Week 1

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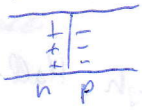
physics.bme.hu/...

Physics of Semiconductors

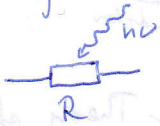
Semiconductors (SC): material whose conductivity can be effected by:
- temperature
- doping (intentional/unintentional)
- external voltage (drain, bias voltage)

- another semiconductor nearby
  - diffusion, charge transfer



depletion layer → charge diffusion junction

- light, photoconductivity (sensors, photovoltaic eff.)



- magnetism (spintronics, magnetic semiconductors)
  Mn ; GaAs

SC materials:

Bulk semiconductors
- IV. group: Si, Ge, (Sn), C
  - allotropes: diamond, graphite, graphene, nanotubes, fullerenes
- IV. group Compounds: SiC
- III-V group Compounds: GaAs, AlP, InSb
- II-VI group Comp.: ZnS, ZnSe, ZnO, PbS_2, $FeSe_2$

Low dimensional semiconductors: 1D: C nanotubes, nanowires GaAs
2D: graphene, transition metal dichalcogenide MoS_2, MoSe

Molecular SC: Buckyball

Diamond: SC or Insulator?

$E_g = 6\,eV \rightarrow SC$

$Si_3N_4 \Rightarrow 4\,eV \rightarrow$ Insulator

B : C $\rightarrow$ Superconductor
4% 96%

Early History of SCs: Fundamental effects

1833 Faraday: AgS heated $\rightarrow$ R decreases

1839 Becquerel: photovoltaic effect

1873 Smith: photoconductivity Se (light $\rightarrow$ R decreases)

1874 Braun: rectification (egyenirányítás) in metal-sulfides
Schuster: CuO rectification

1878 Hall-effect

1900 Baedeker: inverse sign Hall-effect in CuI

$R_H = \frac{1}{n \cdot e}$

$n = \frac{\text{number of } e^-}{cm^3}$ $\hookrightarrow$ charge carriers

1910 Weiss: Halbleiter
semi conductor

1928-1938 Quantum Theory of Semiconductors
Bloch, Schottky, Mott

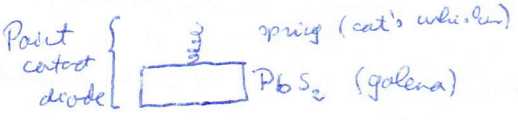
1940 Bardeen: non-reproducing laboratory results are due to about <1ppm unintentional doping

Technology:

1880: Bell voice trasfer Se (piezoelectricity)

1883: Fritts: first solar cell

1904: J.C. Bose sensitive radio detector (rectifying device)

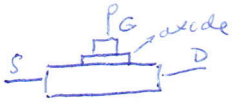


1906 Round: LED

1920 several people $\rightarrow$ CuO + Se: rectifier AC $\rightarrow$ DC

1922 Loser ZnO: amplifier

1926 Lilienfeld FET field-effect transistor



I_{SD} depends on V_{GS}

1941 Ohl: first Si p-n junction

1947 Borden-Brattain-Schodley: bipolar junction transistor

Nobel prices

1956 transistor

1973 Esaki, Giaver tunnel-diode

1985 von Klitzing: quantized Hall-effect

2000 Alferov, Kroemer, Kilby
SC laser IC

2007 Fert, Grünberg GMR effect
↓
giant-magnetoresistance

2009 Boyle, Smith CCD

2010 Geim, Novoselov graphene

2014 Akasaki, Amano, Nakamura: Blue LED (GaN)

Position of SC physics

- prerequisite: quantum mechanics
  solid state physics
  statistical physics
  material science (optics)

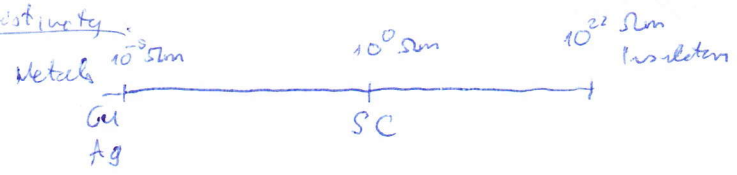
- It gives us: electronics, spintronics, laseroptics, laserphysics

- Ongoing research: fundamental: - new materials
  - low dimensional SCs
  excitons
  fundamental phenomenons: QHE, FQHE

- Applied research: new devices (HEMT) → high e^- mobility transistor

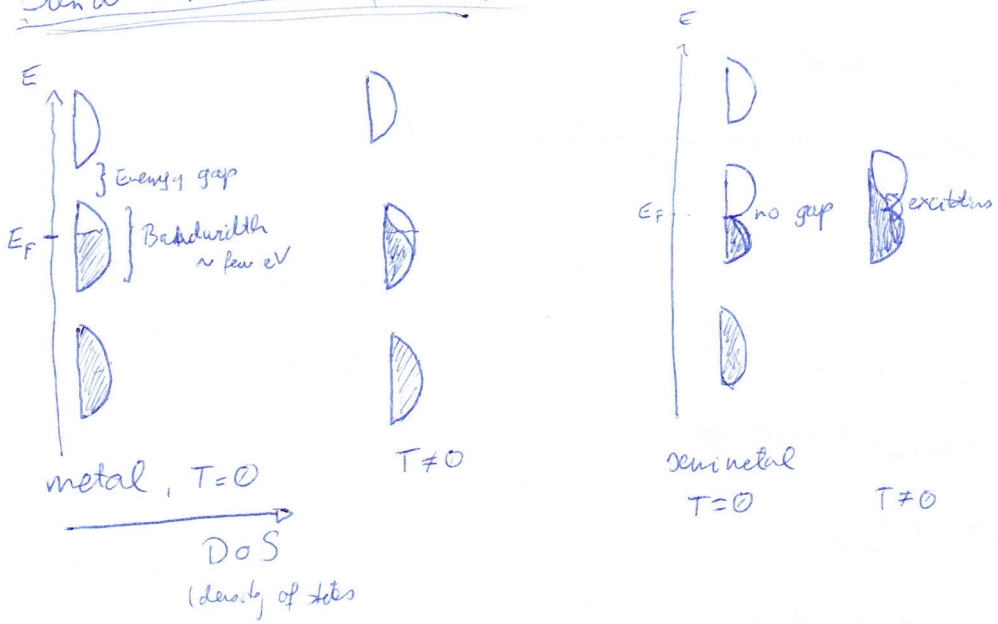
  size ↓
  speed, freq ↑
  power consumption ↓

- Resistivity:



Week 2

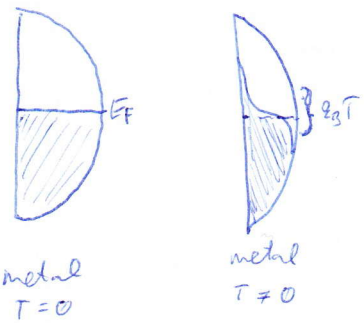
Band structure of SCs



$E_F \longleftrightarrow \mu$

E_F: $T=0$ property

μ: finite temperature, average energy of particles

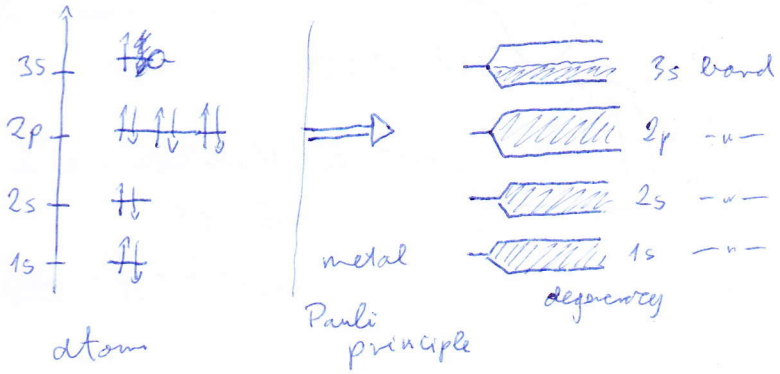


$$f(E) = \frac{1}{1 + e^{\frac{E-\mu}{k_B T}}}$$

$\mu(T \to 0) = E_F$

$\mu \neq E_F$

Na: $1s^2 2s^2 2p^6 3s^1$



Diamond

$1s^2 2s^2 2p^2$

Si

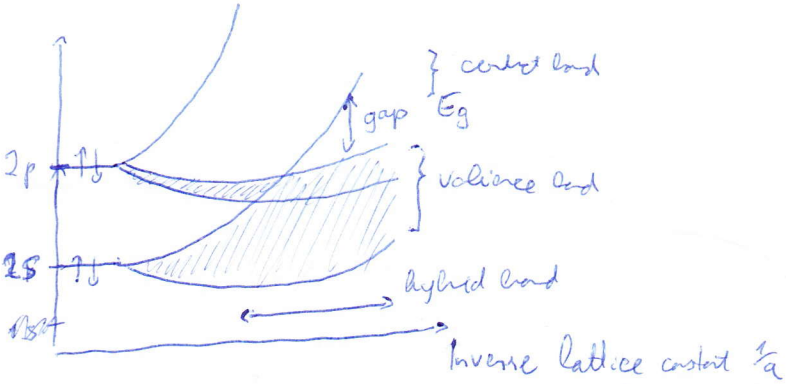
$1s^2 2s^2 2p^6 3s^2 3p^2$

$2p^2$ $2s^2$ } hybridisation $\xrightarrow{sp^3\ hybr.}$

anti-bonding orbital

bonding orbital

CH_4 sp^3



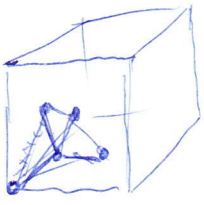
Structure: diamond structure

Bravais-lattice

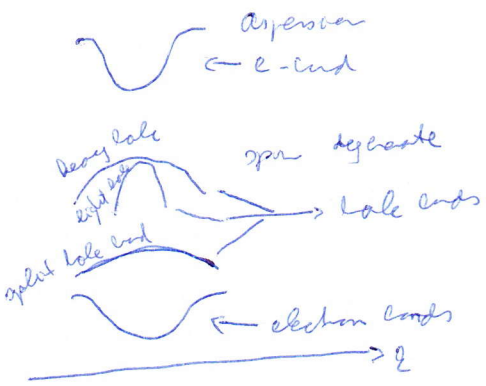
fcc

basis: (0, 0, 0) Ga

$(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})a$ As

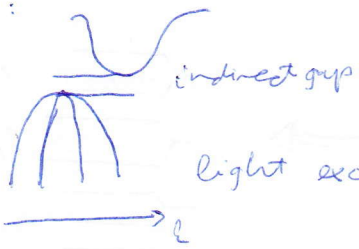


Band structure



LASER ✓

Si:



light excitation

$E = pc$

$p_{light} = \frac{E}{c} = \frac{h\nu}{c}$

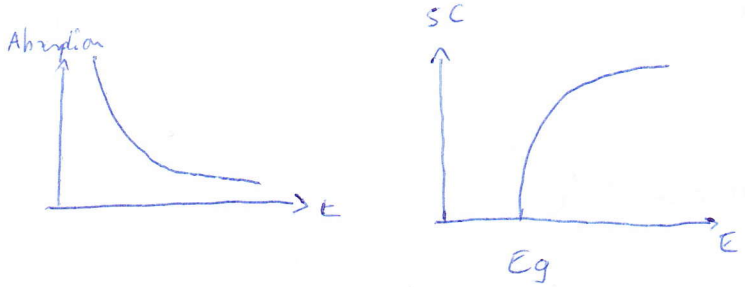
cannot emit or absorb light

~~LASER~~

8 e^- basis closed band structure (Si: 2 atom basis
GaAs:

Bandgap: C Si Ge GeAs AlAs
5eV 1,1eV 0,7eV 1,5eV 2,2eV

Optical properties:



Charge carriers in SCs: (C-C)

n: charge carrier concentration

in a metal: $n = 10^{22} \frac{1}{cm^3}$

Drude-modell:

$ma = F = qE$ plus a viscous force (drag force)

$ma = qE - Kv$

stationary solution $0 = qE - Kv$

we introduce: $\frac{K}{m} = \frac{1}{\tau}$ → relaxation

$ma = qE - Kv \rightarrow a = \frac{qE}{m} - \frac{K}{m} v$ $\quad \left[\frac{K}{m}\right] = \frac{1}{s}$

$qE = Kv \rightarrow \boxed{v_{drift} = \frac{qE\tau}{m}}$

$v_D \approx 10^{-1} \dots 10^{1} \frac{m}{s}$

current density: $j = n \cdot e \cdot v_D$

$[j] = \frac{C}{m^2 s}$

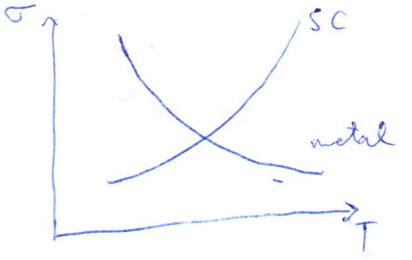
$[n e v_D] = \frac{1}{m^3} C \frac{m}{s} = \frac{C}{m^2 s}$

$\boxed{j \sim n}$

$j = \sigma E$ differential Ohm's laws

$j = n e v_D = \frac{n e^2 \tau}{m} E \longrightarrow \boxed{\sigma = \frac{n e^2 \tau}{m}}$

→ conductivity



metal n x const

σ is dominated by τ shortening

SC: n is strongly T dependent

if dominates σ

Solid state physics revision

1D free electrongas (particle in the box)

