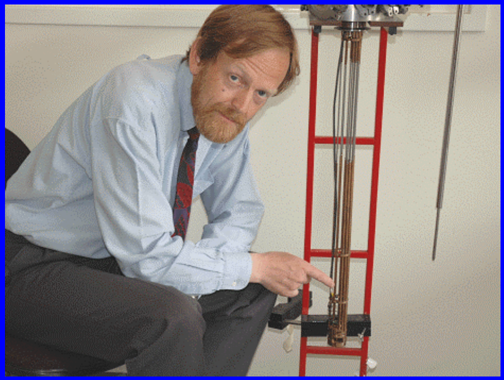
UvA-VU Master Course: Advanced Solid State Physics

Contents in 2005:

- Diffraction from periodic structures (week 6, AdV)
- Electronic band structure of solids (week 7, AdV)
- **Motion of electrons and transport phenomena (week 8, AdV)**
- Superconductivity (week 9&10, RW)
- Magnetism (week 11&12,JB)

Anne de Visser



Rinke Wijngaarden

Jürgen Buschow

Literature, software and homework

The course is based on the book:

H. Ibach and H. Lüth: Solid State Physics

3rd edition (Springer-Verlag, Berlin, 2003)

ISBN 3-540-43870-X

See also:

N.W. Ashcroft and N.D. Mermin: Solid State Physics

(Saunders College Publ.)

ISBN 0-03-083993-9

Computer simulations form an essential part of the course:

R.H. Silsbee and J. Dräger:

Simulations for Solid State Physics

(Cambridge University Press, Cambridge 1997)

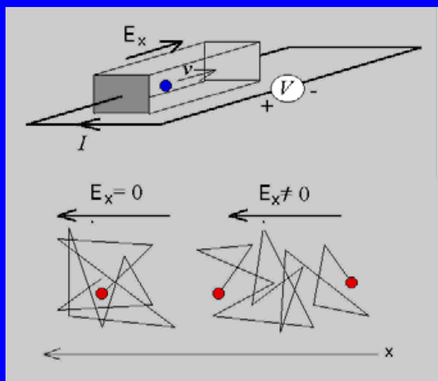
ISBN 0-521-59911-3

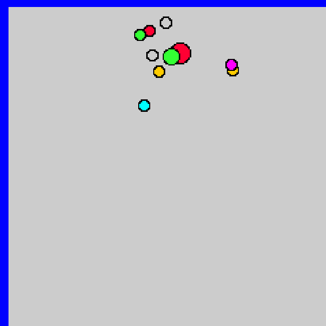
Software (freeware): www.physics.cornell.edu/sss/

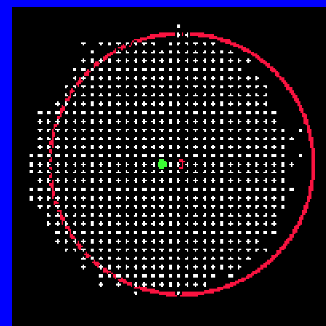
Homework exercises will be distributed throughout the course

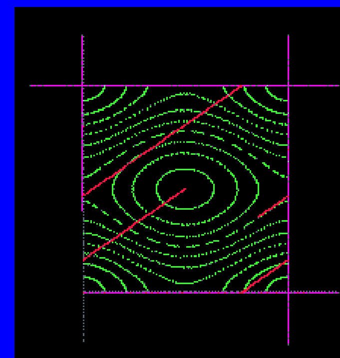
Completing the course gives 6 ECTS $\rightarrow$ ~ 6 x 28 hours

Course 3: Motions of electrons and transport phenomena



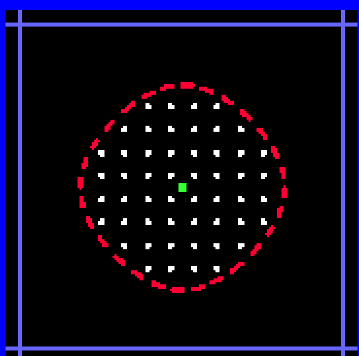


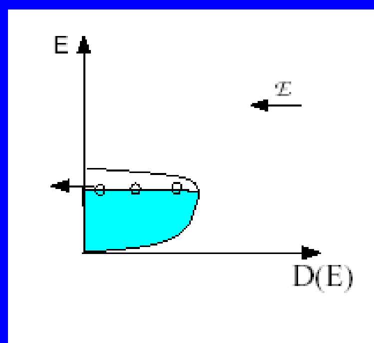


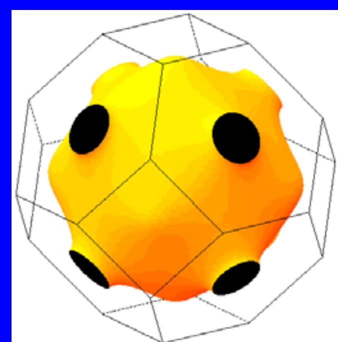


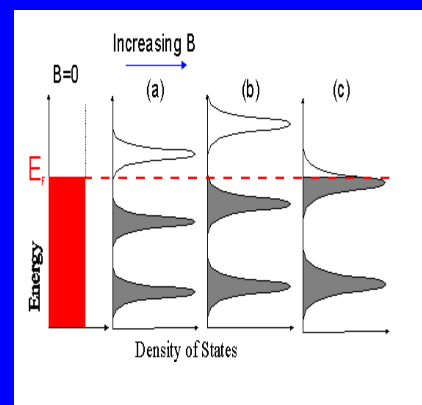
$$\sigma = \frac{ne^2\tau}{m}$$

$$\left(\frac{1}{m^*}\right)_{ij} = \frac{1}{\hbar^2}\sum_j \frac{\partial^2 E(\vec{k})}{\partial k_i \partial k_j}$$









Pictures are taken from the Solid State Course by Mark Jarrel (Cincinnati University), from Ibach and Lüth, from Ashcroft and Mermin and from several sources on the web.

Course 3: Motions of electrons and transport phenomena

- Equation of motion of electrons
- Drude and Sommerfeld models for conductivity
- Crystal momentum is not momentum!
- Motion of electrons in bands and the effective mass tensor
- Currents in bands and holes
- Scattering of electrons in bands
- Electrical conductivity of metals
- Quantum oscillations and the topology of Fermi surfaces
- Quantum Hall effect

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Equation of motion of electrons

Classical equation of motion in **E** and **B** field:

$$\vec{F} = m\frac{d\vec{v}}{dt} = -e\left(\vec{E} + \vec{v}\times\vec{B}\right)$$ without collisions

$$v \sim e^{-t/\tau}$$

v decays exponentially

relaxation time τ

$$\vec{F} = m\left(\frac{d\vec{v}}{dt} + \frac{\vec{v}}{\tau}\right) = -e\left(\vec{E} + \vec{v}\times\vec{B}\right)$$ with collisions

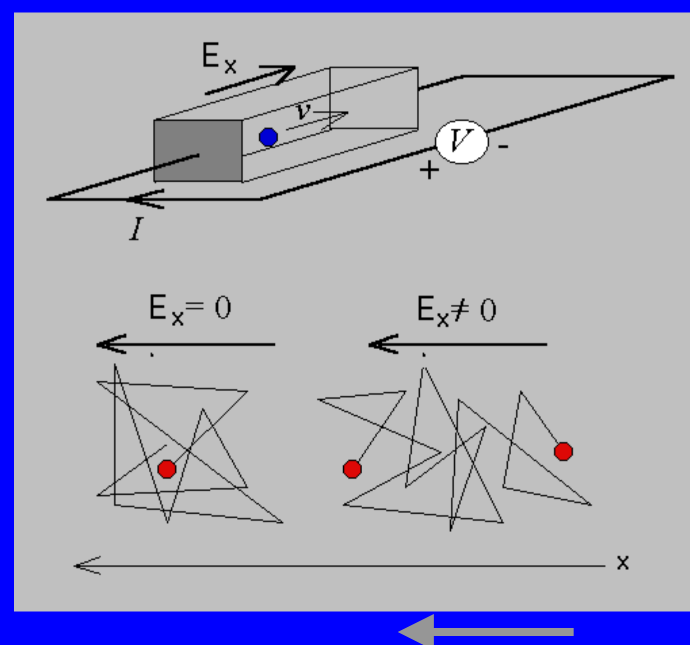
= 0

- steady-state average velocity

$$\vec{v} \equiv \vec{v}_{av} = -\frac{e\vec{E}\tau}{m}$$

- current density

$$\vec{j} = -ne\vec{v}_{av} = -ne\left(-\frac{e\vec{E}\tau}{m}\right)$$



v_{av}

Drude model for conductivity

Classical model: dilute gas of electrons

- neglect interactions with other electrons and ions between collisions
  - independent electron approximation
  - free electron approximation
- collisions probability $1/\tau$ (time between collisions τ)
- thermal equilibrium through collisions

Paul Drude (1863-1906)

- Maxwell-Boltzmann velocity distribution
- equipartition of energy $1/2\ m v_T^2 = 3/2\ k_B T$

$$\vec{j} = -ne\vec{v}_{av} = -ne\left(-\frac{e\vec{E}\tau}{m}\right) = \frac{ne^2\tau}{m}\vec{E}$$

$$\vec{j} = \sigma\,\vec{E} = \rho^{-1}\vec{E}$$

ρ = resistivity
σ = conductivity

$$\sigma = \frac{ne^2\tau}{m}$$

electron transport with $v_{av} = v_D$ = drift velocity

$\tau \sim 10^{-14} - 10^{-15}$ s, $v_T \sim 10^5$ m/s
mean free path $\ell = v_T\tau$ = 1-10 Å

Important failure Drude: mean free path ℓ can be >> interatomic distance

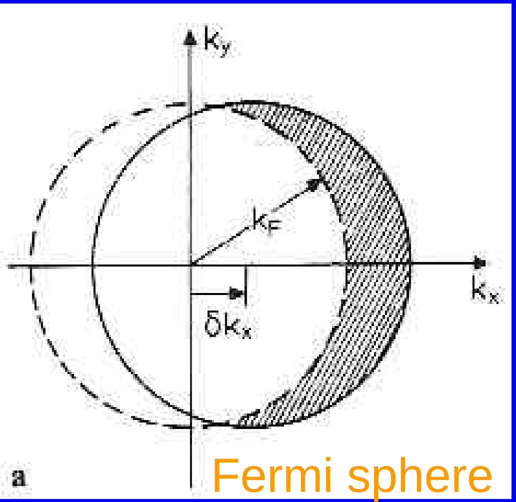
Sommerfeld model for conductivity

- Quantum mechanical description

$$\psi = \frac{1}{\sqrt{V}} e^{i\vec{k}\cdot\vec{r}}$$

Fermi velocity → $$\vec{v}_F = \frac{\hbar \vec{k}_F}{m}$$

Fermi energy → $$E_F = \frac{\hbar^2 |\vec{k}_F|^2}{2m}$$



- Fermi-Dirac velocity distribution
- Semi classical energy gain electrons

$$\delta E = -e\vec{E}\cdot\vec{v}\,\delta t$$
$$\delta E = \vec{\nabla}_k E(\vec{k})\cdot\delta\vec{k} = \hbar\,\vec{v}\cdot\delta\vec{k}$$
$$\hbar\frac{d\vec{k}}{dt} = -e\vec{E}$$

$$\vec{v} = \frac{1}{\hbar}\vec{\nabla}_k E(k) = \frac{\hbar}{m}\vec{k}$$

free electrons only!

