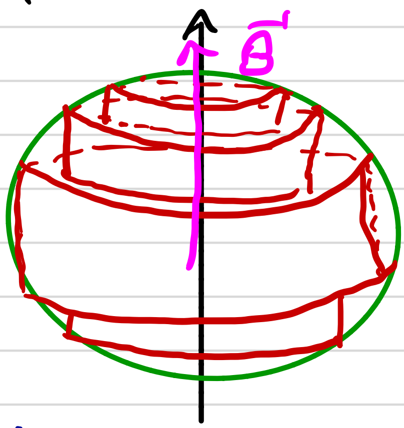
Now, we have: $T = \frac{\hbar^2}{eB} \frac{\partial A}{\partial E}$

$$\Rightarrow \quad \underbrace{\left(E_{n+1} - E_n\right) \frac{\partial A}{\partial E}}_{\simeq A_{n+1} - A_n} = \frac{2\pi e B}{\hbar}$$

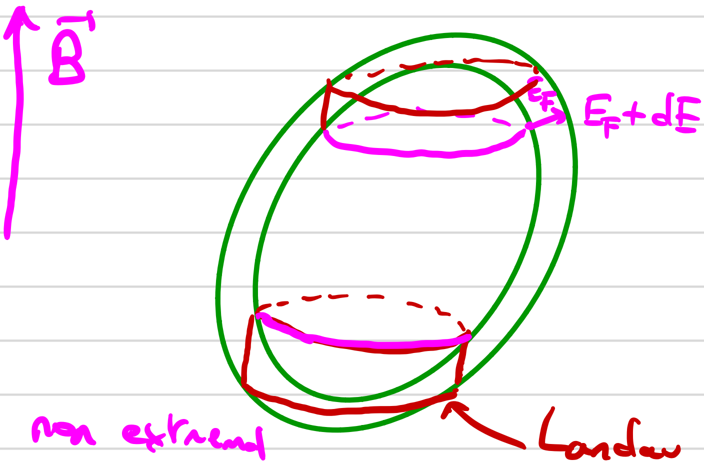
$\left(E_{n+1} - E_n \sim \hbar\omega_c \ll E_F \right)$

Classical orbits at adjacent allowed (quantized) energies and same k_z differ by : $\Delta A = \frac{2\pi e B}{\hbar}$

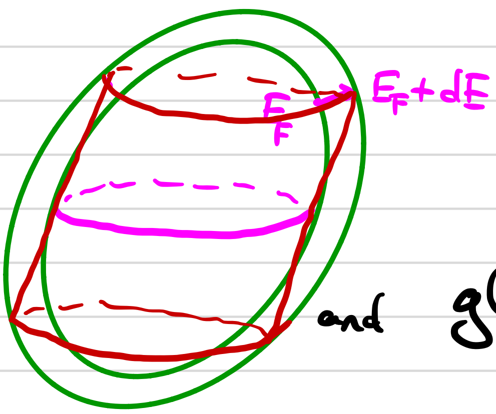
$$\Rightarrow \quad A_n \underset{n \gg 1}{\simeq} n \frac{2\pi e B}{\hbar}$$



Fermi surface is re-arranged into "Landau tubes" whose area is quantized



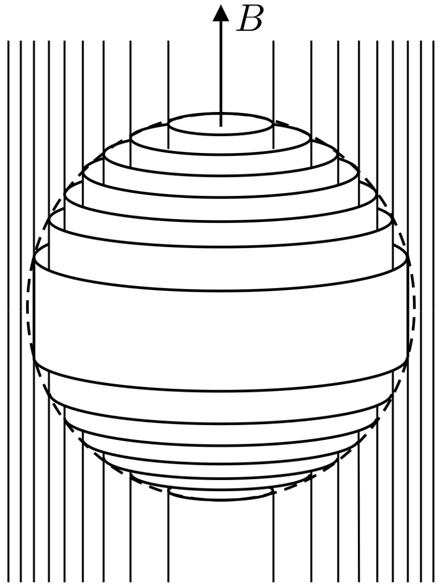
Density of states small
$g(E_F)dE$

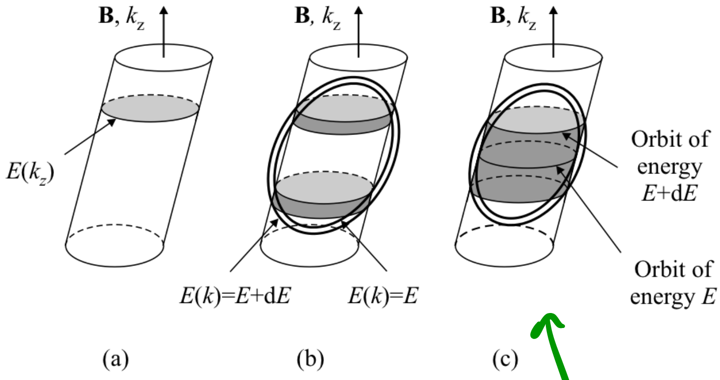


$\rightarrow$ effectively 1d, $g(E) \sim 1/\sqrt{E-E_*}$

$\Rightarrow$ enhanced d.o.s.

and $g(E_F)$ enters all physical quantities!





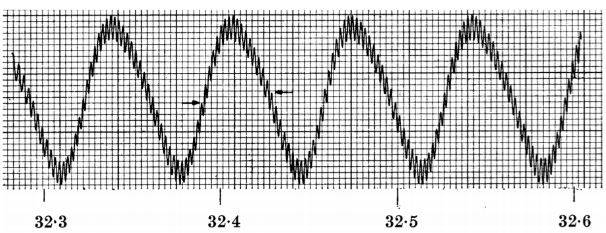
Landau tubes

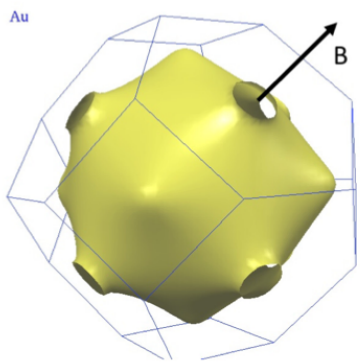
enhanced dos! for extremal orbits

$\Rightarrow$ enhanced (diverging!) d.o.s. for $A_n = \frac{2\pi e B}{\hbar} n + \ldots = A_e$

extremal

$$\Rightarrow \boxed{\Delta\left(\frac{1}{B}\right) = \frac{2\pi e}{\hbar} \frac{1}{A_e}}$$





quantum oscillations for gold