$\psi(q,x) = \frac{1}{\sqrt{L}} e^{iqx}$ plane wave

$p = \hbar q$

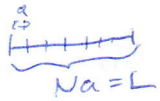
↓ canonical impuls — ↓ crystal momentum

Energy dispersion $\varepsilon(q) = \frac{\hbar^2 q^2}{2m}$

$$\left(H\psi = E\psi \qquad -\frac{\hbar^2}{2m}\Delta\psi = E\psi \right)$$

In a solid q is quantized by periodic boundary conditions

$\psi(0) = \psi(L)$ is single valued

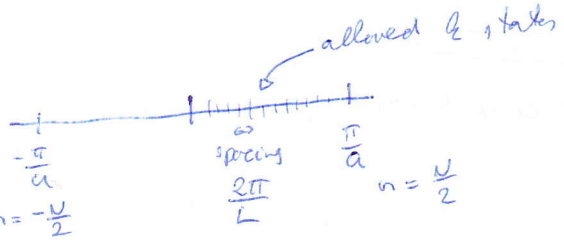


$e^{iqL} = 1$

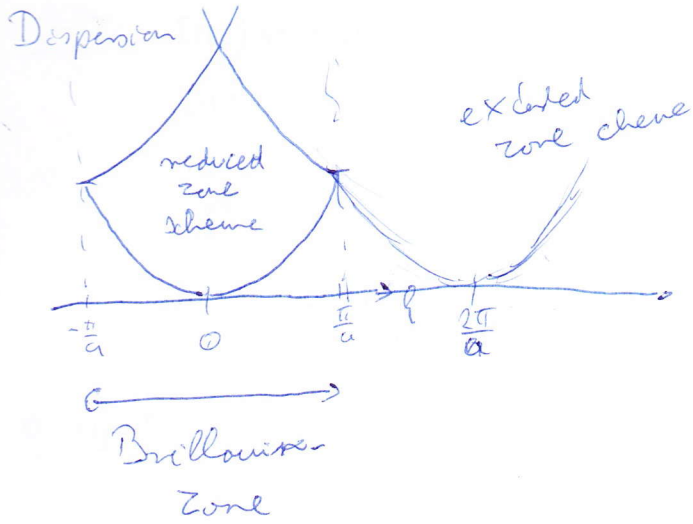
$qL = 2\pi n \qquad n \in 0, 1, 2, \ldots N-1$

$q = \frac{2\pi}{Na} n = \frac{2\pi}{a} \cdot \frac{n}{N}$

1D



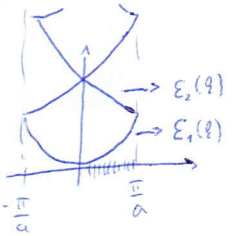
↳ quasi-continous



Week 3

Charge carriers:

free e^- gas: $E_n(q)$ $\quad E(q) = \frac{\hbar^2 q^2}{2m}$



periodic b. c.: $q = \frac{2\pi}{L} n \quad n = -\frac{N}{2} \dots \frac{N}{2}$

separation $\Delta q = \frac{2\pi}{L}$ (Δq quantization)

$v = \frac{1}{\hbar} \frac{\partial E(q)}{\partial q}$ ← velocity

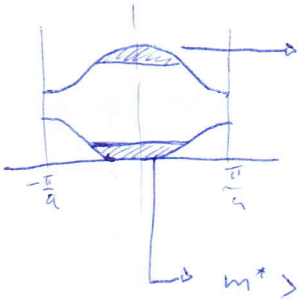
for 1D: $\frac{\hbar q}{m} = v$

$p = \hbar q$

for free e^- gas:

$(m^*)^{-1} = \frac{1}{m} \quad m^* = m \qquad F_{ext} = \hbar \dot{q}$ → crystal momentum

1D free e^- in periodic potential

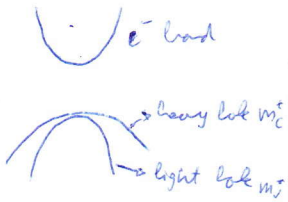


$m^* < 0 \leftarrow ma = F_+$

↳ charge carrier hole h^+

$m^* > 0$ charge carrier → e^-

GaAs



typical values $m_c^* = 0{,}1 \dots 0{,}5\, m_0$

$m_v^* = -1 \dots -3\, m_0$

Density of states:

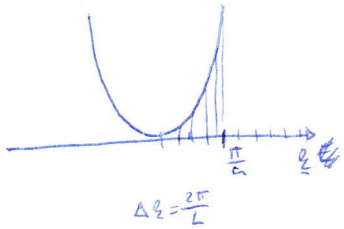
density of states in q-space

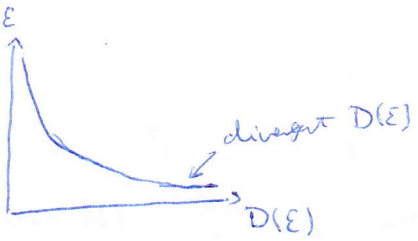
1D $\Delta q = \frac{2\pi}{L}$

$D(q) = \frac{L}{2\pi}$ dimension of m

$$N = \int_{-\pi/a}^{\pi/a} D(q)\, dq = \int_{-\pi/a}^{\pi/a} \frac{L}{2\pi} dq = \frac{L}{2\pi}\frac{2\pi}{a} = \frac{L}{a} = N$$

Go from $D(q) \to D(\varepsilon)$:





1D: $D(q)\, dq = D(\varepsilon)\, d\varepsilon$ ← preservation of states at definition of $D(\varepsilon)$

$D(\varepsilon) = D(q)\frac{dq}{d\varepsilon} =$

$= D(q)\left(\frac{d\varepsilon}{dq}\right)^{-1}$

$\frac{dq}{d\varepsilon} = \left(\frac{d\varepsilon}{dq}\right)^{-1}$ derivation of the inverse function

$y = f(x)$: $\left[f^{-1}(x)\right]' = \frac{1}{f'(f^{-1}(x))}$

$\left(\frac{d\varepsilon}{dq}\right) = \frac{\hbar^2 q}{m^*}$ $\quad D(\varepsilon) = \frac{L}{2\pi}\cdot\frac{m^*}{\hbar^2 q} =$ $\quad q = \sqrt{2m^*\varepsilon}$

$$\boxed{D(\varepsilon) = \frac{L}{\pi}\frac{m^*}{\sqrt{2}\hbar\sqrt{\varepsilon}}}$$

2D:

$D(q)\, 2\pi q\, dq = D(\varepsilon)\, d\varepsilon$

$\frac{2A}{4\pi^2}\, 2\pi \cdot \frac{m^*}{\hbar^2} = D(\varepsilon) = \frac{A m^*}{\pi\hbar^2}$ → Constant no singularity

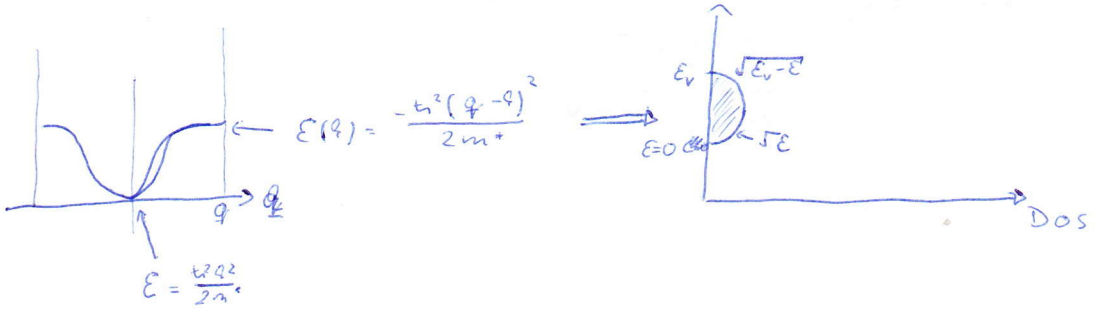
3D: $D(q)\, 4\pi q^2 dq = D(\varepsilon)\, d\varepsilon$

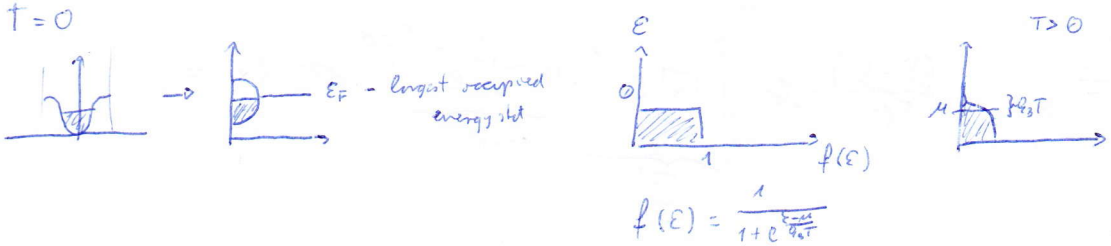
$D(\varepsilon) = \frac{V}{4\pi^3} 4\pi \cdot q^2 \frac{m^*}{\hbar^2 q} =$

$\left(\frac{d\varepsilon}{dq}\right)^{-1} = \left(\frac{\hbar^2 q}{m}\right)^{-1}$

$D(\varepsilon) \sim k \sim \sqrt{\varepsilon}$

Occupation of bands in 3D





$f(\varepsilon) = \frac{1}{1 + e^{\frac{\varepsilon - \mu}{k_B T}}}$

ε_F only makes sense at $T = 0$

$\lim_{T \to 0} \mu(T) = \varepsilon_F$

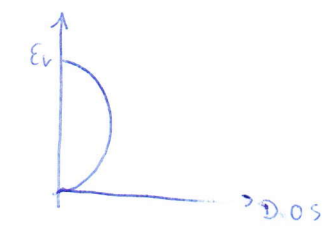
Number of charge carriers

$N_c = n \cdot V = \int D(\varepsilon) f(\varepsilon)\, d\varepsilon$

n : density of electrons — system specific function

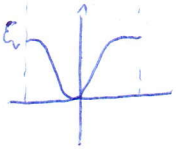
$f(\varepsilon)$: quantum statistics of electrons

Top of the valence band



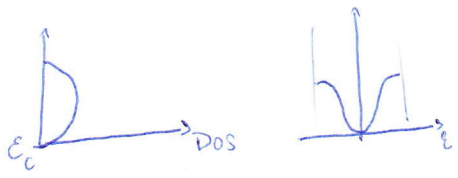
$D_V(\varepsilon) = \frac{V}{2\pi^2} \left(\frac{2m_V^*}{\hbar^2}\right)^{3/2} (\varepsilon_V - \varepsilon)^{1/2}$

(D_V of valence band)

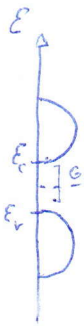


Bottom of conduction band

$$\mathcal{E}(\ell) = \frac{\hbar^2 \ell^2}{2m^* c}$$



$$D_c(\mathcal{E}) = \frac{V}{2\pi^2}\left(\frac{2m^* c}{\hbar^2}\right)^{\frac{3}{2}} (\mathcal{E}-\mathcal{E}_c)^{\frac{1}{2}}$$



$$f(\mathcal{E}) = \frac{1}{1+e^{\frac{\mathcal{E}-\mu}{k_B T}}} \approx$$

$\mathcal{E}_c, \mathcal{E}_g$ ---- $\mu \approx \frac{\mathcal{E}_c + \mathcal{E}_v}{2}$; $|\mathcal{E}-\mu| \approx \frac{1}{2}\mathcal{E}_g$

$\mathcal{E}_g \gg k_B T$

$\mathcal{E}_g$: 1,2 eV ; $k_B T$: 26 meV

density of e^-

$$n = \frac{1}{V}\int_{\mathcal{E}_c}^{\infty} D_c(\mathcal{E}) f(\mathcal{E})\, d\mathcal{E} \qquad p = \frac{1}{V}\int_{-\infty}^{\mathcal{E}_v} D_v(\mathcal{E}) f(\mathcal{E})\, d\mathcal{E}$$

$$n \sim \int_{\mathcal{E}_c}^{\infty} \sqrt{\mathcal{E}-\mathcal{E}_c}\; e^{-\frac{\mathcal{E}-\mu}{k_B T}}\, d\mathcal{E} = \int_0^{\infty} \sqrt{x}\, e^{-x} \cdot \underbrace{(k_B T)^{\frac{3}{2}} e^{-\frac{\mathcal{E}_c-\mu}{k_B T}}}_{\text{const}}\, dx =$$

$\int_0^{\infty} \sqrt{x}\, e^{-x} dx = \frac{\sqrt{\pi}}{2}$

$$\left(\frac{\mathcal{E}-\mathcal{E}_c}{k_B T}\right) = x$$

$$n = 2\left[\frac{m_c^* k_B T}{2\pi\hbar^2}\right]^{\frac{3}{2}} e^{\frac{-(\mathcal{E}_c-\mu)}{k_B T}}$$

$$p = 2\left[\frac{m_v^* k_B T}{2\pi\hbar^2}\right]^{\frac{3}{2}} e^{-\frac{(\mu-\mathcal{E}_v)}{k_B T}}$$

conservation of charge (μ is unknown)

$n = p$ solve the equation for μ gives

$$\mu = \underbrace{\frac{1}{2}(\mathcal{E}_c+\mathcal{E}_v)}_{\mu \text{ is in the middle of the gap}} + \underbrace{\frac{3}{4} k_B T \ln\left[\frac{m_v^*}{m_c^*}\right]}_{\text{small change}}$$

n in sodium (Na) $n \sim 10^{21} - 10^{22} \frac{1}{cm^3}$

calculate n in a SC

$$n_c = 2 \left[\frac{k_B T}{2\pi\hbar^2}\right]^{\frac{3}{2}} (m_c^* m_v^*)^{\frac{3}{2}} e^{-\frac{E_g}{k_B T}} =$$

↑ substitute back μ

$$= \frac{1}{10} \left(\frac{10^{20}}{10^{-22}}\right)^{\frac{3}{2}} \left(10^{-31}\right)^3 \cdot e^{-40} = \boxed{10^{10} \frac{1}{cm^3}}$$