"drift k"

displaced in k space

stationary state $$\delta k_x = -\frac{e\tau}{\hbar}E_x$$

- EOM $$\vec{F} = \hbar\frac{d\vec{k}}{dt} = m\frac{d\vec{v}}{dt} = -e\left(\vec{E} + \vec{v}\times\vec{B}\right)$$

- $$\vec{j} = -ne\vec{v}_{av} = \frac{ne^2\tau}{m}\vec{E}$$ $$\sigma = \frac{ne^2\tau}{m}$$

Like Drude!

mean free: $\ell = v_F\tau$ (use Fermi velocity!)
example copper: $v_F = 1.6\mathrm{x}10^6$ m/s
$\tau \sim 2\mathrm{x}10^{-9}$ at 4K → $\ell_{4K} = 3\mathrm{x}10^{-3}$ m
$\tau \sim 2\mathrm{x}10^{-14}$ at 300K → $\ell_{300K} = 3\mathrm{x}10^{-8}$ m

Sommerfeld works also at low T!

Intermezzo: Crystal momentum is not momentum!

- Free electron with energy ε_k in state ψ_k

$$H\psi_k = \varepsilon_k \psi_k \;\; ; \;\; H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}$$

$$\psi_k = \frac{1}{\sqrt{L}} e^{ikx} \;\; ; \;\; \varepsilon_k = \frac{\hbar^2 k^2}{2m}$$

Momentum expectation value free electrons

$$p_k = \left\langle \psi_k \left| -i\hbar \frac{d}{dx} \right| \psi_k \right\rangle = \int \frac{1}{\sqrt{L}} e^{-ikx} \left(-i\hbar \frac{d}{dx} \right) \frac{1}{\sqrt{L}} e^{ikx} dx = \hbar k$$

- Bloch electrons

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)$$

$$\psi_k(x) = u_k(x) e^{ikx}$$

$$p_k = \int u_k^*(x) e^{-ikx} u_k^*(x) \left(-i\hbar \frac{d}{dx} \right) u_k(x) e^{ikx} dx$$

$$= \hbar k - i\hbar \int u_k^*(x) \frac{du_k}{dx} dx \neq \hbar k$$

real momentum

crystal momentum

Motion of electrons in bands and effective mass tensor

- the real world: electron state is wave packet

$$\psi(x,t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} U(k) e^{i(kx-\omega(k)t)} d\vec{k}$$

delocalized

$$U(k) = const.\delta(k-k_0) \rightarrow \psi(x,t) \propto e^{i(k_0 x - \omega t)}$$

$$U(k) = const. \rightarrow \psi(x,t) \propto \delta(x)$$

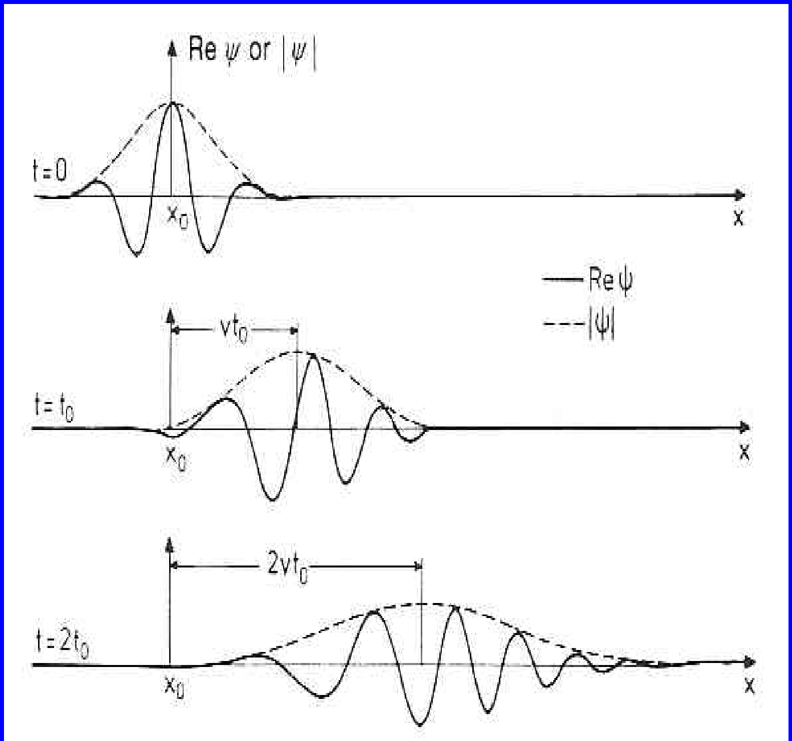
localized

- group velocity and dispersion

$$v = \frac{\partial \omega}{\partial k} \quad ; \quad \omega = c(k)k$$

- velocity of crystal electron depends on dispersion E(**k**)

$$\vec{v} = \vec{\nabla}_k \omega(\vec{k}) = \frac{1}{\hbar}\vec{\nabla}_k E(\vec{k})$$



free electrons:

E= $\hbar^2 k^2/2m$

v = **k**$\hbar$/m = **p**/m

Velocity of crystal electron

Example:
tight binding dispersion relation

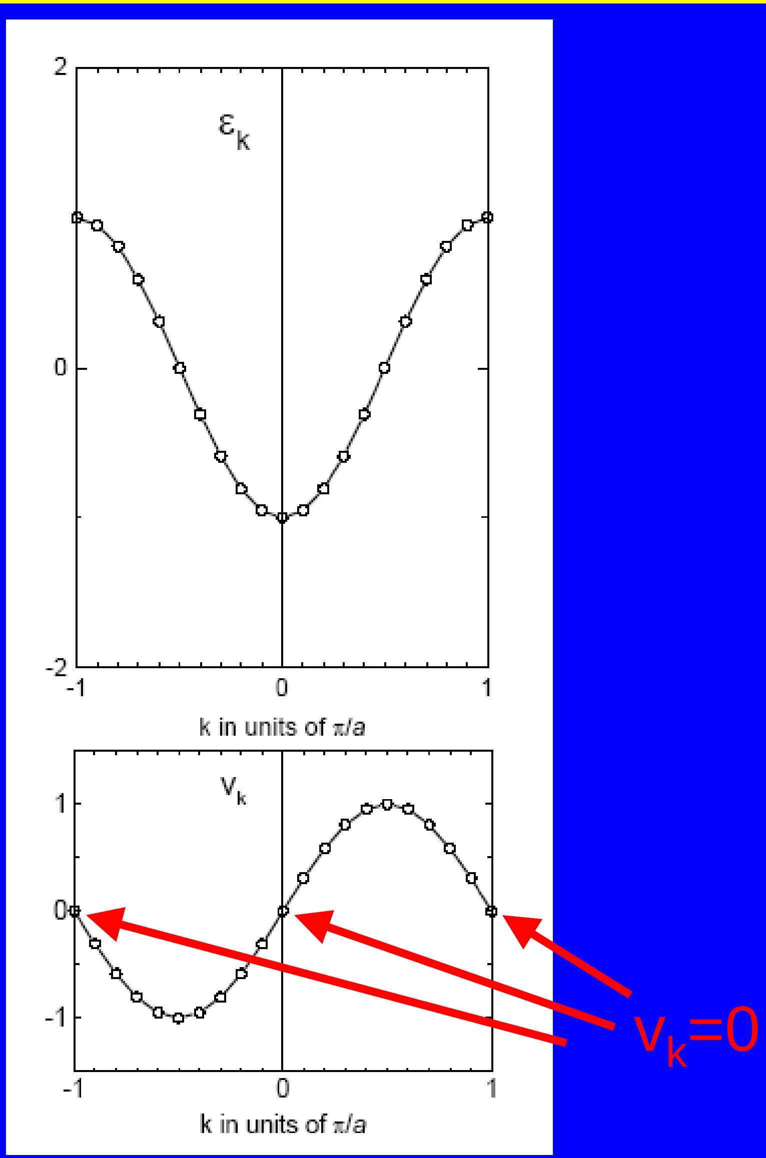
$$\varepsilon_k = E_{at} + A + 2B\cos(ka)$$

velocity

$$\vec{v}_k = \frac{1}{\hbar}\vec{\nabla}_k E(\vec{k})$$

$$\Rightarrow \quad v_k = -2Ba\sin(ka)$$

velocity is constant at fixed k
very different from classical picture



Semi classical eq. of motion in electric field

- rate of change of group velocity component

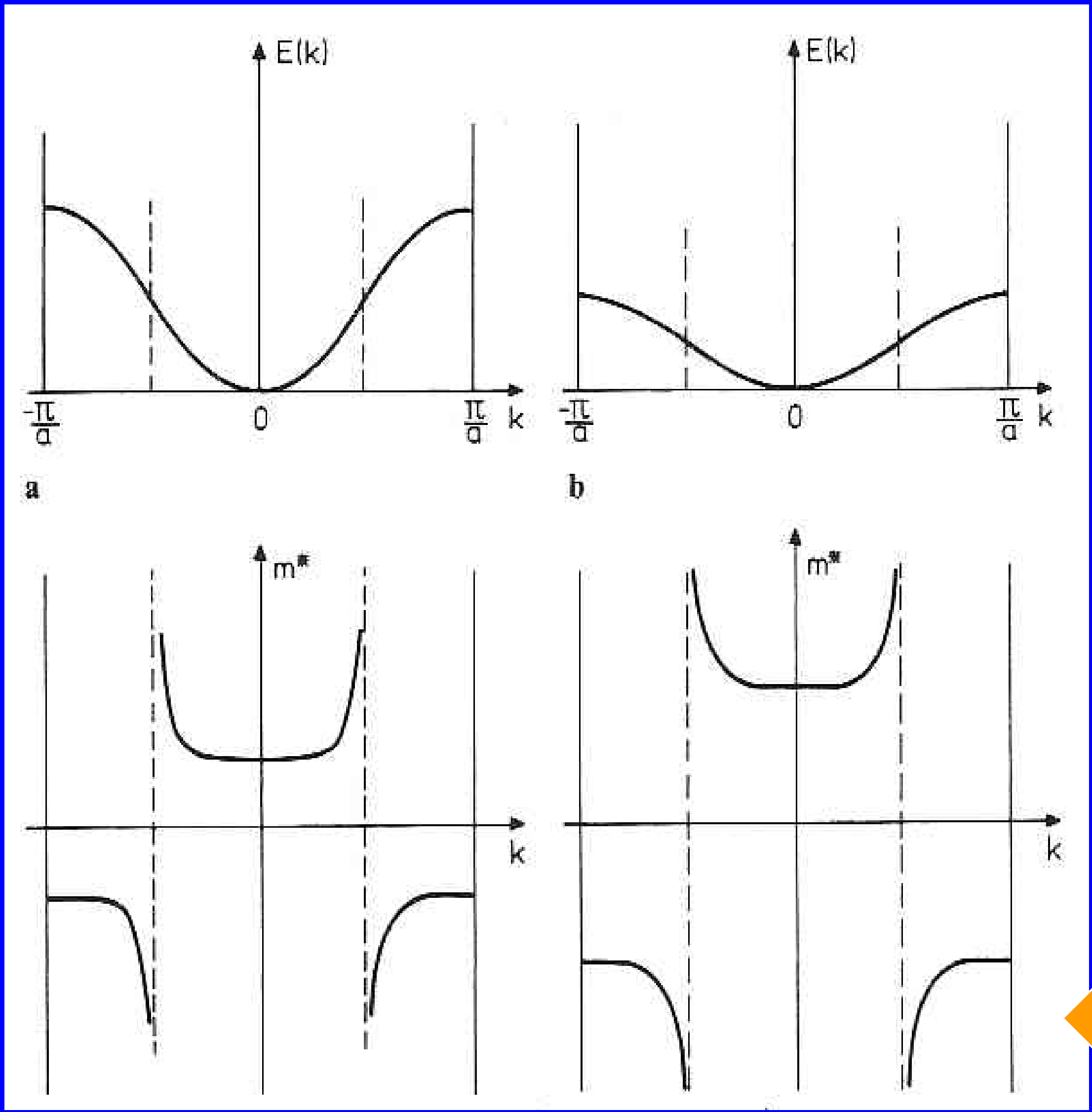
$$\dot{v}_i = \frac{1}{\hbar}\frac{d}{dt}\left(\vec{\nabla}_k E\right)_i = \frac{1}{\hbar}\sum_j \frac{\partial^2 E}{\partial k_i \partial k_j}\dot{k}_j$$