Week 3

Revision: DOS : $D(\varepsilon)$

$$n = \frac{1}{V}\int D(\varepsilon) f(\varepsilon)\, d\varepsilon \qquad 3D: D(\varepsilon) \sim \sqrt{\varepsilon}$$

$$n = p = 2\left[\frac{k_B T}{2\pi\hbar^2}\right]^{\frac{3}{2}} (m_c^* m_v^*)^{\frac{3}{4}} e^{-\frac{E_g}{k_B T}}$$

$$\boxed{n \sim e^{-\frac{E_g}{k_B T}}}$$

$n \cdot p = n_i^2(T)$ ← T dependence is const

is always valid not only for intrinsic (Law of Mass Action)

$$c = \frac{[OH^-][H^+]}{[H_2O]} = 10^{-14} \qquad pH = \frac{[H^+]}{[H_2O]}$$

Mobility vs charge concentration

Drude

$$ma = -eE - Kv \quad \Rightarrow \quad a = -\frac{eE}{m} - \underbrace{\frac{K}{m}v}_{\frac{v}{\tau}}$$

→ relaxation time approximation

stac.

$$0 = -Ee - Kv$$

$$j = \sigma E = n e v_D \qquad \boxed{\frac{|v_D|}{E} = \mu}$$ mobility

	Electron	Holes
Drift velocity	$v_{De} = \frac{-eE\tau_e}{m_e^*}$	$v_{Dh} = \frac{eE\tau_h}{m_h^*}$
curr density	$j_e = n \cdot e \cdot v_{De}$	$j_h = p \cdot e$
conductivity $j = \sigma E$	$\sigma = \frac{n e^2 \tau_e}{m_e^*}$	$\sigma_n \frac{p e^2 \tau_h}{m_h^*}$
mobility μ	$\mu_e = \frac{e\tau_e}{m_e^*}$	$\mu_h = \frac{e\tau_h}{m_h^*}$

Full conductivity: $\boxed{\sigma = n e \mu_e + p e \mu_h}$

HEMT: high electron-mobility transistor

$[\mu] = \frac{m\,m}{s\,V} = \frac{cm^2}{Vs}$ ("the larger, the better")

typical values: Si $\mu_e = 1000 \frac{cm^2}{Vs}$ → e^--phonon scattering

$\mu_h = 100 \frac{cm^2}{Vs}$ → intervalend scattering

GaAs $\mu_e = 30000 \frac{cm^2}{Vs}$

$\mu_h = 1000 \frac{cm^2}{Vs}$

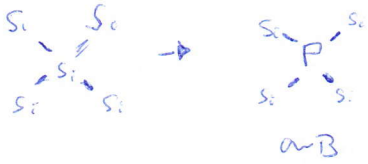
poly-silic $\mu_e \approx 1$

Pur Copper $\mu \sim 0{,}1 \frac{cm^2}{Vs}$

graphene $\mu = 2\,000\,000 \frac{cm^2}{Vs}$

Doping:

- replacing some atoms by heteroatoms

eg: 

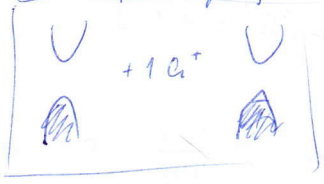
a-B

III → Al: Si p doped

V → As: Si n doped

Band picture: n-doping

p-doping



p: extra electron, extra proton [+ H atom]

n: extra hole, extra e⁻

 → band state

Schrödinger-eq. for Si

$$\left[-\frac{\hbar^2}{2m}\Delta + U(r)\right]\Psi(r) = E\,\Psi(r)$$

kinetic — atomic pot

we have the neutron

+ are Si replaced by P → same Sch. + Sch for H

H-atom, Bohr-radii: $\frac{mv^2}{r} = \frac{1}{4\pi\varepsilon_0}\frac{e^2}{r^2}$

$L = mvr = n\hbar$

$$r = \frac{1}{4\pi\varepsilon_0}\frac{e^2}{mv^2}$$

$$\boxed{v = \frac{e^2}{4\pi\varepsilon_0}\frac{1}{n\hbar}}$$

introduce: $\alpha = \frac{e^2}{\hbar c\, 4\pi\varepsilon_0} \approx \frac{1}{137}$

fine structure constant

$$v_n = \alpha\cdot\frac{c}{n}$$

$$r_n = \frac{1}{4\pi\varepsilon_0}\frac{e^2}{m\alpha^2c^2}n^2 = \frac{e^2}{4\pi\varepsilon_0\hbar c}\frac{\hbar}{mc}\frac{n^2}{\alpha^2} = \frac{n^2\hbar}{mc}\frac{1}{\alpha}$$

introduce: $a_B = \frac{\hbar}{mc}\frac{1}{\alpha} \approx 0{,}5\,\text{Å} = 5\cdot10^{-11}\,m$

↳ Bohr radius

Binding energy:

$$E = \frac{1}{2}mv_n^2 - \frac{1}{4\pi\varepsilon_0}\frac{e^2}{r_n} = \frac{1}{2}m\alpha^2\frac{c^2}{n^2} - \frac{\alpha^2\hbar c\, mc}{n^2\hbar} = -\frac{1}{2}mc^2\alpha^2\frac{1}{n^2}$$

10^{-4}

$0{,}5\,\text{MeV}$

$E_1 = -13{,}6\,eV$

In a SC: $m \to m_e^*$ $\quad (m_e^* = 0{,}1 \dots 1\ m_0)$

$\varepsilon_0 \to \varepsilon_0\varepsilon_r$ → extra $e^- + p^+$ coulomb potential is screened

$\varepsilon_r(Si) = 11{,}9$

Bohr-radius of a dopant:

$$a_B^* = \frac{m}{m_e^*}\cdot\varepsilon_r\cdot a_B \approx 100\,a_B$$

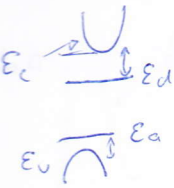
$a_B^* \gg a_B$

$$E_1^* = E_1\cdot\frac{m^*}{m}\frac{1}{\varepsilon_r^2} \longrightarrow E_1^* \ll E_1$$

E_1^*: Binding E

10 meV – 100 meV

typically



ε_d – donor energy $\quad \varepsilon_d - \varepsilon_c$ binding energy

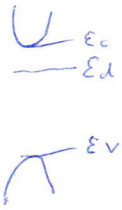
ε_a – acceptor energy $\quad \varepsilon_a - \varepsilon_v$

densities: donor density: n_D

average distance between donors: d

- if $d \ll a_B^*$ P – discrete state < 1 ppm doping
- if $d \lesssim a_B^*$ B – donor band 1000 ppm
- if $d \approx a_B^*$ B – degenerate SC few % doping

Doping & charge carrier concentration



intrinsic SC: $\mu \approx \frac{1}{2}(\varepsilon_c + \varepsilon_v)$

extrinsic SC: $\mu \approx \frac{1}{2}(\varepsilon_c + \varepsilon_d)$ → derivation complicated

Grand canonical ensemble $\langle n \rangle = \dfrac{\sum n \cdot e^{-\beta(\varepsilon_n - \mu n)}}{Z}$

→ partition function

for donor levels: $n = \emptyset, \uparrow, \downarrow, \not{2}$ → due to Coulomb repulsion

probability for single occupation

$$f_d(\varepsilon_d) = \frac{2\, e^{-\beta(\varepsilon_0 + \varepsilon_d - \mu)}}{e^{-\beta(\varepsilon_0 + 0)} + 2e^{-\beta(\varepsilon_0 + \varepsilon_d - \mu)}} =$$

ε_0: ground state

$\varepsilon_0 + \varepsilon_d$: ground + donor is occupied

↑ donor statistics

$$= \frac{1}{1 + \frac{1}{2} e^{\beta(\varepsilon_d - \mu)}}$$

$\Longrightarrow$ Fermi function

Probability of ionizing the donor state

$$1 - f_d(\varepsilon_d) = \frac{1 + \frac{1}{2} e^{\beta(\varepsilon_d - \mu)}}{1 + \frac{1}{2} e^{\beta(\varepsilon_d - \mu)}} - \frac{1}{1 + \frac{1}{2} e^{\beta(\varepsilon_i - \mu)}} = \frac{1}{1 + 2e^{\beta(\mu - \varepsilon_i)}}$$

(the first fraction equals 1)

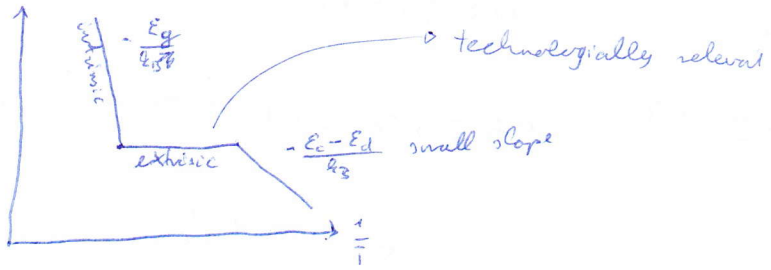
charge carrier concentration in the conduction band

$$n = n_d \frac{1}{1 + \frac{1}{2} e^{\beta(\mu - \varepsilon_d)}} \qquad \mu - \varepsilon_d = \underbrace{\frac{1}{2}(\varepsilon_c - \varepsilon_d)}_{\text{donor binding energy}}$$

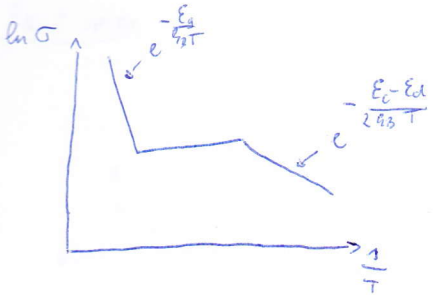
1. $T \to 0$ $\quad n = 0$
2. $k_B T \approx \varepsilon_c - \varepsilon_d$ donors are ionized
   $n \approx n_d$; depletion or extrinsic regime

3. $k_B T \gg \varepsilon_c - \varepsilon_d$ and $k_B T \approx \varepsilon_c - \varepsilon_v = \varepsilon_g$ intrinsic regime
   band - band excitations

$\sigma \sim n$ $\quad \ln \sigma$



Week 5

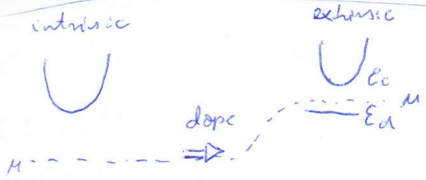


Law of mass action intrinsic $n = p = \sqrt{np}$

$$np = n_i^2(T) = n_c n_v e^{-\frac{E_g}{k_B T}}$$

$$\left.\begin{aligned} n &= n_c e^{-\frac{E_c - \mu}{k_B T}} \\ p &= n_v e^{-\frac{\mu - E_v}{k_B T}} \end{aligned}\right\}$$

Handwaving proof of law of mass action



$\mu \approx \frac{1}{2}(E_c + E_v)$

$$\left.\begin{aligned} n = n_d &= n_c e^{-\frac{E_c - \mu}{k_B T}} \\ p &= n_v e^{-(\mu - E_v)\beta} \end{aligned}\right\} \begin{array}{l} \rightarrow \text{goes up} \\ \rightarrow \text{goes down} \end{array}$$

their product remains the same

Band structure calculations

importance: - understand conduction properties (m^*, E_g)
- understand optical properties (E_g)
- intelligent design (band-engineering)

Band structure calculation methods

- empty lattice model (handwaving model) gives $\vec{q}$-space quantized
- ↓
- quasi-free electron approximation $\left(\frac{\hbar^2 q^2}{2m} + U(r)\right)$ ($U(r)$: periodic potential)
- ↓
- semi-empirical methods (tight-binding, TB, pseudopotential methods)
- ab initio (first principles) DFT
- interacting e^- model, GW...

$$H\Psi = E\Psi$$

$$H = \frac{-\hbar^2}{2m}\Delta + U(\underset{\sim}{r})$$

$$U(\underset{\sim}{r}) = \sum_{\substack{\text{atoms} \\ \text{ion-e} \\ \text{interact}}} H_{at} + \sum_{\substack{\text{for} \\ \text{all } e^-}} H_{e\text{-}e}$$

Simplification: use 1 e^- wavefunctions

$$\left[-\frac{\hbar^2}{2m} + U(\underset{\sim}{r})\right]\psi(\underset{\sim}{r}) = E\psi(\underset{\sim}{r})$$

↑ 1 e^- wavefunct.

In solids: $U(\underset{\sim}{r}) = U(\underset{\sim}{r} + \underset{\sim}{R})$ $\underset{\sim}{R}$ lattice vector

↳ lattice periodic

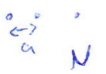
Bloch theorem: $\psi_{\underset{\sim}{q}}(\underset{\sim}{r}) = e^{i\underset{\sim}{q}\underset{\sim}{r}}\, u_{\underset{\sim}{q}}(\underset{\sim}{r})$

when $u_{\underset{\sim}{q}}(\underset{\sim}{r}) = u_{\underset{\sim}{q}}(\underset{\sim}{r} + \underset{\sim}{R})$

↳ $e^{i\underset{\sim}{q}\underset{\sim}{r}}$: plane wave

$\underset{\sim}{q}\in$ are given by the Born - Karman periodic boundary conditions

eg 1D



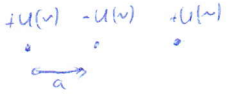
$$q = \frac{2\pi}{Na}n \qquad n = -\frac{N}{2} \cdots \frac{N}{2}$$

q: crystal wave number, crystal momentum

$n\hbar q$ ——————→

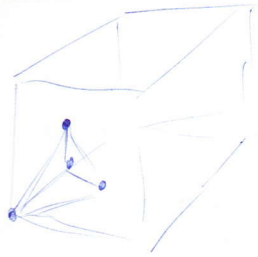
when $q = 0 \longrightarrow \psi_{q=0}(\underset{\sim}{r}) = u_{\underset{\sim}{q}}(\underset{\sim}{r})$ ↳ same for each lattice site

in 1D when $q = \pm\frac{\pi}{a}$, then



Structure and k-space

Real space

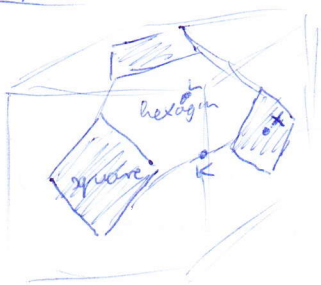


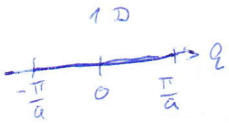
diamond

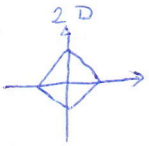
fcc + 2 atom basis

$(0,0,0)\ \left(\frac{1}{4},\frac{1}{4},\frac{1}{4}\right)a$

q-space







Distinguished points in q-space

Γ: BZ center $(0,0,0)$

L: middle of Hexagon

X: middle of square

K: middle point on two touching hexagons

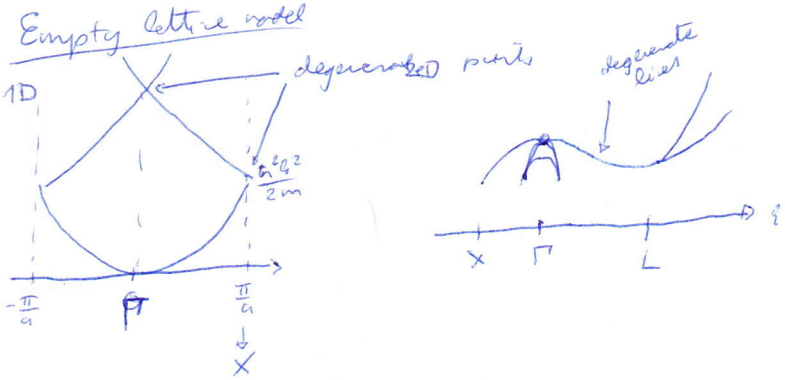
distinguished direction

100 Γ —Δ— X

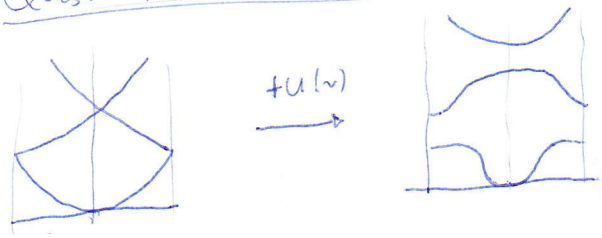
111 Γ —Λ— L

110 Γ —Σ— K

Empty lattice model



Quasi-free e^- approximation



$U(r) = U(x+n\,a)$

$H = \frac{\hbar^2}{2m}\partial_x^2 + U(x)$ ← solves E_q

$\Psi_q = \frac{1}{\sqrt{V}} e^{iqr}$

$E_q = \mathcal{E}_q + \langle \Psi_q | U(x) | \Psi_q \rangle$

good for away from degenerate points

$\mathcal{E} = \frac{\hbar^2 q^2}{2m}$

$H = \frac{\hbar^2}{2m}\partial_x^2$

$H\Psi_k = \mathcal{E}(q)\Psi_q$

Degenerate perturbation calculation

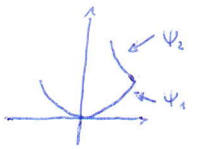
$$H = \begin{pmatrix} U_{11} & U_{12} \\ U_{21} & U_{22} \end{pmatrix} = \begin{pmatrix} \frac{\hbar^2 q^2}{2m} & U \\ U^* & \frac{\hbar^2(\frac{2\pi}{a}-q)^2}{2m} \end{pmatrix}$$

where $U = \int e^{-iqr} U(r)\, e^{i(q-G)r}\, dr = U(G)$

↕ Fourier integral

$U_{11} = \langle \Psi_{1q} | U | \Psi_{1q} \rangle$

$U_{12} = \langle \Psi_{1q} | U | \Psi_{2q} \rangle$

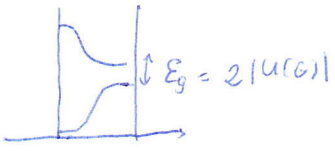


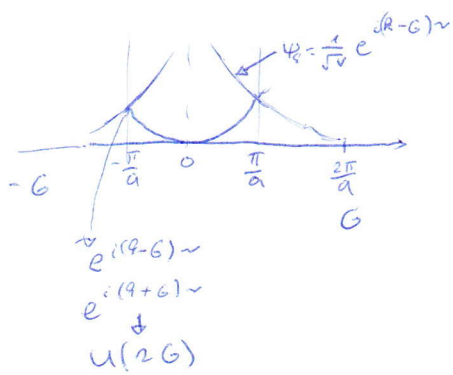
$\Psi_1 = \frac{1}{\sqrt{V}} e^{iqr}$

$\Psi_2 = \frac{1}{\sqrt{V}} e^{i(q-G)r}$

1D: $G = \frac{2\pi}{a}$

Solutions at degeneracy





Tight-binding approximation TBA

1D, 1 atom lattice $H\psi = E\psi$

$$H = -\frac{\hbar^2}{2m}\Delta + U(r)$$

$U(r) = \sum_R V_{atom}(r - R)$ — sum of atomic potentials

assume atomic solution is known

$$H_{at}\varphi_a = \varepsilon_a \varphi_a$$

$H_{at} = -\frac{\hbar^2}{2m}\Delta + V_{atom}$

Ansatz ("trial")

$$\psi_q(r) = \frac{1}{\sqrt{N}} \sum_n e^{iqa}\varphi_a(r - na)$$

short notation $\psi_q(r) = \sum_n e^{iqna}\underbrace{|n\rangle}_{\varphi_a(r-na)}$

substitute into Sch. eq.

$$H\psi = \sum_h e^{iqna}\left[-\frac{\hbar^2}{2m}\Delta + \sum_{q'} V_{at}(r - n'a)\right]|n\rangle = E(q)\sum_n e^{iqna}|n\rangle$$

project multiply $\langle n''|$ left $\longrightarrow$ $\langle n''|n\rangle = \delta_{n,n''}$ — wave functions are orthogonal

$$\sum_n e^{iqna}\left[\varepsilon_a \delta_{n''n} + \sum_{n''\neq n}\langle n''|V_{at}(r - n'a)|n\rangle\right] = E(q)\sum_n e^{iqn}\underbrace{\langle n''|n\rangle}_{\delta_{n''n}}$$

result:

$$E(q) = \varepsilon_a + \sum_{n,n'\neq n} e^{iq(n-n'')a}\langle n''|V_{at}(r - na)|n\rangle$$

From the sum: nearest-neighbour tight binding

Lets call

$$\langle n-1|V_{at}|n\rangle = -|t| = \langle n+1|V_{at}|n\rangle$$

$V<0$ (Coulomb int)

$$E(q) = \varepsilon_a + \underbrace{\left(e^{iqa} + e^{-iqa}\right)}_{2\cos(qa)} \cdot (-|t|) =$$

$$\boxed{E(q) = \varepsilon_a - 2|t|\cos(qa)}$$

BS calculations II.

TB version. $H\psi = E\psi$ $\quad H = \frac{-\hbar^2}{2m}\Delta + U(r)$ $\quad U(r) = \sum V_{at}(r - na)$

$H_{at}\varphi_a = \varepsilon_a \varphi_a$

$H_{at} = -\frac{\hbar^2}{2m}\Delta + V_{at}(r)$

Anzats $\quad \psi_q(r) = \frac{1}{\sqrt{N}} e^{iqna} \varphi_a(r - na)$ $\quad$ (satisfies Bloch-th.)

⇕ new notation

$\psi_q(r) = \sum_n e^{iqna} |n\rangle$ $\qquad \langle n'|n\rangle = \delta_{nn'}$

$$H\psi = \sum_n e^{iqna}\left[-\frac{\hbar^2}{2m}\Delta + \sum_{n'} V_{at}(r - n'a)\right]|n\rangle = E(q)\sum_n e^{iqna}|n\rangle \qquad / \langle n'| \text{ project}$$

$$\sum_{n'} V_{at}(r - n'a) = V_{at}(r - na) + \sum_{n' \neq n} V_{at}(r - n'a)$$

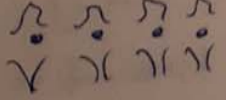
$$\sum_n e^{iqna}\left[\varepsilon_a \delta_{nn''} + \sum_{n' \neq n}\langle n''|V_{at}(r - n'a)|n\rangle\right] = E(q)\underbrace{\sum_n e^{iqna}\delta_{n,n''}}_{e^{iqn''a}}$$

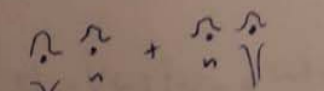
$$\boxed{E(q) = \varepsilon_a + \sum_{n,n' \neq n} e^{iq(n-n')a}\langle n''|V_{at}(r - na)|n\rangle}$$

Approximations: ① NNTB (nearest neighbour tight binding)

$\varphi_a(r - na)$ s-type

$V_{at}(r - na)$ central pt



NNTB: 

$n' = n'' = n+1$ $\qquad n'' = n' = n+1$

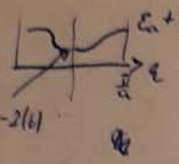
and $\langle n-1|V_{at}(r - (n-1)a)|n\rangle =$

$= \langle n+1|V_{at}(r - (n+1)a)|n\rangle =$

$= \int \varphi_a^*(r - (n-1)a)\, V(r - (n-1)a)\cdot \varphi_a(r - na)\, d^3r = -|t| \qquad |t| > 0$

t: overlap integral

NNTB: $E(q) = \varepsilon_a + \underbrace{\left(e^{iqa} + e^{-iqa}\right)}_{2\cos(qa)} \cdot (-1) \cdot |t| = \varepsilon_a - 2|t|\cos(qa)$



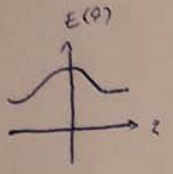
$m^* > 1$ ⟺ sss type overlap

⟺ ppσ type overlap

sign of overlap: +

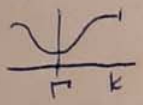
$E(q) = \varepsilon_a + 2|t|\cos(qa)$

hole type band.



$m^* < 0$

ppπ: overlap is negative



2nd NNTB:

$n' = n'' = n - 2$

$n' = n'' = n + 2$

$\left(e^{i2qa} + e^{-i2qa}\right)|t|$

$E(q) = \varepsilon_a - 2|t|\cos(qa) - \underbrace{2|t_{2nnn}|\cos(2qa)}_{\text{double periodically}}$

TB is semi-empirical:

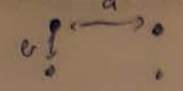
- DFT band structure + fitting with TB parameters
- fit t's from experiment like E_g, m^*

Example effective mass: $(m^*) = \frac{1}{a^2}\frac{\partial^2 E(q)}{\partial q^2}$

$E(q) = \varepsilon_a - 2|t|\underbrace{\cos(qa)}_{\approx 1 - \frac{q^2a^2}{2}} = \varepsilon_a - 2|t|\left[1 - \frac{q^2a^2}{2}\right] \longrightarrow (m^*)^{-1} = \frac{2|t|a^2}{\hbar^2}$

2D TB

$$E(q) = \varepsilon_a - 2|t_a|\cos(q_x a) - 2|t_e|\cos(q_y a)$$



"$\underline{q}\cdot\underline{p}$ model" – good semi-empirical model near band extrema ⟷ ideal for SC

– gives clear results for transport, optics, magnetic properties

$H\Psi = E\Psi$ solution obeys Bloch theorem

$$\Psi_{n,\underline{q}}(\underline{r}) = e^{i\underline{q}\underline{r}}\underbrace{u_{n\underline{q}}(\underline{r})}_{\text{lattice periodic function}}$$

$\underline{q}$: crystal momentum, generally $\hbar\dot{\underline{q}} = \underline{F}$ external

$\underline{p} = -i\hbar\nabla$ canonical impulse

$\hbar\underline{q} \neq \underline{p}$ except for plane waves

substitute $\Psi_{n,\underline{q}}(\underline{r})$ into $H\Psi$: $\Delta\Psi_{n,\underline{q}}(\underline{r}) = (i\underline{q})^2 e^{i\underline{q}\underline{r}} u_{n\underline{q}}(\underline{r}) + (i\underline{q}) e^{i\underline{q}\underline{r}} \nabla u_{n\underline{q}}(\underline{r}) +$

$+ e^{i\underline{q}\underline{r}} \Delta u_{n\underline{q}}(\underline{r})$ → write into $H\Psi$

$$\left[\frac{\hbar^2\underline{q}^2}{2m} - \frac{i\hbar^2\underline{q}}{m}\nabla - \frac{\hbar^2}{2m}\Delta + V(\underline{r})\right] u_{n\underline{q}}(\underline{r}) = E_{n\underline{q}}\, u_{n\underline{q}}(\underline{r})$$

$\underline{p} = -i\hbar\nabla$ put at $H\Psi$ gives

$$\left[\frac{\hbar^2\underline{q}^2}{2m} + \frac{\hbar\underline{q}\underline{p}}{m} + \frac{\underline{p}^2}{2m} + V(\underline{r})\right] u_{n,\underline{q}}(\underline{r}) = E_{n,\underline{q}}\, u_{n\underline{q}}(\underline{r})$$

so far exact!

$\underline{q}\cdot\underline{p}$ approximation: consider solution of $H\Psi = E\Psi$ near band edges where $\underline{q}=0$ (like Γ)

then $\left[\frac{\underline{p}^2}{2m} + V(\underline{r})\right] u_{n,0}(\underline{r}) = E_{n,0}\, u_{n0}(\underline{r})$ Schrödinger equation at the zone center

+ consider $\frac{\hbar^2\underline{q}^2}{2m} + \frac{\hbar\underline{q}\underline{p}}{m}$ as perturbation! → if $\underline{q}$ is small, it works

2nd order perturbation theory

Suppose: $H|n\rangle = \mathcal{E}_n|n\rangle$ is solved $|n\rangle$ is a set of orthonormal wave functions

$\langle n'|n\rangle = \delta_{nn'}$

$(H+V)\Psi = E\Psi$ what is E and Ψ?