with $\dot{k}_j = -\frac{e}{\hbar}E_j$ $\rightarrow$ $\dot{v}_i = \frac{1}{\hbar^2}\sum_j \frac{\partial^2 E}{\partial k_i \partial k_j}\left(-eE_j\right)$

- effective mass tensor (inverse) $\left(\frac{1}{m^*}\right)_{ij} = \frac{1}{\hbar^2}\sum_j \frac{\partial^2 E(\vec{k})}{\partial k_i \partial k_j}$

- eq. of motion

$$\dot{v}_i = \left(\frac{1}{m^*}\right)_{ij}\left(-eE_j\right)$$



Effective mass

2nd derivative

$$m^* = \frac{\hbar^2}{d^2E/dk^2}$$

flatter band
→ higher m*

$$dv/dk > 0 \rightarrow m^* > 0$$
$$dv/dk < 0 \rightarrow m^* < 0$$

Negative effective mass !

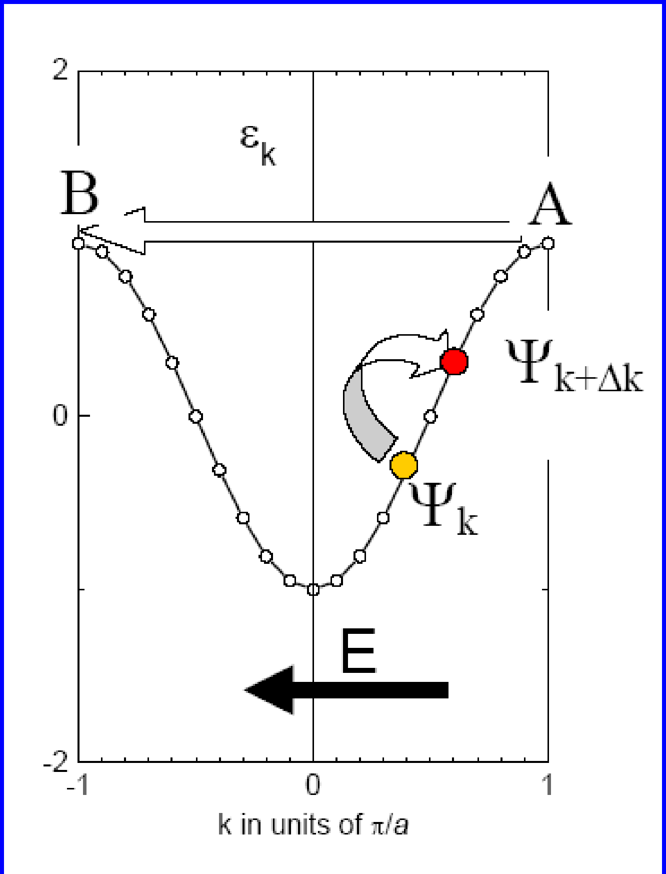
effective mass approximation
m* constant when

$$E(\vec{k}) = E_0 + \frac{\hbar^2}{2m^*}(k_x^2 + k_y^2 + k_z^2)$$

Crystal (Bloch) electron in electric field

Force due to electric field
is equal to time derivative of
crystal momentum

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



Bloch state evolves,
after time Δt: $\psi_k \rightarrow \psi_{k+\Delta k}$

when state reaches BZ
k= π/a → -π/a
Bloch oscillations

NB Scattering prevents
observation Bloch osc.

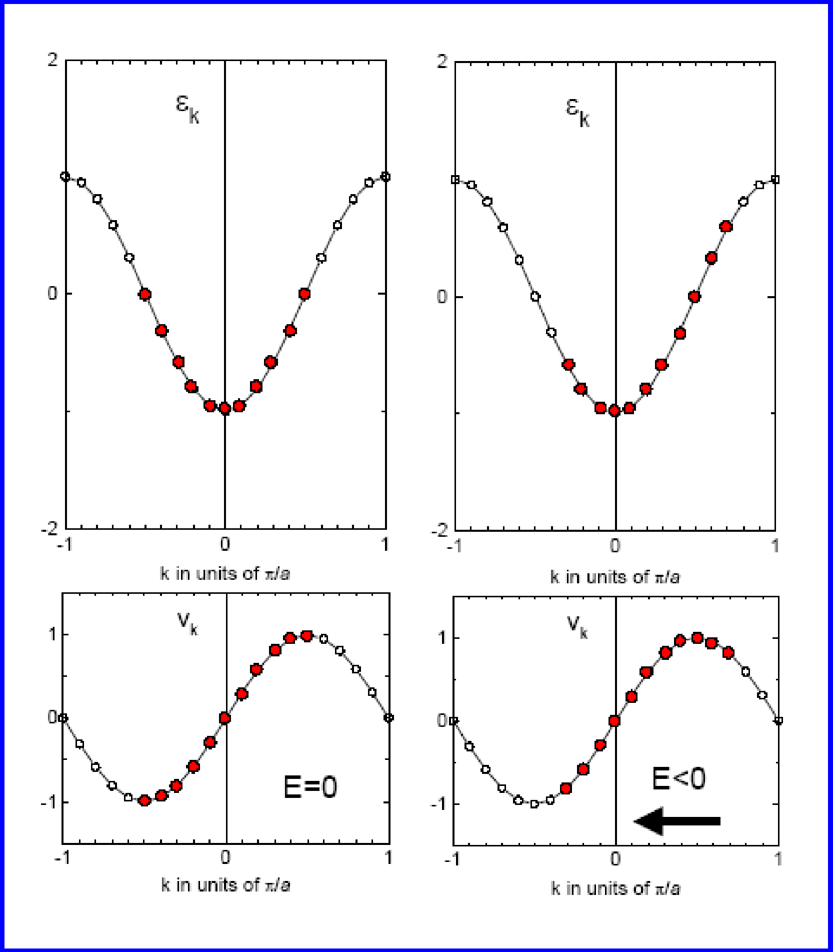
Current for Bloch states in a half filled band

Scattering produces steady state

$$\psi_k \rightarrow \psi_{k+\Delta k}$$

$$\Delta\vec{k} = -\frac{e\vec{E}}{\hbar}\tau$$

τ = relaxation time



netto velocity E≠0

→ current

$$I = -2e \sum_{occup.\,states} v_k$$

$|\Delta k| = eE\tau/\hbar \sim 15\ m^{-1}$

With $\tau \sim 10^{-14}$ s and E ~1 V/m

<< BZ ~10^{10} m^{-1}

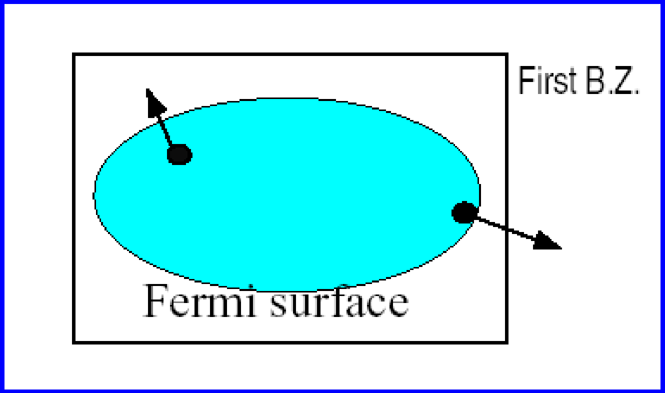
→ in reality small change

Currents in bands and holes

- particle current density of d**k** at **k**

$$d\vec{j}_n = \vec{v}(\vec{k})\frac{d\vec{k}}{8\pi^3} = \frac{1}{8\pi^3\hbar}\vec{\nabla}_k E(\vec{k})d\vec{k}$$

density states in d**k** $1/(2\pi)^3$



- electrical current density

integrate over first Brillouin zone

$$\vec{j} = \frac{-e}{8\pi^3\hbar}\int_{1st\ Br.z.}\vec{\nabla}_k E(\vec{k})d\vec{k}$$

different occupied states make different contributions to the current density

- full band

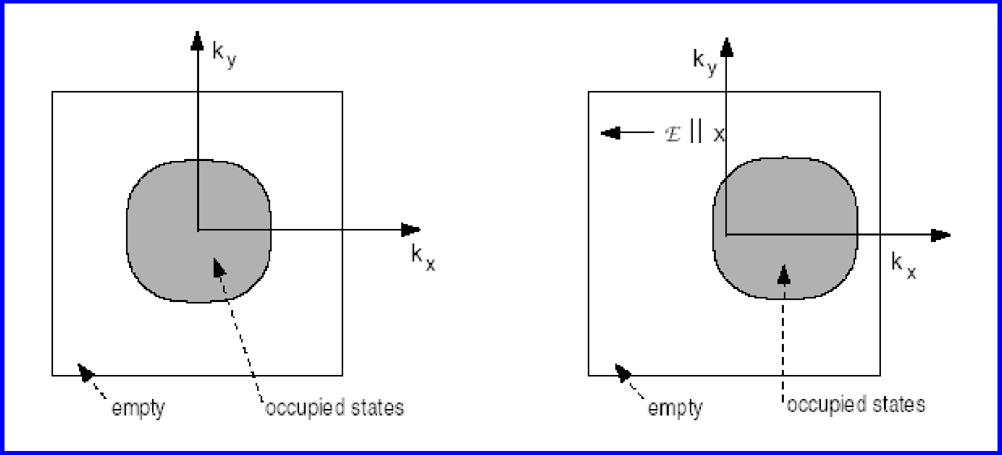
$$\vec{v}(-\vec{k}) = \frac{1}{\hbar}\vec{\nabla}_{-k}E(-\vec{k}) = -\frac{1}{\hbar}\vec{\nabla}_k E(\vec{k}) = -\vec{v}(\vec{k})$$

current = 0 $\rightarrow$ insulator

lattice with inversion symmetry

$$E(\vec{k}\uparrow) = E(-\vec{k}\downarrow)$$

- partially filled band: **E** field redistributes k states symmetry around k=0 lost