Answer

$$E_n = \mathcal{E}_n + \langle n|V|n\rangle + \sum_{n'\neq n} \frac{|\langle n'|V|n\rangle|^2}{\mathcal{E}_{n'} - \mathcal{E}_n}$$

$$\Psi_n = |n\rangle + \sum_{n'\neq n} \frac{\langle n'|V|n\rangle |n'\rangle}{\mathcal{E}_{n'} - \mathcal{E}_n}$$

my basis $u_{n,0}(r)$:

Result: $u_{n,\underline{q}} = u_{n0} + \frac{\hbar}{m} \sum_{n'\neq n} \frac{\langle u_{n'0}|\underline{q}\cdot\underline{p}|u_{n0}\rangle}{E_{n0} - E_{n,0}} |u_{n'0}\rangle$

$$\langle u_{n0}| \underbrace{\frac{\hbar^2 q^2}{2m}} + \frac{\hbar \underline{q}\underline{p}}{m} |u_{n,0}\rangle$$

1st term is 0

$$\frac{\hbar^2 q^2}{2m}\langle u_{n'0}|u_{n0}\rangle \simeq \delta_{nn'}$$

but $n \neq n'$

Energy:

$$E_{n,\underline{q}} = E_{n,0} + \frac{\hbar^2 q^2}{2m} + \frac{\hbar^2}{m^2} \sum_{n'\neq n} \frac{|\langle u_{n',0}|\underline{q}\cdot\underline{p}|u_{n,0}\rangle|^2}{E_{n'} - E_n}$$

$$\langle u_{n,0}| \frac{q^2\hbar^2}{2m} + \frac{\hbar}{m}\underline{q}\underline{p}|u_{n,0}\rangle$$

gives $\frac{\hbar^2 q^2}{2m} \neq 0$ → linear term in q disappears in the band edge

Effective mass approximation

$$E_{n,q} = E_{n,0} + \frac{\hbar^2 q^2}{2m^*}$$

$$\frac{1}{m^*} = \frac{1}{m} + \frac{2}{mq^2} \sum_{n\neq n} \frac{|\langle u_{n0}|\underline{q}\cdot\underline{p}|u_{n0}\rangle|^2}{E_{n'0} - E_{n0}}$$

the matrix element is reasonable

$$\mathcal{P}^2 = \frac{1}{k^2} |\langle u_{n'0}|\underline{q}\,\underline{p}|u_{n,0}\rangle|^2$$

experimentally determined

$\frac{2P^2}{m} \approx 20\,eV$ for most groups IV and III-V SCs

this goes $\frac{1}{m^*} = \frac{1}{m} + \frac{2P^2}{mE_g}$ ← describes m^* well for IV and III-V SCs

Week 7 ppt

Week 8

Envelope function method

- works well in a SC with slowly varying external fields (magnetic, electric, doping, heterostructures, Band-gap engineering)

slowly: characteristic length scale of V is longer than the lattice constant

$H_0 \psi(\underset{\sim}{r}) = E \psi(\underset{\sim}{r})$ ↕ $E_{n,\underset{\sim}{q}}$

original H includes periodic potential

solution w/o fields (doping) is known

$\psi_{n\underset{\sim}{q}}(\underset{\sim}{r}) = e^{i\underset{\sim}{q}\underset{\sim}{r}} u_{n\underset{\sim}{q}}(\underset{\sim}{r})$ $\quad u_{n\underset{\sim}{q}}(\underset{\sim}{r}) = u_{n\underset{\sim}{q}}(\underset{\sim}{r} + \underset{\sim}{R})$

External Field: perturbation $V(\underset{\sim}{r})$

$H_0 + V(\underset{\sim}{r}) = H$

↑ slowly varying function $\quad V(\underset{\sim}{q}) = \int e^{i\underset{\sim}{q}\underset{\sim}{r}} V(\underset{\sim}{r})\, d^3r \sim \delta_{\underset{\sim}{q}} V_0$

$H\phi = E\phi$ / Ansatz $\quad \phi(\underset{\sim}{r}) = \sum_{n\underset{\sim}{q}} F_n(\underset{\sim}{q})\, \psi_{n\underset{\sim}{q}}(\underset{\sim}{r})$

linear combination of atomic orbitals

$F_n(\underset{\sim}{q})$: envelope function

Substitute into Sch-eqn:

$$\sum_{n\underset{\sim}{q}} \psi_{n,\underset{\sim}{q}} \left[E_{n,\underset{\sim}{q}}(\underset{\sim}{r}) - E + V(\underset{\sim}{r}) \right] F_n(\underset{\sim}{q}) = 0 \qquad (*)$$

$\psi_{n,\underset{\sim}{q}}(\underset{\sim}{r})$ forms an orthonormal set of functions

$$\int \psi^*_{n',\underset{\sim}{q}'}(\underset{\sim}{r})\, \psi_{n,\underset{\sim}{q}}(\underset{\sim}{r})\, d^3r = \delta_{nn',\underset{\sim}{q}\underset{\sim}{q}'} = \delta_{nn'}\delta_{\underset{\sim}{q}\underset{\sim}{q}'}$$

we $\int \psi^*_{n'\underset{\sim}{q}'}(\underset{\sim}{r})$ the (*) equation $\quad \langle \psi_{n'\underset{\sim}{q}'}(\underset{\sim}{r}) |$

$\langle \psi_{n'\underset{\sim}{q}'} | \psi_{n\underset{\sim}{q}} \rangle = \delta_{nn'}\delta_{\underset{\sim}{q}\underset{\sim}{q}'}$

$$\sum_{n\underset{\sim}{q}} \left[(E_{n\underset{\sim}{q}}(\underset{\sim}{r}) - E)\, \delta_{nn'}\delta_{\underset{\sim}{q}\underset{\sim}{q}'} + \langle \psi_{n'\underset{\sim}{q}'} | V(\underset{\sim}{r}) | \psi_{n\underset{\sim}{q}} \rangle \right] F_n(\underset{\sim}{q}) = 0 \qquad (**)$$

set of linear equations for $F_n(\underset{\sim}{q})$

$$\langle \psi_{n'\underset{\sim}{q}'}(\underset{\sim}{r}) | V(\underset{\sim}{r}) | \psi_{n,\underset{\sim}{q}}(\underset{\sim}{r}) \rangle = \int \underbrace{u^*_{n'\underset{\sim}{q}'}(\underset{\sim}{r}) u_{n\underset{\sim}{q}}(\underset{\sim}{r})}_{\text{atomic (fast)}} \underbrace{e^{i(\underset{\sim}{q}-\underset{\sim}{q}')\underset{\sim}{r}} V(\underset{\sim}{r})}_{\text{slowly varies}}\, d^3r$$

Envelope Function Approximation is

- Separation of the integral

$$\langle \psi_{n',q'} | V(\sim) | \psi_{nq} \rangle \approx \underbrace{\int u^*_{n'q'}(\sim)\, u_{nq}(\sim)\, d^3\sim}_{\text{Bloch's theorem says } \delta_{nn'}\,\delta_{qq'}} \underbrace{\int e^{i(q-q')r} V(\sim)\, d^3\sim}_{V(q-q')}$$

substitute back to (**)

$$\sum_q \left[\left(E_{n'q}(\sim) - E \right) \delta_{qq'} + V(q-q') \right] F_{n'}(q) = 0$$

Schrödinger equation for $F_{n'}(q)$

particle in a box

example: plane wave solution + effective mass approximation

$E_n(q) = E_c + \frac{\hbar^2 q^2}{2m_c^*}$ with this we get the EFA equation as

$$\frac{\hbar^2 q^2}{2m^*c} F_c(q) + \sum_q V(q-q') F_c(q) = (E - E_c) F_c(q)$$

↑ envelope fn. for cond. band; set of linear equations

We approximate canonical impulse with $-i\hbar\nabla \equiv q$ (is valid for plane waves)

(**) becomes

the Schrödinger equation for $F_c(q)$

$$\left[\frac{-\hbar^2 \Delta}{2 m_c^*} + E_c + V(\sim) \right] F_c(\sim) = E\, F_c(\sim)$$

FT both sides $F_c(\sim) \to F_c(q)$

$FT(q'(\sim)) = iq\, \phi(q)$

$$\boxed{FT\left(V(\sim) F_c(\sim)\right) = \int V(q-q') F_c(q)\, d^3\sim}$$

Substituting it back:

$$\frac{\hbar^2 q^2}{2m^*c} F_c(q') + \sum_q V(q-q') F_c(q) = (E - E_c(q)) F_c(q)$$

Semiempirical methods, it needs E_c and m_c^* as input

Example: extra charge (doping)

charge density $n(r) = \sum |\psi(r)|^2 \underbrace{f(E_i)}_{\text{Fermi fn}} = \underbrace{n_{c0}}_{\text{original charge density}} \sum F_c(r) f(E_c)$

i: band index

EFA is self consistent

works well if $a_B^* >> d$

eg.: doped Si: Si Si

current: j

thermal current j_Q

magnetoresistance

frequency dependent conductivity

Peltier & Seebeck effect

size (length) scales

- charge carrier length
  - diffusion

charge is created, annihilated

(example: solar cells)

Diffusion $l = v_F \cdot \tau$

τ: momentum scattering time
—"— relaxation time

τ_c charge carrier lifetime

Fick's law $j = -D \nabla n$

D: diffusion constant

$D \approx \frac{1}{3} v_F^2 \tau$

$D \approx \frac{1}{3} v_F l$

charge carrier diffusion length:

$\sigma_c = \sqrt{D \tau_c}$ solution of the diffusion eq.

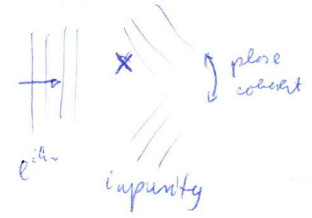
 $\rightarrow \langle \Delta x^2(t) \rangle = D t$

spin diffusion length

τ_s: spin lifetime

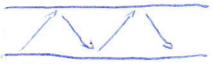
$\tau_s = 1\,ns - 1\,\mu s$ $\sigma_s = \sqrt{D \tau_s}$

Phase coherence length



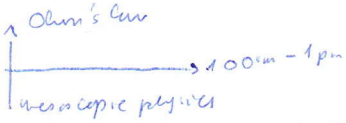
important for
- weak localization
- ballistic transport

optical analogy of ballistic transport is optical fiber



momentum relaxation time 10^{-13} - 10^{-15}

mean free path ~100nm $\quad l = v_F \tau$



Week 9

Transport in semiconductor

Diffusion → Ohm's law

	Free electrons (Sommerfeld-model)	Bloch-electrons
Quantum number	k ∈ periodic boundary condition	k ∈ periodic b.c. + n: band index
velocity	$\underline{v} = \frac{\hbar \underline{q}}{m} \frac{1}{\hbar} \frac{\partial \mathcal{E}}{\partial \underline{q}} = \frac{\hbar \underline{q}}{m}$	$\underline{v}(\underline{q}) = \frac{1}{\hbar} \frac{\partial \mathcal{E}}{\partial \underline{q}} = \frac{1}{\hbar} \nabla_{\underline{q}} \mathcal{E}(\underline{q})$
Energy dispersion	$\mathcal{E}(\underline{q}) = \frac{\hbar^2 q^2}{2m}$	$\mathcal{E}_n(\underline{q}) = \mathcal{E}_n(\underline{q}+\underline{G})$ $\quad G$ ∈ reciprocal lattice
wave fn	$\psi_{\underline{q}}(\underline{r}) = \frac{1}{\sqrt{V}} e^{i \underline{q} \underline{r}}$	$\psi_{n,\underline{q}}(\underline{r}) = e^{i \underline{q} \underline{r}} u_{n,\underline{q}}(\underline{r})$ where $u_{n,\underline{q}}(\underline{r}) = u_{n,\underline{q}}(\underline{r}+\underline{R})$
effective mass	$m^* = m$	$(\underline{\underline{m}}^*)^{-1} = \frac{1}{\hbar^2} \frac{\partial^2 \mathcal{E}}{\partial \underline{q}^2}$ $\quad \underline{\underline{m}}^*$ tensor

Reminder: Drude-modell

$$m\underline{a} = -e\underline{E} - K\underline{v}$$

+ damping parameter

$$m\dot{\underline{v}} = -e\underline{E} - \frac{m}{\tau}\underline{v} \longrightarrow \boxed{\sigma = \frac{ne^2\tau}{m}}$$

Drude: - resistivity is due to collisions with ions, viscous movement

Bloch-modell: motion of electrons in a perfect lattice (ions at equilibrium position)

$\sigma = \infty \quad v = \text{constant}$

$\tau = \infty$

resistivity is given by impurities and lattice vibrations (phonons)

Canonical vs crystal momentum

conservation of momentum → result of translational invariance

in a crystal: discrete translational invariance $\underline{r} \to \underline{r} + \underline{R}$

→ crystal momentum is conserved ($\hbar \underline{q}$)

Forces: $F_{ext} = \hbar \dot{\underline{q}}$ ← periodic potential is transformed out from the problem

Price paid: - $u_{n,q}(\underline{r})$ are not nice

- canonical impulse ≠ crystal momentum ↔ $p \neq \hbar q$

$$\hat{p}\,\psi_{n,q}(\underline{r}) = \frac{\hbar}{i}\nabla\left[e^{i\underline{q}\underline{r}}\,u_{nq}(r)\right] = \hbar q\,\psi_{n,q}(\underline{r}) + \frac{\hbar}{i}e^{i\underline{q}\underline{r}}\nabla u_{n,q}(\underline{r})$$

Bloch functions are not eigenstates of canonical impulse

Contribution of a closed electron band to conduction

$$\underset{\text{at } T=0}{\underline{j}} = -e\int \frac{d^3q}{4\pi^3}\underbrace{\frac{1}{\hbar}\frac{\partial \varepsilon}{\partial \underline{q}}}_{\underline{v}(q)}$$

$$\underline{j} = -e\int D(\underline{q})\,f(\underline{q})\,\underline{v}(q)\,d^3\underline{r}$$