- current of positive charge, particles in unoccupied states (holes)

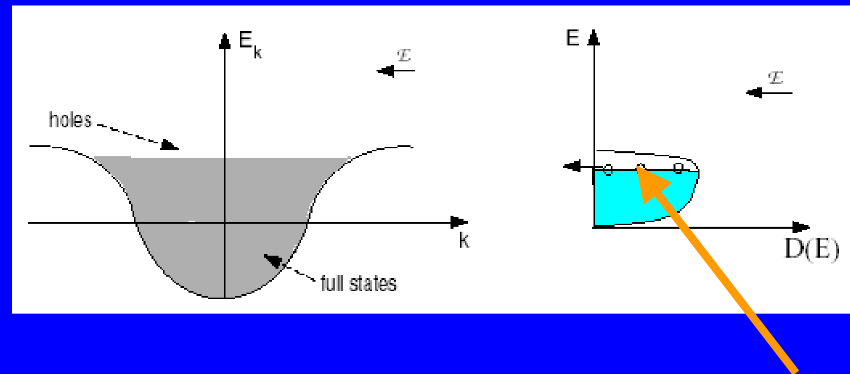
$$\vec{j} = \frac{-e}{8\pi^3} \int_{k\ occupied} \vec{v}(\vec{k}) d\vec{k}$$

$$= \frac{-e}{8\pi^3} \int_{1st\ Br.z.} \vec{v}(\vec{k}) d\vec{k} - \frac{-e}{8\pi^3} \int_{k\ empty} \vec{v}(\vec{k}) d\vec{k}$$

$$= \frac{+e}{8\pi^3} \int_{k\ empty} \vec{v}(\vec{k}) d\vec{k}$$

- near top of the band
  (k taken from top)

$$E(\vec{k}) = E_0 - \frac{\hbar^2 k^2}{\left|2m^*_\wedge\right|}$$

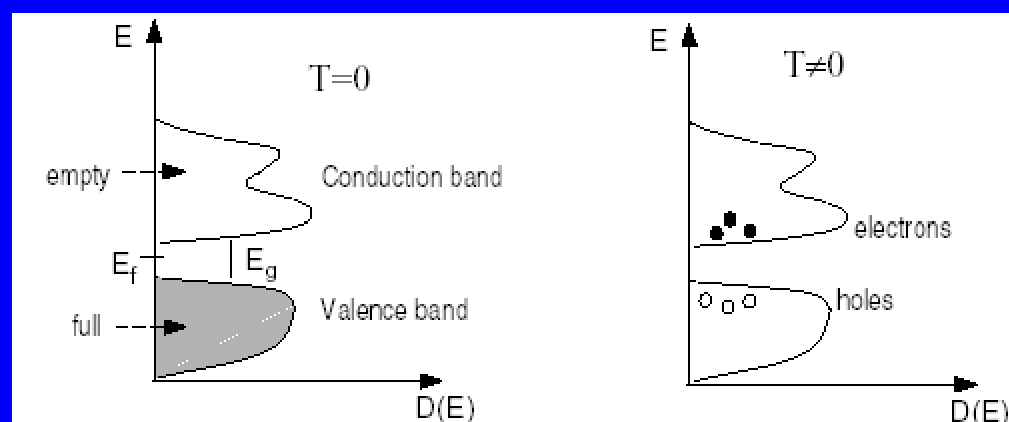


holes

- holes at the top of the band have positive effective mass!

$$\dot{\vec{v}} = \frac{1}{\hbar}\frac{d}{dt}\vec{\nabla}_k E(\vec{k}) = -\frac{1}{\left|m^*_\wedge\right|}\hbar\dot{\vec{k}} = \frac{e}{\left|m^*_\wedge\right|}\vec{E}$$

- insulators
  conduct at T≠0
  n ~ exp($-E_g/k_BT$)



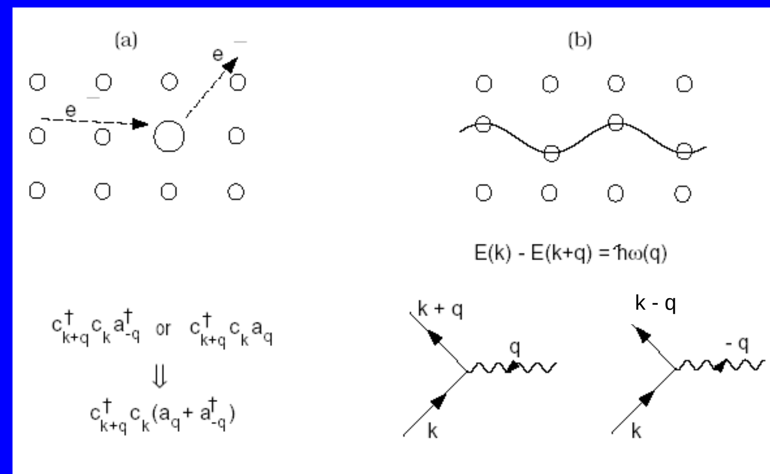
Scattering of electrons in bands

What did we learn:

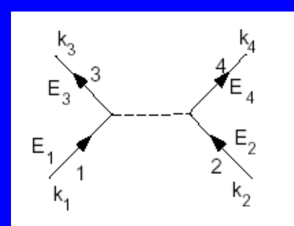
- equation of motion $\rightarrow$ electrons/holes accelerate
- Bloch waves in perfect lattice $\rightarrow$ no resistivity

This cannot be true:

- scattering!
  - deviations from periodicity (defects, lattice vibrations)
  - electron-electron collisions



scattering at a defect or phonon



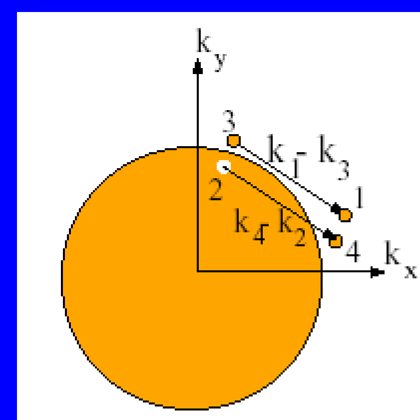
momentum and energy conservation

$$E_1 + E_2 = E_3 + E_4 \quad ; \quad \vec{k}_1 + \vec{k}_2 = \vec{k}_3 + \vec{k}_4$$

scattering restricted to narrow k-shell near k_F

$$\frac{1}{\tau_{e-e}} \sim \rho_{e-e} \sim \left(\frac{k_B T}{E_F}\right)^2$$

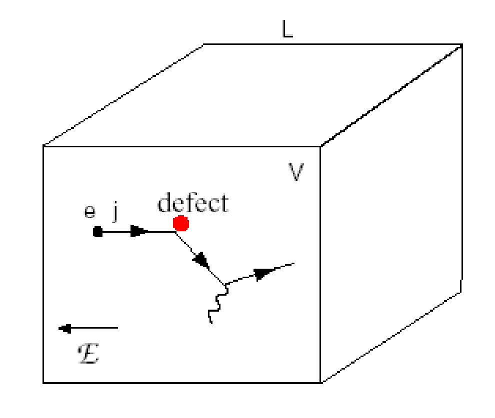
near 300 K τ_{e-e}~10^{-10} s >> τ_{e-ph} or τ_{e-d}



k_1,k_2 scatters into k_3,k_4

Boltzmann equation and relaxation time approximation

Boltzmann eq. describes
“non-equilibrium steady state”
- driving force due to **E** and **B** field
- dissipation due to scattering



thermal equilibrium distribution E=B=0

$$f_0(\vec{k}) = f(\vec{r},\vec{k},t)\Big|_{\vec{E}=0} = \frac{1}{e^{(E(\vec{k})-E_F)/k_BT}+1}$$

change of f in time (t-dt) $\rightarrow$ t + effect of scattering

$$f(\vec{r},\vec{k},t) = f(\vec{r}-\vec{v}dt,\vec{k}+\frac{e\vec{E}}{\hbar}dt,t-dt) + \left(\frac{\partial f}{\partial t}\right)_s dt$$

expanding up to terms linear in dt
$\rightarrow$ Boltzmann equation

$$\frac{\partial f}{\partial t} + \vec{v}\cdot\vec{\nabla}_r f - \frac{e}{\hbar}\vec{E}\cdot\vec{\nabla}_k f = \left(\frac{\partial f}{\partial t}\right)_s$$

Relaxation time approximation:
rate at which f returns to equilibrium
$\propto$ deviation of f from f_0

$$\left(\frac{\partial f}{\partial t}\right)_s = -\frac{f(\vec{k})-f_0(\vec{k})}{\tau(\vec{k})}$$

Electrical conductivity of metals

Particle current density

insert distribution function

$$\vec{j}_n = \frac{1}{8\pi^3}\int_{1st\ BZ} \vec{v}(\vec{k})\, f(\vec{k})\, d\vec{k}$$

- linear effects in electric field (Ohms law)
- isotropic medium, cubic lattice
- linearized Boltzmann eq.

only states at Fermi surface important

$$\sigma = j_x / E_x = -\frac{e^2}{8\pi^3}\int v_x^2(\vec{k})\tau(\vec{k})\frac{\partial f_0}{\partial E}\, d\vec{k}$$

Fermi surface

$$\Rightarrow \quad \sigma \cong \frac{e^2}{8\pi^3\hbar}\int_{E=E_F} \frac{v_x^2(\vec{k})}{v(\vec{k})}\tau(\vec{k})\, df_E$$

Conductivity expressed as integral over the Fermi surface, depends on **v**(E_F) and τ(E_F)