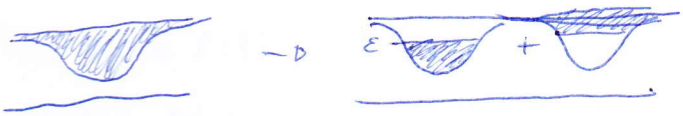
$D(\underline{q})$: DOS; $f(\underline{q})$: occupation (Fermi)

$$\underline{j} = -e\int_{\text{closed band}} \frac{d^3q}{4\pi^3}\frac{1}{\hbar}\frac{\partial \varepsilon}{\partial \underline{q}} = 0 \quad \text{(strong)}$$

$$\underbrace{\int \frac{d^3q}{4\pi^3}}_{\text{symmetric domain}}\frac{\partial \varepsilon}{\partial \underline{q}} = 0 \longrightarrow \text{odd function}$$

Concept of holes:

$$0 = \int_{\text{closed band}} \frac{d^3q}{4\pi^3}\underline{v}(\underline{q}) = \int_{\text{states until } \varepsilon} \frac{d^3q}{4\pi^3}v(\underline{q}) + \int_{\text{states above } \varepsilon} \frac{d^3q}{4\pi^3}v(q)$$



$$-e\int_{\text{states below } \varepsilon} \frac{d^3q}{4\pi^3}\underline{v}(\underline{q}) = +e\int \frac{d^3q}{4\pi^3}v(q)$$

Boltzmann equation

We describe the system with a particle distribution function

$f(q, v, t)$ distribution funct

simplest form $f_0(E(q), q \approx, t) = \frac{1}{e^{\frac{E(q)-\mu}{k_B T}} + 1}$

measurable quantities:

$$j(q) = -e \int D(\underline{q})\, f(E(q))\, \underline{v}(\underline{q})\, d^3q$$

Boltzmann

$$\frac{df}{dt} = \frac{\partial f}{\partial t} + \dot{\underline{q}} \nabla_q f + \dot{\underline{v}} \nabla_v f = \left.\frac{\partial f}{\partial t}\right|_{\text{collision term}}$$

L.B. introduced Heuristically

$\dot{\underline{q}} \nabla_q f$ → Force term $\quad \dot{\underline{q}} \sim \underline{F}_{ext}$

$\dot{\underline{v}} \nabla_v f$ → Diffusion term we neglect

Assume: force term only

$$\frac{\partial f}{\partial t} + \frac{1}{\hbar} F_{ext} \frac{\partial f}{\partial \underline{q}} = \left.\frac{\partial f}{\partial t}\right|_{coll} = \frac{-g(t,q)}{\tau}$$ relaxation time approximation

$$f(q,t) = f^0(q,t) + g(q,t)$$

f^0: equil. distrib.; g: difference from equil.

τ: relaxation time

scattering probability per unit time from $\underline{q} \to \underline{q}'$

usually $\tau = \tau(\underline{q})$

τ is the same as τ in Drude model

Assume: ① external Force

$$\frac{\partial f}{\partial t} = \frac{\partial f^\circ}{\partial t} + \frac{\partial g(\underline{q},t)}{\partial t} = \frac{-g(\underline{q},t)}{\tau} \rightarrow \boxed{g(\underline{q},t) = g(\underline{q},0)\, e^{-\frac{t}{\tau}}}$$

$\frac{\partial f^\circ}{\partial t} = 0$

origin of the name

Week 10 | Week 11

B.E.:

$$\frac{df}{dt} = \frac{\partial f}{\partial t} + \overbrace{\nabla_{\underline{x}} f \cdot \dot{\underline{x}}}^{\text{Force}} + \overbrace{\nabla_{\underline{v}} f \cdot \dot{\underline{v}}}^{\text{diffusion}} = \left.\frac{\partial f}{\partial t}\right|_{coll}$$

f distribution fn: $f^\circ(\underline{\epsilon}) = \frac{1}{1 + e^{\frac{\epsilon(\underline{q}) - \mu}{k_B T}}}$

$m\dot{\underline{v}} = \underline{F}_{ext}$

assume: $f(\underline{q},t) = f_e^\circ(\underline{q}) + g(\underline{q},t)$

relax. time approx: $\left.\frac{\partial f}{\partial t}\right|_{coll} = \frac{-g(\underline{q},t)}{\tau(\underline{q})} = \frac{-g(\underline{q},t)}{\tau}$

stat case: $\frac{\partial f}{\partial t} = 0$ + $\underline{F}_{ext} = -e\underline{E}$

neglect diffusion $\nabla_v f = 0$

Force term $\nabla_{\underline{x}} f = \frac{\partial f}{\partial \underline{x}} = \frac{\partial f}{\partial \epsilon}\frac{\partial \epsilon(\underline{q})}{\partial \underline{x}} = \frac{\partial f}{\partial \epsilon} m \underline{v}(\underline{q})$

$$\boxed{\underline{v}(\underline{q}) = \frac{1}{m}\frac{\partial \epsilon(\underline{q})}{\partial \underline{q}}}$$ Substitute back to B.E.

$$-\frac{e\underline{E}}{m}\frac{\partial f}{\partial \epsilon} m \underline{v}(\underline{q}) = -\frac{g(\underline{q},t)}{\tau}$$

Solution: $g(\underline{q},t) = \frac{\partial f}{\partial \epsilon} e\underline{E}\, \underline{v}(\underline{q})\, \tau$

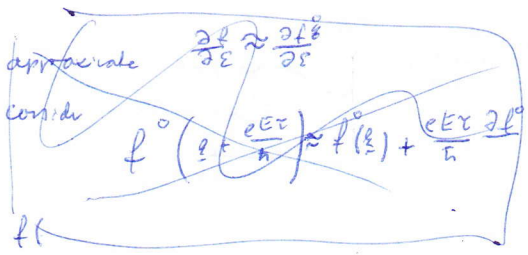
With this

$$f(\underline{q},t) = f^\circ(\underline{q}) + \frac{\partial f}{\partial \epsilon} e\underline{E}\, \underline{v}(\underline{q})\, \tau$$

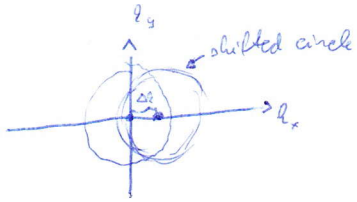
approx: $\frac{\partial f}{\partial \epsilon} \approx \frac{\partial f^\circ}{\partial \epsilon}$

consider $f^\circ\left(\underline{q} + \frac{e\underline{E}\tau}{m}\right) \approx f^\circ(\underline{q}) + \frac{e\underline{E}\tau}{m}\frac{\partial f^\circ}{\partial \epsilon}\underbrace{\frac{\partial \epsilon}{\partial \underline{q}}}_{m\underline{v}(\underline{q})} =$

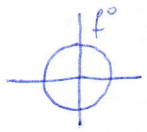
$$= f^\circ(\underline{q}) + e\underline{E}\tau\frac{\partial f}{\partial \epsilon}\underline{v}(\underline{q})$$



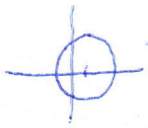
perturbed distribution function looks like as it was shifted in $\underline{q}$-space by $\boxed{\Delta\underline{q} = \frac{-e\underline{E}\tau}{m}}$



net current:



no net current



net current!

→ net drift velocity from BE

$$v_d = \frac{\hbar \Delta q}{m^*}$$

$$v_d = \frac{-eE\tau}{m^*}$$ Boltzmann-eq. → same as Drude model

Drude

many, slow electrons

$v_d \ll v_f$

$j = nev_d$

Boltzmann

a few electrons on the Fermi-surface

v_f (fast)

$$j = ev_F \frac{n v_d}{v_F}$$

number of charge carr.

Transport in SCs II

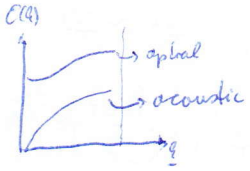
τ is principal quantity

origins: phonons, impurities, defects

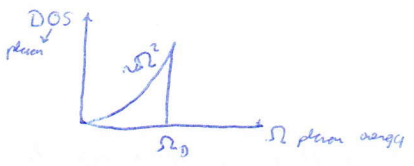
Matthiesen's rule: $\frac{1}{\tau} = \frac{1}{\tau_{e\text{-}e}} + \frac{1}{\tau_{e\text{-}ph}} + \frac{1}{\tau_{imp}} + \dots$

e-e interact. | e-ph interaction

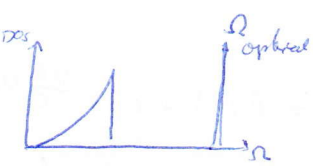
phonon-dispersion:



Debye-model



Debye-Einstein:



Eliashberg - formalism: $\frac{\hbar}{\tau} = 2\pi k_B T \lambda$ λ: e-ph coupling const

$0,1 - 1$ typical value

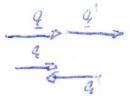
τ is always around $10^{-13} - 10^{-15}$ sec.

only valid if T is large

$\lambda = 2\int \frac{d\Omega}{\Omega} \alpha^2 F(\Omega)$ $\alpha^2 F(\Omega)$ material when $F(\Omega) \sim$ DOS

$\frac{\alpha^2}{L_D}$ e-ph coupling

$\alpha^2 F(\Omega)$ contains the so-called $(1 - \cos\theta)$ term



Bloch - Grüneisen fn

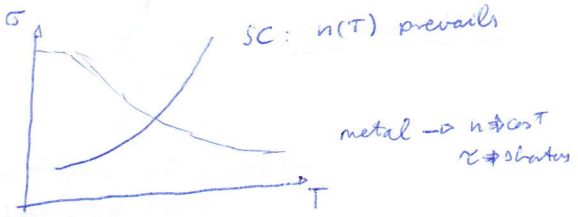
- Debye model with a single T_D

$$\frac{\hbar}{\tau} = 2\pi \lambda k_B T \int_0^{\Omega_D} \frac{d\Omega}{\Omega} \left(\frac{\Omega}{\Omega_D}\right)^2 \left[\frac{\hbar\Omega / k_B T}{\sinh\left(\frac{\hbar\Omega}{k_B T}\right)}\right]^2$$

is 1 if $T \to \infty$

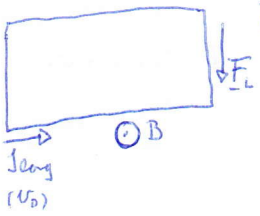
$\sim T^4$ if $T \to 0$

in semiconductors: $\sigma = \frac{n e^2 \tau}{m^*}$



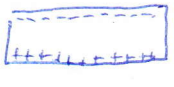
Magneto-transport

Hall-effect:



$\underline{F} = q\,\underline{v} \times \underline{B}$

Stationary conditions: internal field builds up to compensate for it



$v_D = \frac{e E_e \tau}{m^*}$ E_e: Longitud. electric field

$e E_t = e v_D B \rightarrow E_t = v_D B = \frac{e E_e \tau}{m^*} B$

Hall voltage $V_H = d \cdot v_D \cdot B = \frac{d e E_e B \tau}{m^*}$

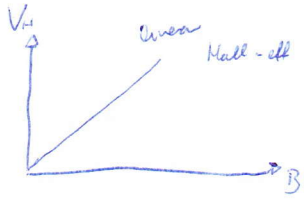
Def: R_H: Hall resistivity $\quad j = \sigma E \;;\; j\varrho = E$

$$R_H = \frac{E_t}{j_{exp}} = \frac{v_D B}{j_{exp}} = \frac{v_D B}{n e v_D} = \frac{B}{ne}$$

$$[R_H] = \frac{V_S\, m^3}{m^2 A_S} = \frac{V}{A} m = \Omega m$$

Hall constant

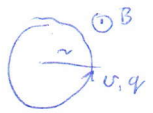
$$R \triangleq \frac{R_H}{B} = \frac{1}{ne} \qquad \text{charge carrier sensitive!}$$



QHE.