For parabolic band this reduces to: $\sigma = \dfrac{e^2\tau(E_F)}{m^*}n$

Electrical conductivity of metals

Matthiesen's rule

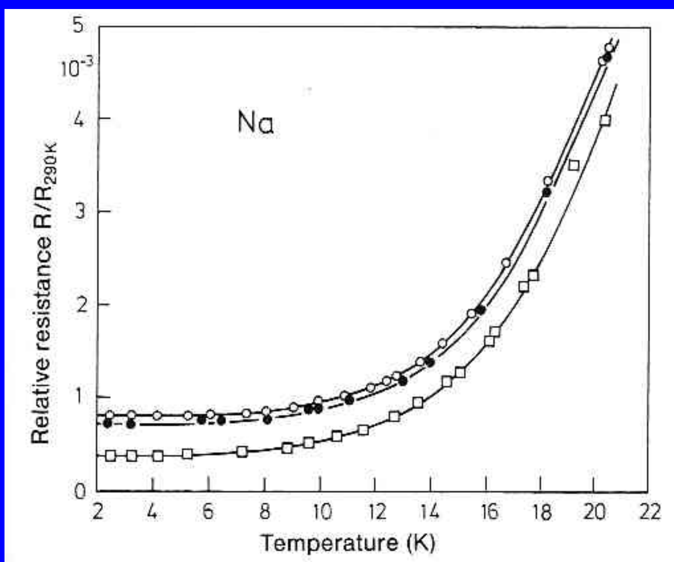
$$\frac{1}{\tau} = \frac{1}{\tau_{def}} + \frac{1}{\tau_{e-e}} + \frac{1}{\tau_{ph}} + \frac{1}{\tau_{mag}} + \frac{1}{\tau_{CEF}} + ...$$

$$\rho = \rho_0 + \rho_{e-e} + \rho_{ph} + \rho_{mag} + \rho_{CEF} + ...$$

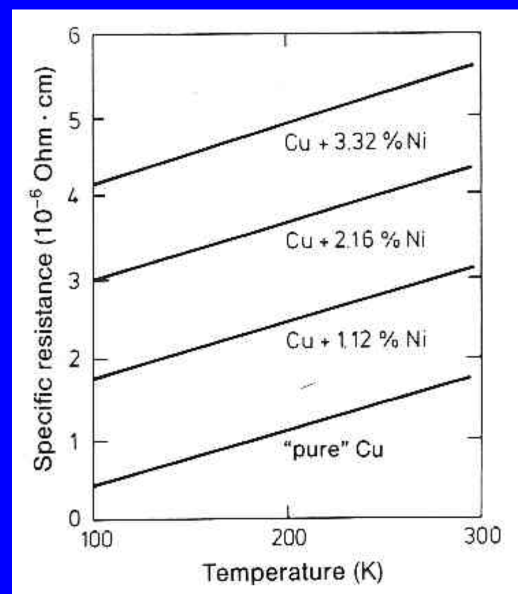
$$\rho_0 = constant$$

$$\rho_{e-e} = AT^2$$

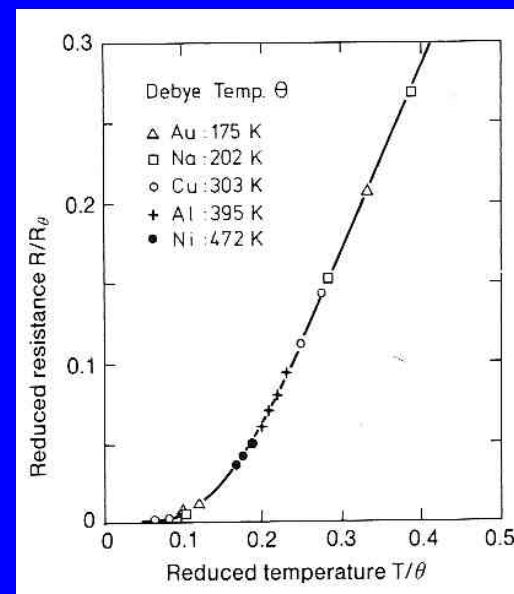
$$\rho_{ph} = a(T/\theta)^5 \int_0^{\theta/T} \frac{x^5 dx}{(e^x - 1)(1 - e^{-x})}$$



resistance of sodium
3 diff. defect concentrations

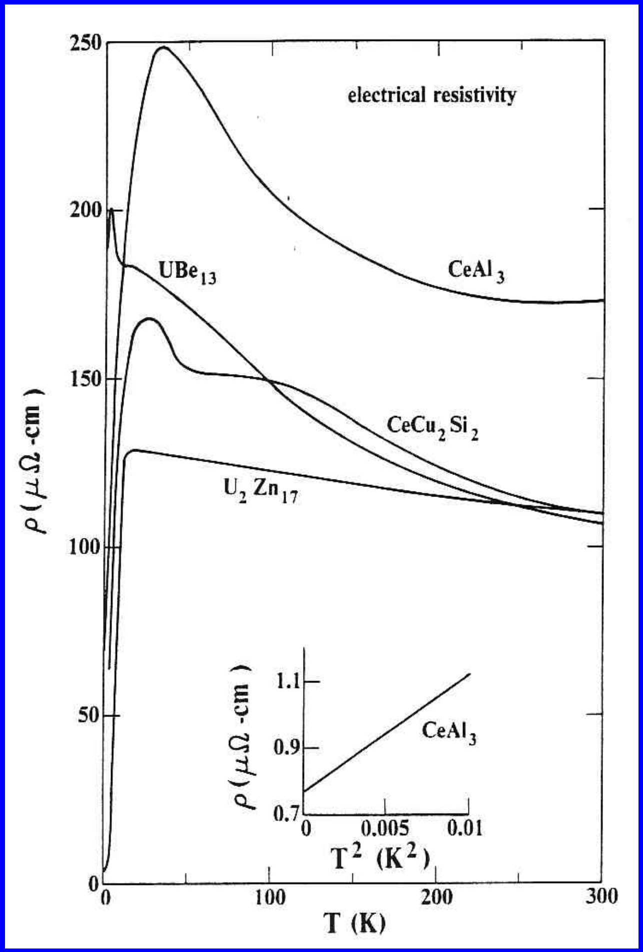


resistivity of copper-nickel alloys

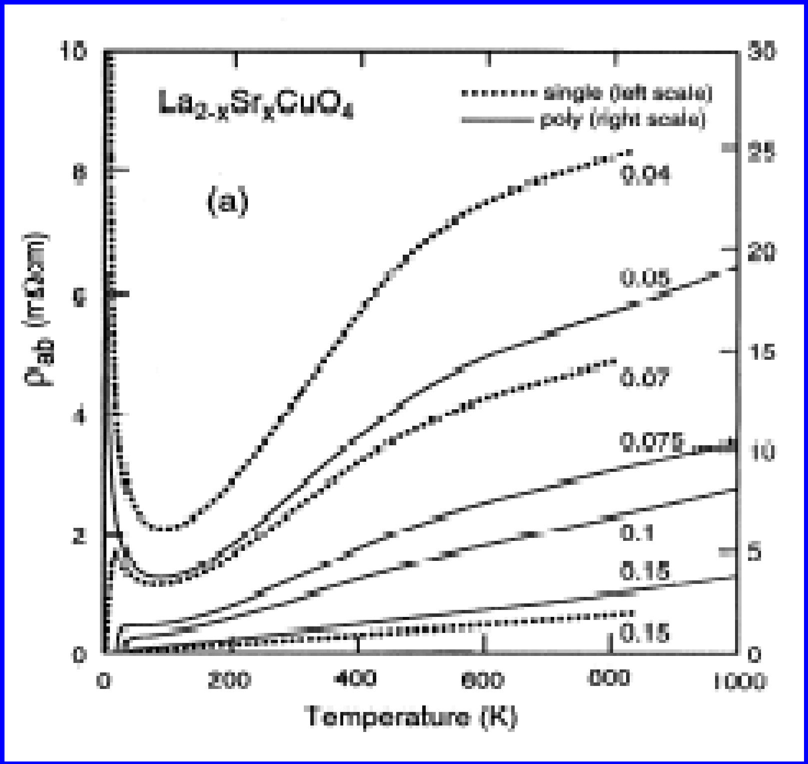


phonon (Debye) resistance

Electrical conductivity of metals: examples



resistivity of heavy-fermion compounds



resistivity of superconducting cuprates: $La_{2-x}Sr_xCuO_4$

Quantum oscillations and the topology of Fermi surfaces

Motion of electrons and holes in magnetic field

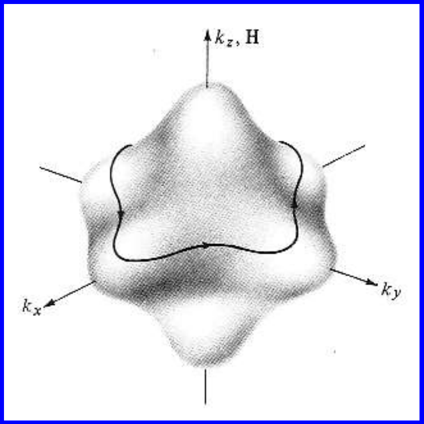
Lorentz force

$$m\frac{d\vec{v}}{dt} = -e(\vec{v}\times\vec{B})$$

for wave packet m**v**=ℏ**k**

$$\frac{d\vec{k}}{dt} = -\frac{e}{\hbar^2}\left[\vec{\nabla}_k E(\vec{k})\times\vec{B}\right]$$

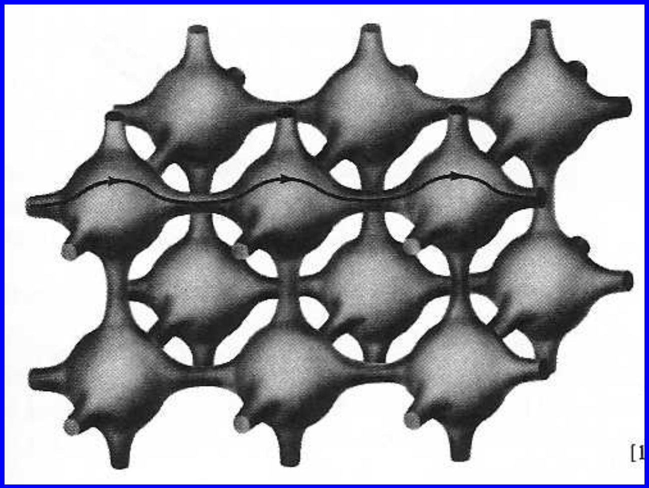
closed orbits



Electrons move:

- in plane ⊥ B
- tangential to surface of constant E(**k**)