$\mu_B B >> \frac{\hbar}{\tau}$

$\frac{\hbar}{\tau}$ – broadening parameter



$\boxed{\omega = \frac{qB}{m}}$ cyclotron freq

$\hbar\omega_c$ = level spacing $\quad \frac{q\hbar}{m} B$, with $\mu_B = \frac{e\hbar}{2m}$

QHE appears when: $\hbar\omega_c > \frac{\hbar}{\tau}$

$\omega_c > \frac{1}{\tau}$

$\omega_c \tau > 1$

– close a cyclotron orbit before scattering

No simple inversion $\quad \varrho \neq \frac{1}{\sigma}$

$$\varrho_{xx} = \frac{\sigma_{xx}}{\sigma_{xy}^2 + \sigma_{yx}^2} = \frac{m^*}{ne^2\tau} = \frac{1}{n\mu e}$$

$\varrho_{xx} = \frac{1}{\sigma_{xx}}$ if σ_{xy} is small

$$\varrho_{xy} = \frac{\sigma_{xy}}{\sigma_{yx}^2 + \sigma_{xx}^2} = \frac{B}{|e|n} \quad \leftarrow \text{Hall resistivity}$$

in practice: $\quad n = \frac{1}{|e|\left(\frac{\partial \varrho_{xy}}{\partial B}\right)\Big|_{B=0}}$ $\qquad \mu = \frac{\left(\frac{\partial \varrho_{xy}}{\partial B}\right)_{B=0}}{\varrho_{xx}}$

μ: carrier mobility

Magnetothermal effects

B.E.

$$\frac{df}{dt} = \frac{\partial f}{\partial t} + \dot{\underline{q}}\,\underline{\nabla}_q f + \dot{\underline{v}}\,\underline{\nabla}_v f = \frac{-g}{\tau}$$

$f(\underline{q}, \underline{v}, t)$ Experiment shows $\underline{\nabla} T \longrightarrow \underline{j}$ (Seebeck-effect)

$\underline{j} \longrightarrow \underline{j}_Q$ (Peltier-effect)

$\mu(\underline{r}), T(\underline{r}), c(\underline{r}) \longrightarrow$ spatial variation

- neglect diffusion $\dot{\underline{v}}\,\underline{\nabla} f = 0$
- $\dot{f} = \frac{\partial f}{\partial t} + \dot{\underline{q}}\,\underline{\nabla}_q f + \cancel{\frac{\partial f}{\partial x}\frac{\partial x}{\partial t}} \frac{\partial f}{\partial x}\frac{\partial x}{\partial T}\underbrace{\frac{\partial T}{\partial \underline{r}}}_{\underline{\nabla} T}\underbrace{\frac{\partial \underline{r}}{\partial t}}_{\dot{\underline{r}}} + \dots$

$$f^\circ = \frac{1}{e^x + 1}$$

Week 12

$$\frac{df}{dt} = \frac{\partial f}{\partial t} + \nabla_{\vec{r}} f \cdot \dot{\vec{r}} + \nabla_{\vec{p}} f \cdot \dot{\vec{p}} = -\frac{f}{\tau}$$

$$f^\circ = \frac{1}{e^{\beta(\varepsilon-\mu)}+1}$$

$$\frac{\partial f}{\partial \varepsilon}\frac{\partial \varepsilon}{\partial x}\nabla T \cdot \dot{\vec{r}} + \dot{\vec{r}} \cdot (\vec{n}\cdot\vec{j})\nabla\left(\frac{(\mu-\varepsilon)e}{T e}\right)$$

Collect all terms:

$$\boxed{\frac{df}{dt} = \frac{\partial f}{\partial t} + \frac{\partial f}{\partial \varepsilon}\cdot \vec{v}(\vec{p})\left[\vec{F}_{ext} - \nabla\mu + \frac{\varepsilon(\vec{p})-\mu}{T}(-\nabla T)\right]}$$

Force: $\dot{\vec{p}}\, f\, \nabla_{\vec{p}}$

$$\dot{\vec{p}} = \vec{F}_{ext}$$

$$\vec{v}(\vec{p})\cdot\frac{\partial f}{\partial \varepsilon} = \frac{\partial \varepsilon}{\partial \vec{p}}\frac{\partial f}{\partial \varepsilon} = f\,\nabla_{\vec{r}}$$

$$\varepsilon = \varepsilon(\vec{p})$$

$$\frac{\partial \varepsilon}{\partial \vec{r}} = \vec{v}(\vec{p})$$

Remember:

$$\frac{df}{dt} = \frac{\partial f}{\partial \varepsilon}\vec{v}(\vec{p})\cdot(-e)\vec{E} = -\frac{f}{\tau}$$

solution $f = f^\circ + e\vec{E}\tau\vec{v}(\vec{p})\cdot\frac{\partial f}{\partial \varepsilon}$

$-\nabla\mu$, $-\nabla T$ act as forces

Particle current:

$$\vec{j}_n = \int \frac{d^3p}{h^3}\vec{v}(\vec{p})f(\vec{p})$$

$$\vec{j} = -e\int \frac{d^3p}{h^3}\vec{v}(\vec{p})f(\vec{p})$$

$$\vec{j}_Q = \int \frac{d^3p}{h^3}\vec{v}(\vec{p})f(\vec{p})\left[\varepsilon(\vec{p})-\mu\right]$$

$dU = \delta Q + \delta W$

$\hookrightarrow dU = TdS + \mu dn$

heat transfer

$TdS = dU - \mu dn$

$\downarrow$

$\int \varepsilon(\vec{p})\vec{v}(\vec{p})f(\vec{p})\frac{d^3p}{h^3}$

Without derivation

$$\vec{j} = K_0\left(\vec{E} + \frac{\nabla\mu}{e}\right) - K_1\left(\frac{\nabla T}{T}\right)$$

$$\vec{j}_Q = K_1\left(\vec{E} + \frac{\nabla\mu}{e}\right) + K_2\left(-\frac{\nabla T}{T}\right)$$

$K_{0,1,2}$ → integrals of $v(\vec{p})f(\vec{p})$

→ two K_1's are the same cross-coefficient

Onsager-relation ("4th law of thermodynamics")

principle of detailed balance

Examples: ① Heat conductivity

$$j_Q = -K \nabla T \quad \text{Fourier-law}$$

$$j = 0$$

$$K_0\left(E + \frac{\nabla \mu}{e}\right) - K_1\left(-\frac{\nabla T}{T}\right) = 0 \quad \text{substitute into } j_Q$$

$$K = \frac{K_2}{T} - \frac{K_1^2}{K_0 T}$$

② Seebeck-effect

$\nabla T \neq 0$, $E = 0$ $\Big\}$ $j \neq 0$ or open circuit $j = 0$, $\nabla T \neq 0$, $E \neq 0$

definition: $\left(E + \frac{\nabla \mu}{e}\right) \triangleq S \nabla T$

↳ Seebeck coefficient

$$\boxed{S = \frac{-1}{T}\frac{K_1}{K_0}}$$

③ Peltier-eff

$\nabla T = 0$, $j \neq 0 \rightarrow j_Q \neq 0$

definition $j_Q = \Pi j$

↳ Peltier-constant

$$\boxed{\Pi = \frac{-K_1}{K_0}}$$

$$\boxed{\Pi = S T} \quad \text{Kelvin-relation} \quad \text{(spec. case of Onsager)}$$

Wiedemann-Franz law: (in metals)

thermal conductivity $\frac{K}{\sigma} = L T$ ← electric conductivity

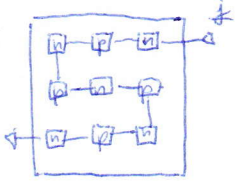
$$L = \frac{\pi^2}{3}\left(\frac{k_B}{e}\right)^2$$

↳ free electron

$$\boxed{\frac{K}{\sigma} = \frac{K_2}{K_0 T}} \quad \text{gives} \quad \boxed{L = \frac{K_2}{K_0 T^2}}$$

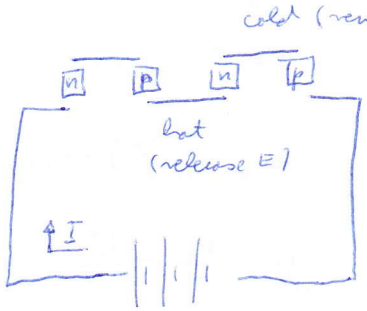
Thermoelectric (Peltier) cooler:

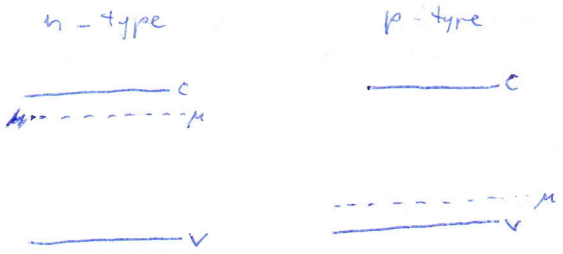
Front:

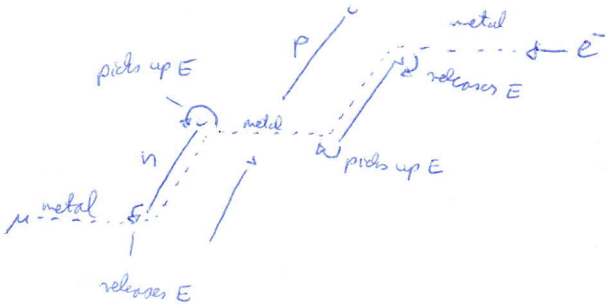


Side: cold, hot, ice

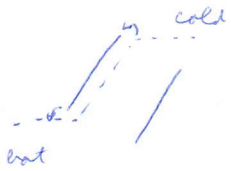
heat flow in parallel







• single n is also peltier cooler



 ← this would not work

Diffusion effects in SCs

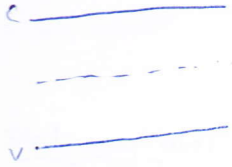
intrinsic SCs

$$n = p = n_i(T) = 2\left(\frac{k_B T}{2\pi\hbar^2}\right)^{3/2}\left(m_e^* m_p^*\right)^{3/4} e^{-\frac{E_g}{k_B T}}$$ depends on T

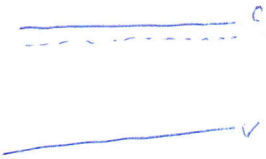
Law of mass action: $np = n_i^2(T)$

~~for extrinsic~~

intrinsic



extrinsic



doped: majority charge carriers
↓
minority cc.

n-type: n: majority p: minority

p-type: p: majority n: minority

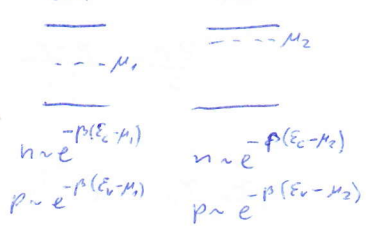
Important: $np = n_i^2(T)$ still valid

why is $n \cdot p = n_i^2(T)$ retained

n increased by $e^{-\beta(\mu_1 - \mu_2)}$

p decreased by $e^{-\beta(\mu_2 - \mu_1)}$

→ product stays the same



a non-equilibrium c-c

excitation (by light, injection, thermal excitation)

equilibrium n_0, p_0

non-equal n, p

Recombination rate $R \sim np$

thermal excitation $G_{thermal} = c \cdot n_0 p_0 = R^0$
↓
const

Net recombination rate $U = R - G_{thermal} = c(np - n_0 p_0)$

$$U = c\left[\underbrace{(n-n_0)(p-p_0)}_{\text{2nd order (Yeet is out)}} + n_0(p-p_0) + p_0(n-n_0)\right]$$

$$U \approx c\left[n_0(p-p_0) + p_0(n-n_0)\right]$$

n type $n_0 >> p_0 \rightarrow U \approx c\, n_0 (p-p_0)$

p type $p_0 >> n_0 \rightarrow U \approx c\, p_0 (n-n_0)$

} recombination is given by minority c-c. concentration

$\dot{n} = -c(n-n_0)$; $\dot{n} = \frac{-n-n_0}{\tau_n}$

$\dot{p} = \frac{-p-p_0}{\tau_p}$

τ_n, τ_p → cc. lifetime

Week 13

n-type $n >> p$ $n \approx n_d$ ← donors

p-type $p >> n$ $p \approx n_a$ ← acceptors

in equilibrium

$$n_0 p_0 = n_i^2(T) \quad \text{always}$$

recombination is given by the minority c-c

in n-type: $\frac{\partial n}{\partial t} = \frac{p - p_0}{\tau_p}$ $p_0 << n_0$

$p > p_0 \rightarrow$ annihilation

$$\frac{\partial p}{\partial t} = \frac{-p - p_0}{\tau_p} \quad \text{eq. if } p > p_0$$

τ_n τ_p c-c lifetime $\tau_n \tau_p >> \tau$

up to 1ms

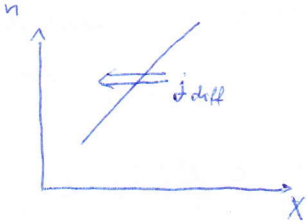
Continuity equation: $\frac{\partial \rho}{\partial t} + \nabla j = \sigma$

For our case

n-type
$$\begin{cases} \frac{\partial n}{\partial t} - \frac{1}{e} \nabla j_n = - \frac{p - p_0}{\tau_p} \\ \frac{\partial p}{\partial t} + \frac{1}{e} \nabla j_p = - \frac{p - p_0}{\tau_p} \end{cases}$$

p-type
$$\begin{cases} \frac{\partial n}{\partial t} - \frac{1}{e} \nabla j_n = - \frac{n - n_0}{\tau_n} \\ \frac{\partial p}{\partial t} + \frac{1}{e} \nabla j_p = - \frac{n - n_0}{\tau_p} \end{cases}$$

Case of spatial inhomogeneity:



$j_{diff} = -D \nabla n$ Fick-eq

diffusion const

$D \approx v^2 \tau$

mean free path approximation

v usually v_F

in the presence of an external field → drift current

$$\underline{j} = n e \underline{v}_{drift} = n e \mu \underline{E} = -n e \mu \underline{\nabla} V$$

(μ: mobility; $\underline{E} = -\underline{\nabla} V$: potential)

Stationary case:

$$\underline{j}_{Diff} + \underline{j}_{Drift} = \underline{0}$$

$$e D \underline{\nabla} n + (-e) n \mu \underline{\nabla} V = 0 \qquad (*)$$

$$n \approx f(\mathcal{E} - eV, T) = \frac{1}{e^{\frac{\mathcal{E} - eV - \mu}{k_B T}} + 1} \approx e^{-\frac{\mathcal{E} - eV - \mu}{k_B T}}$$

$$\boxed{\nabla n = \nabla f = n \cdot \frac{e}{k_B T} \underline{\nabla} V} \qquad \text{if } V = V(x)$$

Write back to (*)

$$\left(\frac{e^2 D n}{k_B T} - n e \mu \right) \underline{\nabla} V = 0$$

$$\boxed{\mu = \frac{e}{k_B T} D} \quad \text{Einstein-relation}$$

mobility, special case of fluctuation-dissipation theorem

Charge inhomogeneity + stationary condition

n-type SC inject holes

$$\frac{1}{e} \underline{\nabla} p = -\frac{p - p_0}{\tau_p} \quad \text{eq. continuity}$$

$$j_p = -e D \underline{\nabla} p \quad \left(\underline{\nabla} p = \frac{\partial p}{\partial x} \right)$$