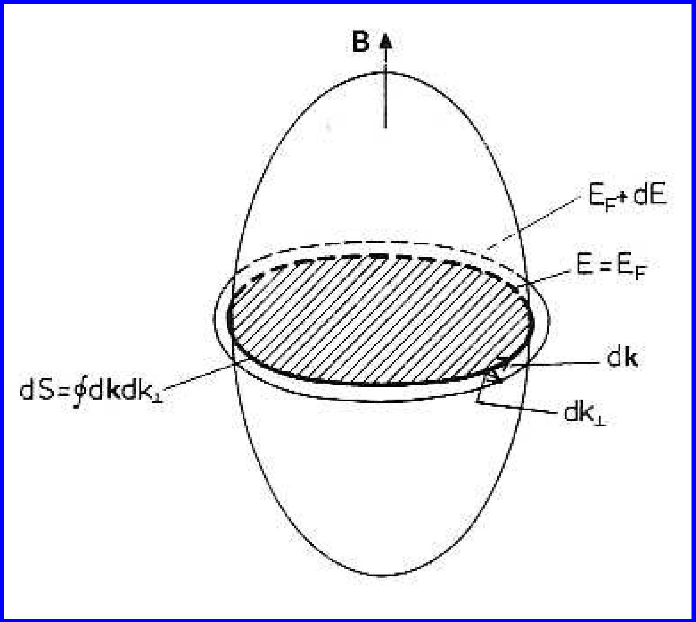
open orbits



Period of orbit in magnetic field

$$T = \int dt = \frac{\hbar^2}{eB} \oint \frac{d\vec{k}}{[\vec{\nabla}_k E(\vec{k})]_\perp}$$

$$\oint \frac{dk_\perp}{dE} d\vec{k} = \frac{dS}{dE}$$



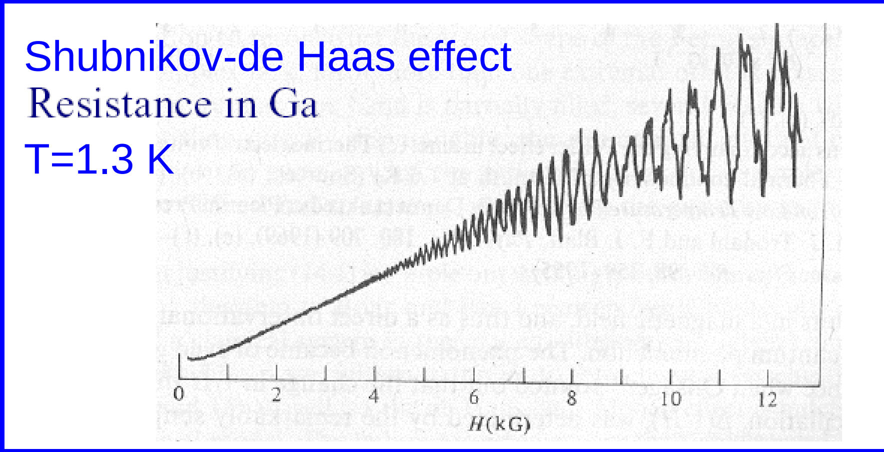
Free electrons

$S = \pi k^2$ and $E = \hbar^2 k^2 / 2m$

$$T = \frac{\hbar^2}{eB}\frac{dS}{dE} = \frac{2\pi\, m^*}{eB}$$

$$\omega_c = \frac{2\pi}{T} = \frac{eB}{m^*}$$

cyclotron frequency



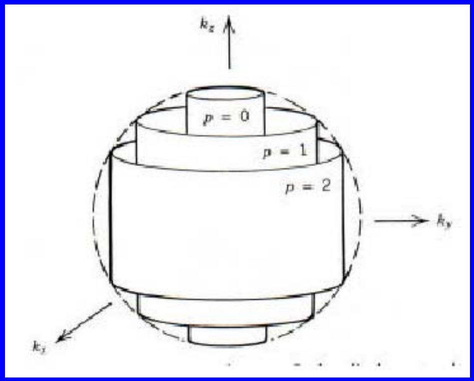
why oscillations?

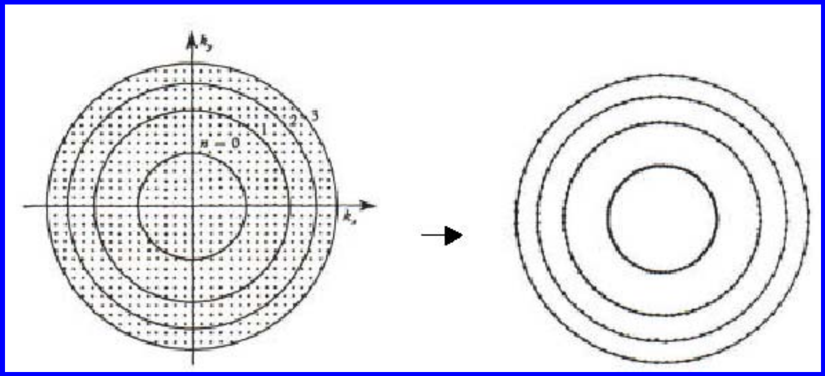
de Haas-van Alphen effect

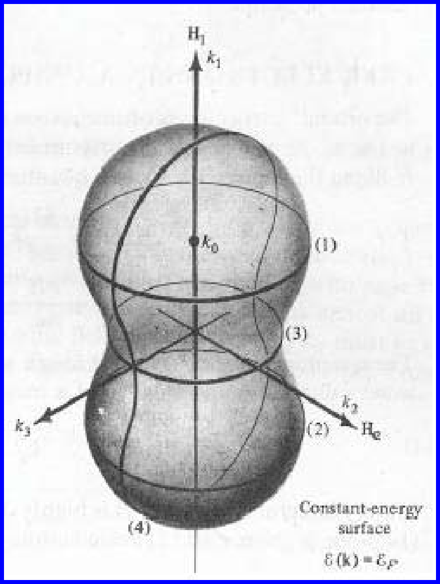
de Haas (1878-1960)   van Alphen (1906-1967)

Landau quantization

$$E_n = (n + \tfrac{1}{2})\hbar\omega_c \quad ; \quad \omega_c = \frac{eB}{m^*}$$







Landau tubes

$$\textit{Energy splitting}: \quad E_{n+1} - E_n = \hbar\omega_c = \hbar\frac{eB}{m^*} = \frac{2\pi\hbar}{T}$$

$$\textit{Fermi surface area's}: \quad S_{n+1} - S_n = \frac{2\pi eB}{\hbar}$$

$$\textit{Period of oscillations}: \quad \Delta\left(\frac{1}{B}\right) = \frac{\hbar S_{F,extr}}{2\pi e}$$

$S_{F,extr} = (\lambda + n)\Delta S$

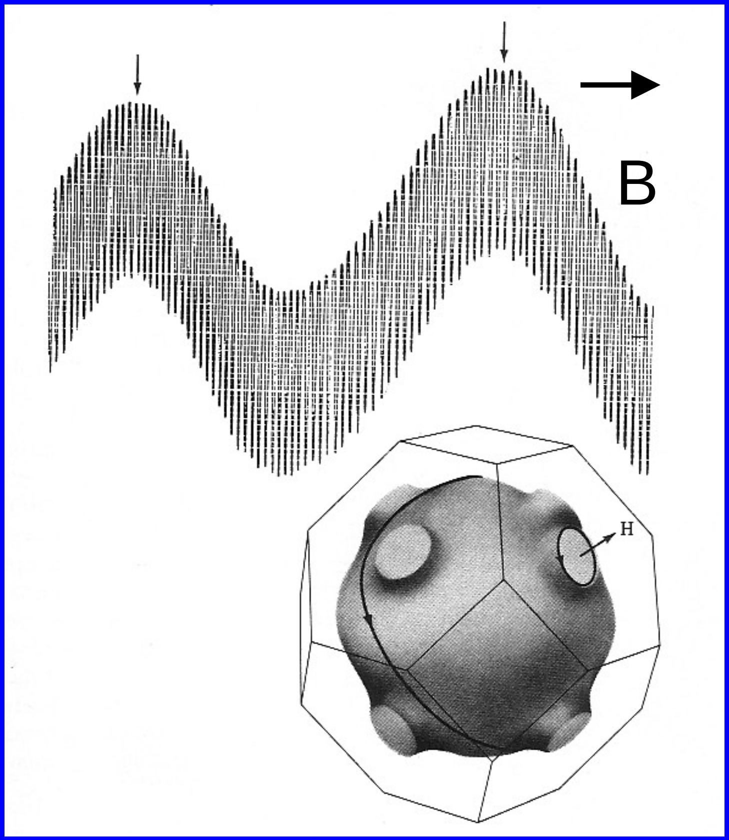
Landau tubes cross E_F with period $\Delta(1/B)$

Some numbers:

- period $T = 2\pi/\omega_c = 3.6\times10^{-11}$ s in 1 T

- quantum number: $(n+1/2)\hbar\omega_c \sim E_F$
  $\rightarrow$ for silver $E_F = 5.5$ eV
  $\rightarrow n \sim 4.6\times10^4$ for B = 1 T

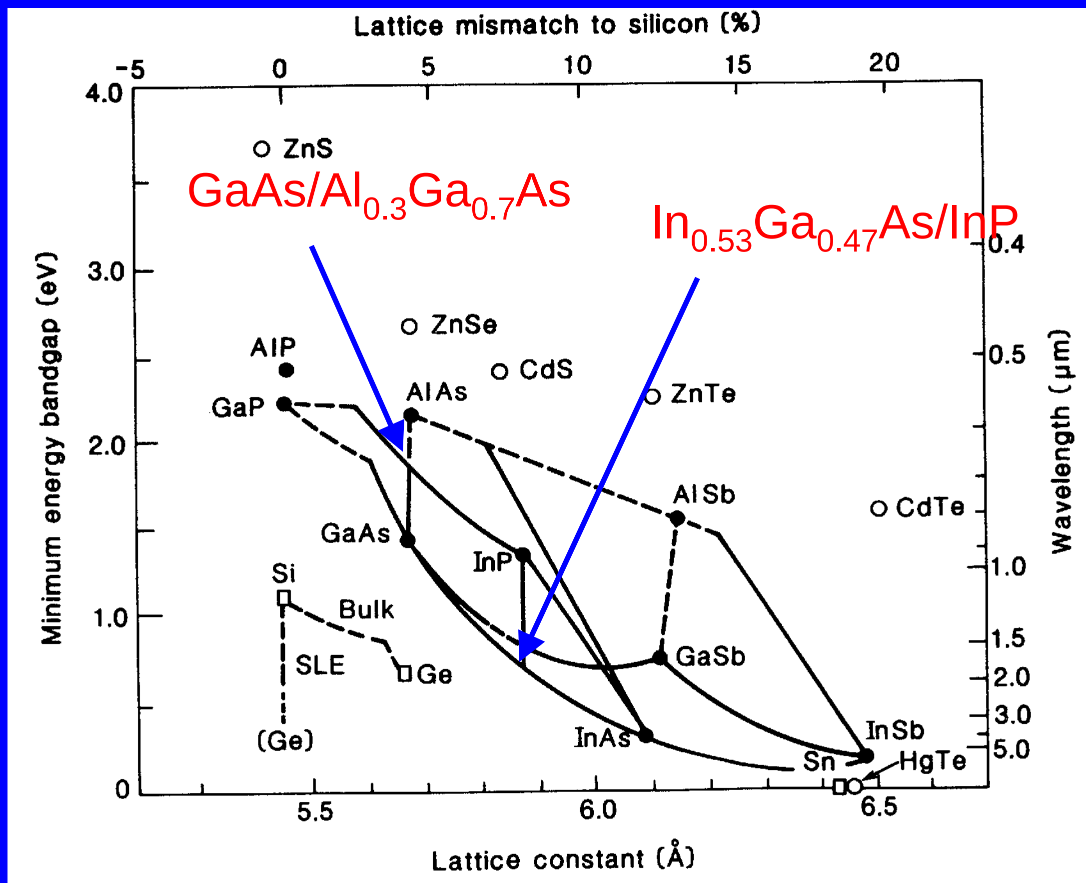
- absence of thermal smearing:
  $k_BT/\hbar\omega_c < 1$
  $k_BT/\hbar\omega_c = k_Bm/\hbar e(T/B)=1.34(T/B)$
  $\rightarrow$ low T & high B



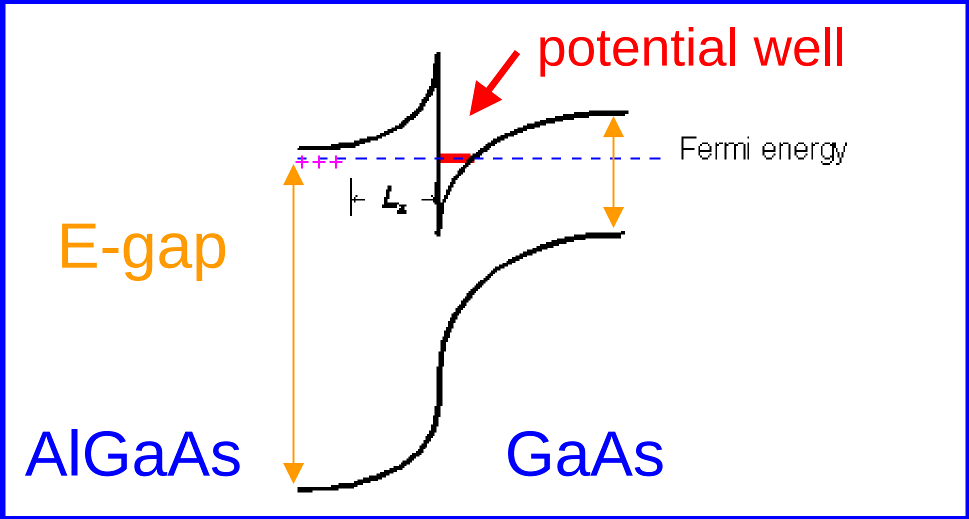
dHvA signal (magnetization)
in silver
B || [1,1,1]   T=1.3 K
two periods$\rightarrow$
neck and belly orbits
$S_{111}(\text{belly})/S_{111}(\text{neck}) = 51$

Quantum Hall effect in 2D systems

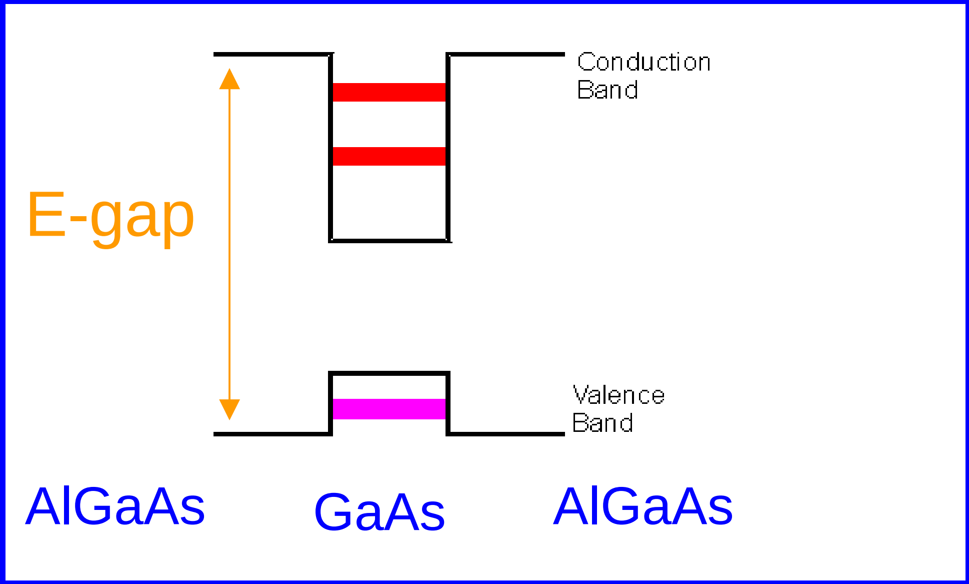
2D electron gas formed at interface of
lattice matched heterostructures or quantum wells



Heterostructures and quantum wells

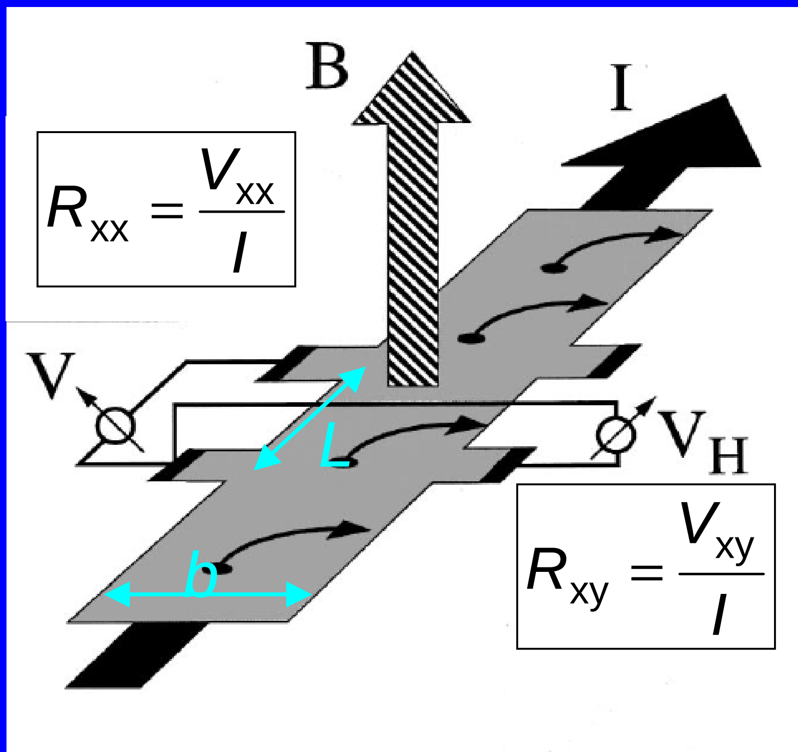


Heterostructure



Quantum well

Magnetotransport in Hall bar geometry



- Classically

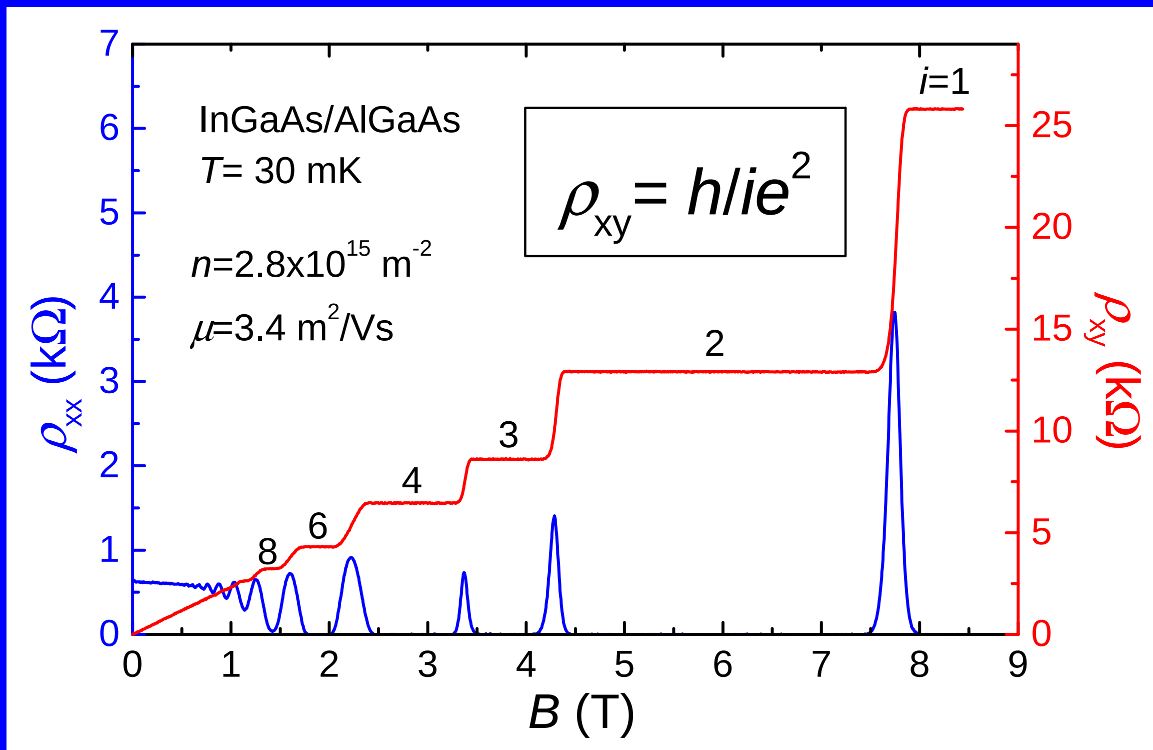
$$\rho_{xx} = R_{xx}\frac{b}{L} = \frac{V_{xx}}{I}\frac{b}{L} = \frac{m^*}{ne^2\tau} = \frac{1}{ne\mu}$$

mobility $\mu = v_D/\mathbf{E}$

$$\rho_{xy} = R_{xy} = \frac{V_{xy}}{I} = \frac{B}{ne}$$

- Hall resistance
  - linear in field
  - gives carrier concentration and type (electrons or holes)

The quantum Hall effect



Klaus von Klitzing
Nobel Prize Physics 1985
“for the discovery of the quantum Hall effect”

- QHE: ρ_{xy} quantized (resistance standard)
- allows precise determination fine structure constant

$$\rho_{xy} = \frac{h}{ie^2} = \frac{25.812}{i}(k\Omega)$$

$$\alpha = \frac{e^2}{h}\frac{\mu_0 c}{2} \cong \frac{1}{137}$$

Landau quantization

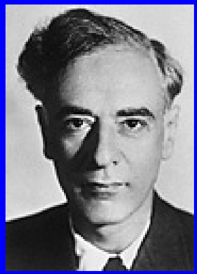
Energy levels in band *i* split into discrete Landau levels in magnetic field

$$E_{i,n} = (n + \tfrac{1}{2})\hbar\omega_c + g\mu_B B$$

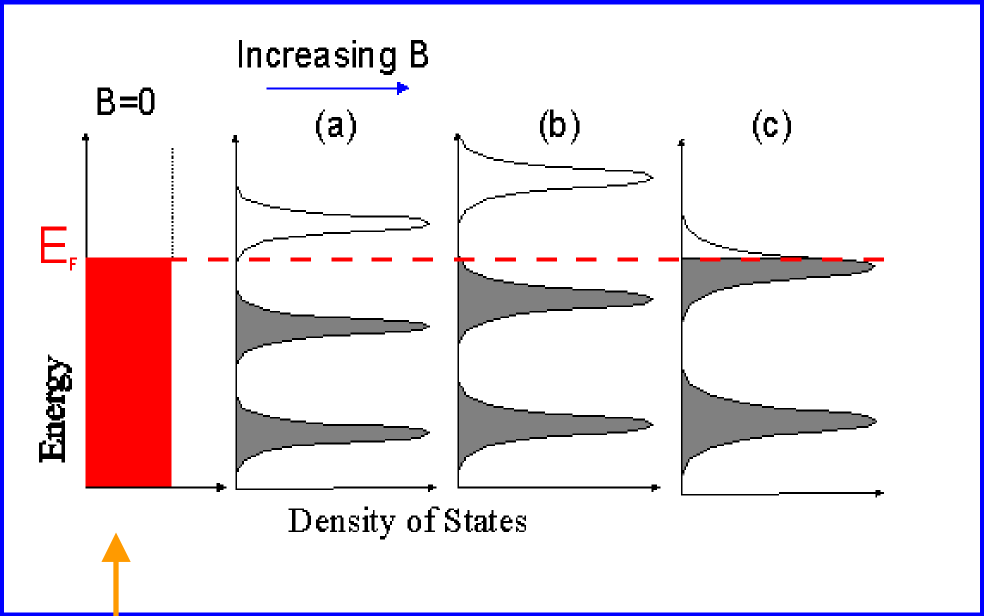
$$\omega_c = \frac{eB}{m^*}$$ cyclotron frequency

n = integer

Zeeman term



Lev Landau
1908-1968
Nobel Prize Physics 1962
"for his pioneering theories for condensed matter"



$$DOS_{2D} = \frac{m^*}{\pi\hbar^2}$$

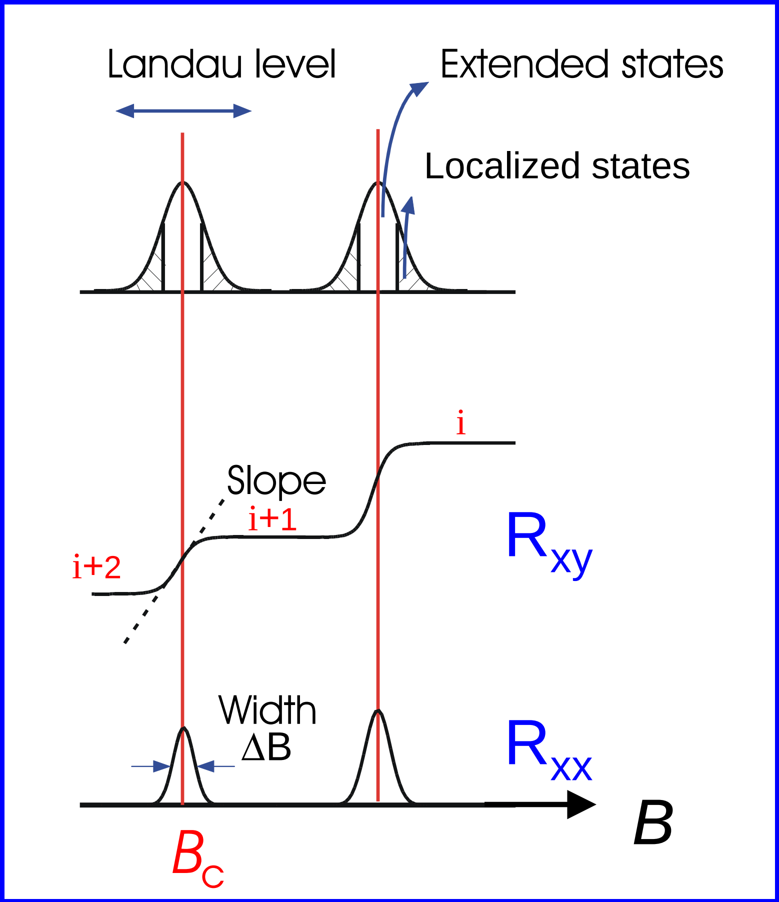
N_L states per unit area per Landau level

$$N_L = \frac{eB}{h}$$

Filling factor ν

$$\nu = \frac{n_{2D}}{N_L} = \frac{n_{2D}h}{eB}$$

Simple "explanation" QHE



- disorder/impurities → extended and localised states in Landau levels
- with increasing field B Landau levels pushed to above E_F → plateau-plateau transitions
- conduction when Landau level in extended states
- width extended states → 0 when T → 0

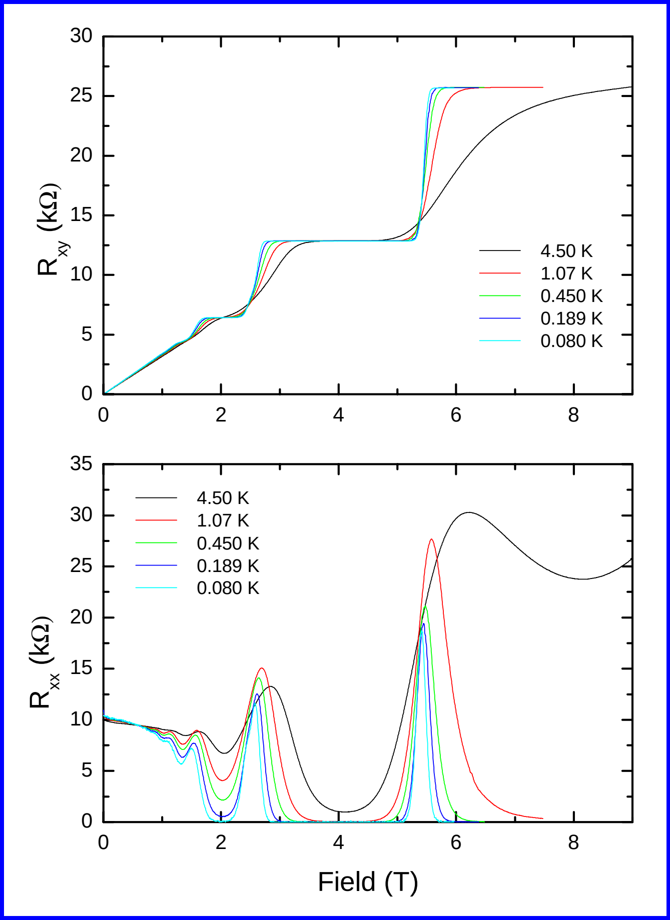
Typical numbers

- Energy distance between levels
  - $k_B T$ ~ 25 meV near 300 K
  - $\hbar\omega_c$ ~ 1.6 meV/T (m^*= 0.067m_e)
  - $k_B T \ll \hbar\omega_c \rightarrow$ T< 4 K

$$\omega_c = eB/m^*$$

- Filling fraction
  - typical n_{2D}= 2x10^{15} m^{-2}
  - quantum limit ν =1 $\rightarrow$ B~ 8.25 T

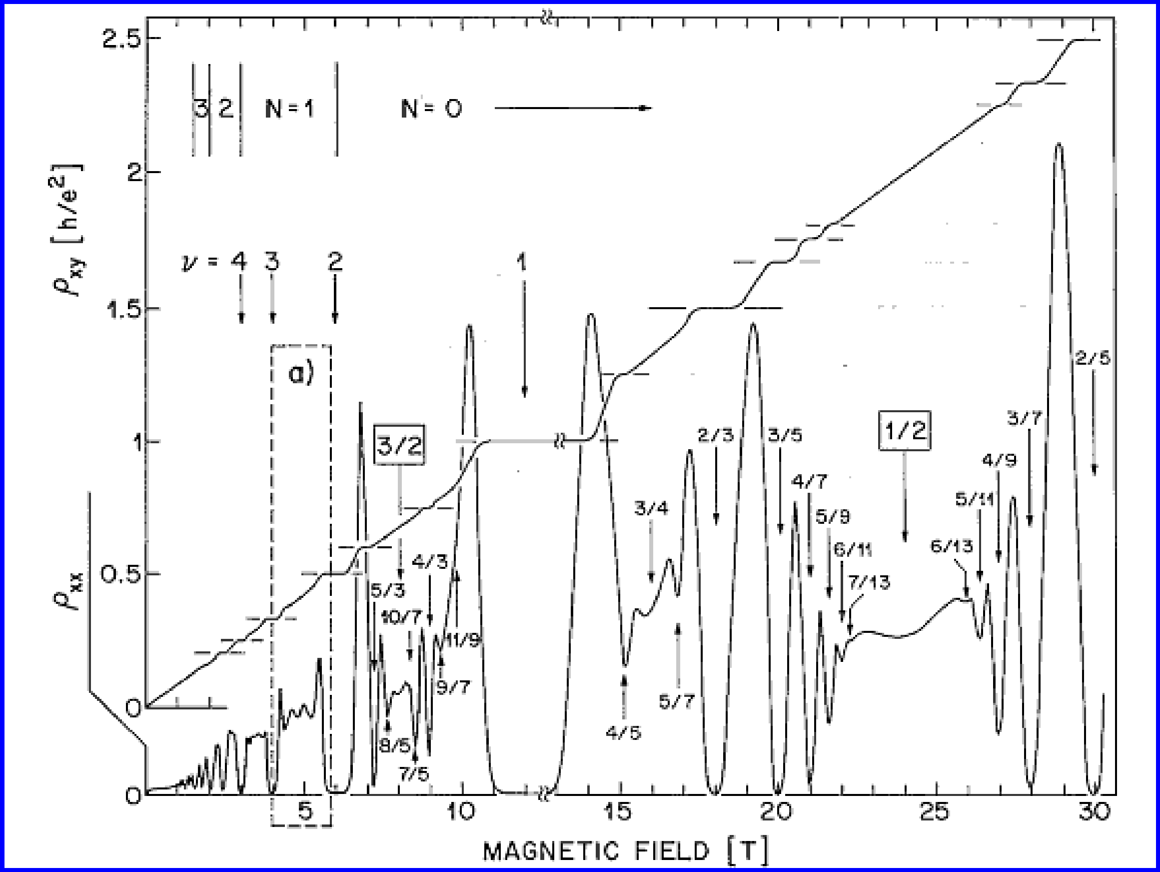
$$\nu = \frac{n_{2D}}{N_L} = \frac{n_{2D}h}{eB}$$



high B/T needed

InGaAs/GaAs quantum well
n = 2x10^{15} m^{-2}
T = 0.08-4.2 K

Fractional quantum Hall effect



$$\rho_{xy} = \frac{h}{\nu e^2} = \frac{25.812}{\nu}(k\Omega)$$

ν = 1/3, 2/3, 1/5, 2/5 etc.

fractional quantum Hall effect in high mobility GaAs/AlGaAs heterostructure
T= 0.15 K