} combine in 1D

$$\frac{\partial^2 p}{\partial x^2} = \frac{1}{D} \frac{p - p_0}{\tau_p}$$

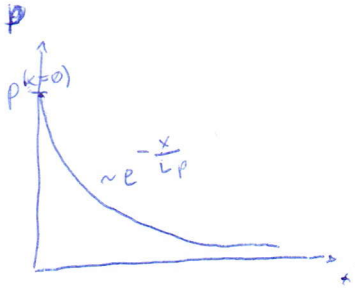
$$\frac{\partial^2 p}{\partial x^2} = \frac{1}{D} \frac{p - p_0}{\tau_p} \qquad \frac{\partial^2 f}{\partial x^2} = a \rightarrow e^{-x\sqrt{a}}$$

solutions: $p(x) = p_0 + [p(x=0) - p_0] e^{-\frac{x}{L_p}}$

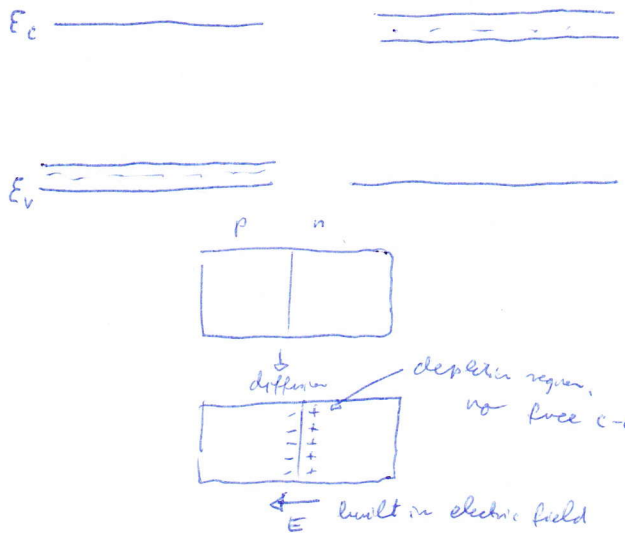
where $L_p = \sqrt{D \tau_p}$ charge diffusion length

$$\boxed{L_p = v_F \sqrt{\tau \tau_p}}$$

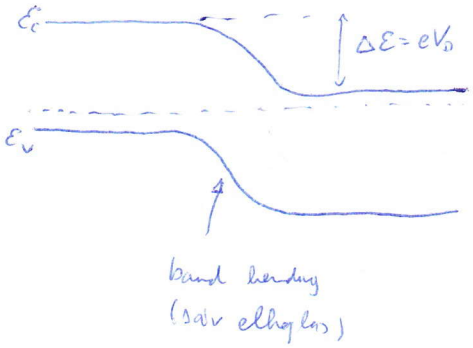
L_p can be up to 1 cm



SC devices



band structure after contact:

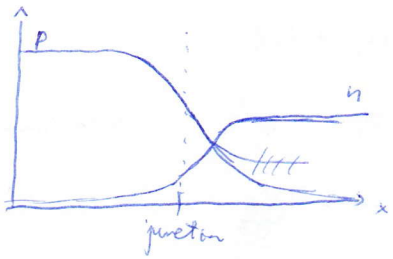


contact or diffusion potential

Driving force of diffusion

$$\underline{j}_{drift} + \underline{j}_{diffusion} = \underline{0}$$

$$n e \mu \underline{E} + eD \underline{\nabla} n = 0$$



Schottky - approximation

charge neutrality

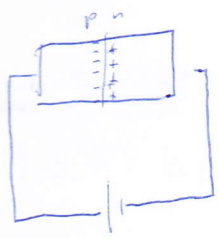
$p l_p^\circ = n l_n^\circ$

$n_a l_p^\circ = n_d l_n^\circ$

heavily doped → small depletion layer

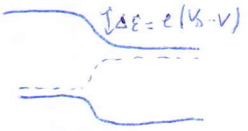
lightly doped → thicc depletion layer

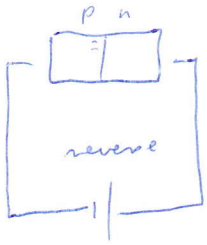
p-n junction + bias

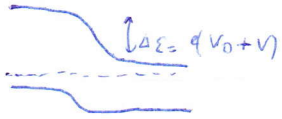


forward

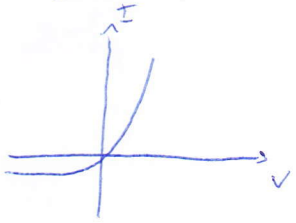
depletion is smaller

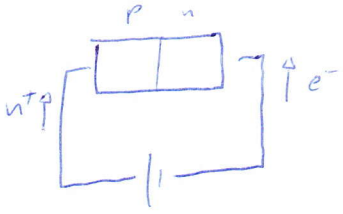


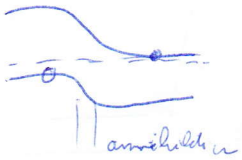




Diode characteristics:







usually light is emitted (LED)

avalanche breakdown

- reverse bias

minorities are accelerated

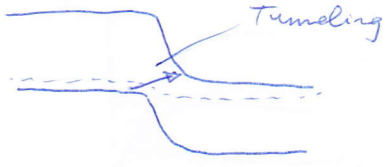
↓

excite additional minority

C-C

- destroys
- occurs in weakly doped SCs

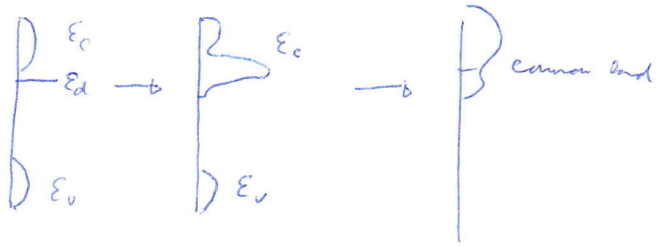
Zener-effect

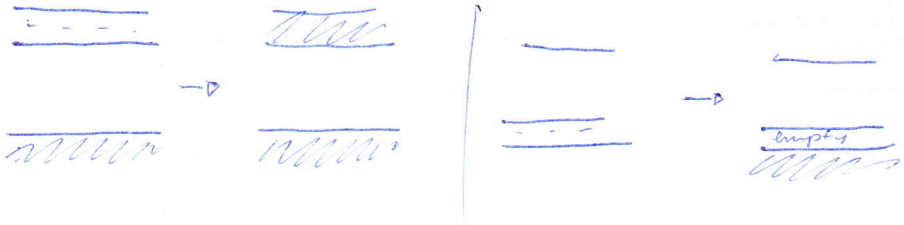


- thin depletion layer
  heavily doped
- reversible, doesn't destroy
- similar physics to tunnel ~~diode~~ diode

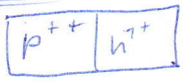
Tunnel diode

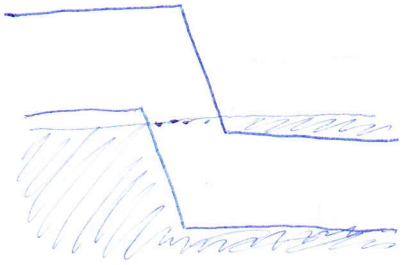
degenerate doping





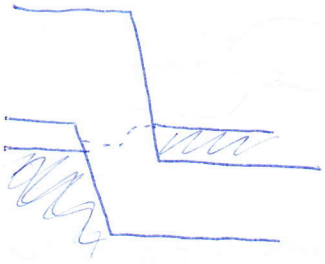
Esaki diode:



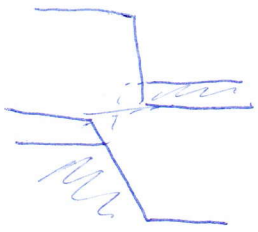


$V \neq 0$

tunnel current

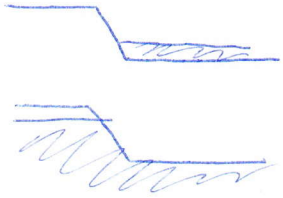


tunnel current increases

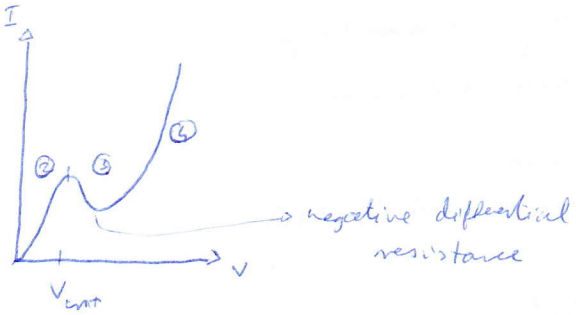


$V > V_{crit}$

tunnel stops



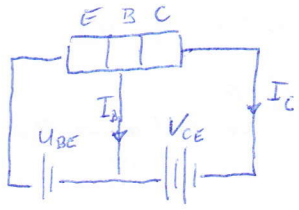
again current flows just like a normal diode



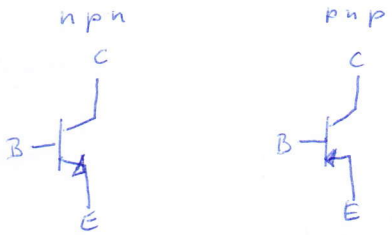
Week 14

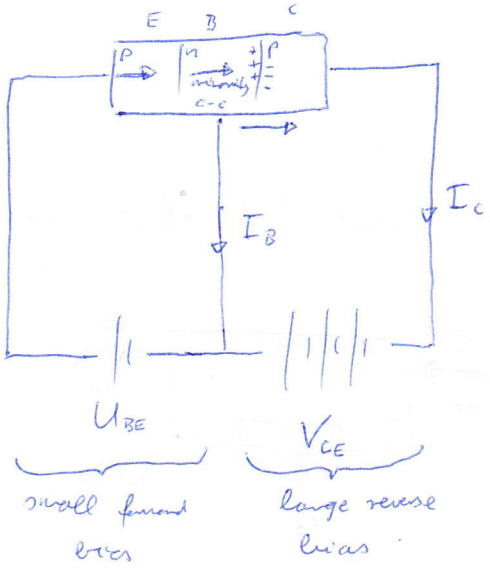
SC devices:

BJT: bipolar junction transistor



- emitter
- base
- collector





BJT ≠ np + pn diode

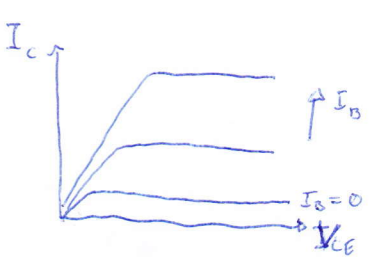
Base is thin $l_B << L_{diff}$

Large E field sweeps e^- to collector

BJT: minority carrier device

I_C depends on injected charges (V_{BE}) and is prop to I_B

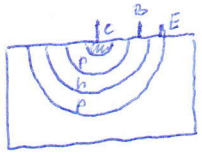
→ I_B controls I_C construction is such that $\frac{I_C}{I_B} = \beta = 10, \ldots 100$ current amplification factor



① digital device

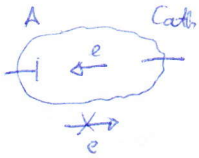
② analoge amplifier

Technically

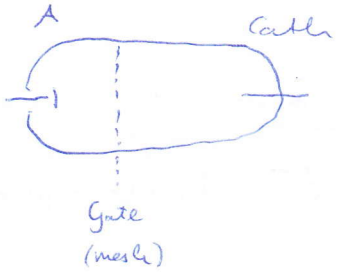


Analogy: vacuum tubes

diodes



triodes



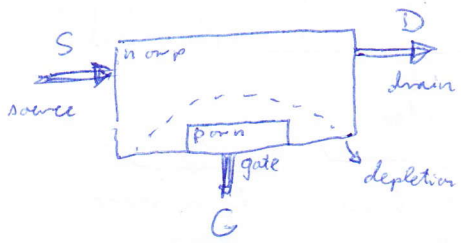
I_A controlled by V_{GG}

here $I_G = 0$

⇒ voltage controlled device

~~I_A controlled by V~~

JFET: junct. field effect. transistor

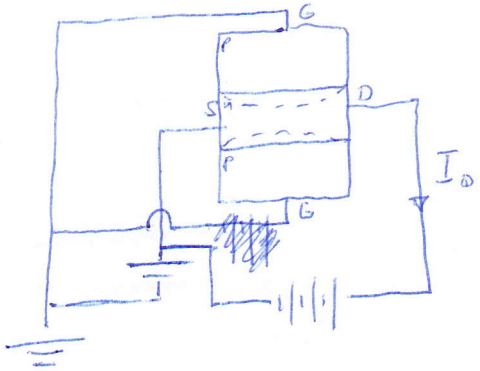


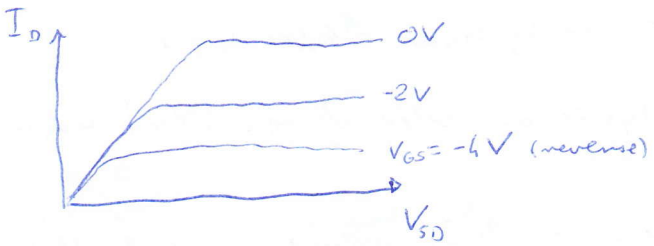
- if: gate-source forward
  → I_{SD} large
- if: gate-source reverse
  → I_{SD} small

I_{SD} controlled by voltage V_{GS}

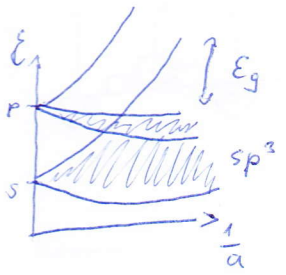
$I_G = 0$

in practice:

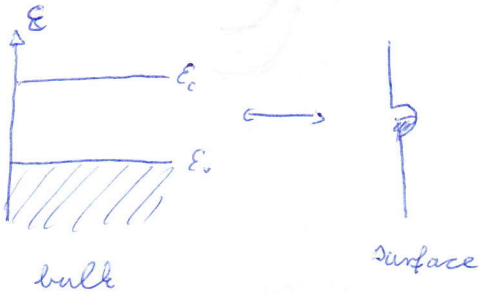




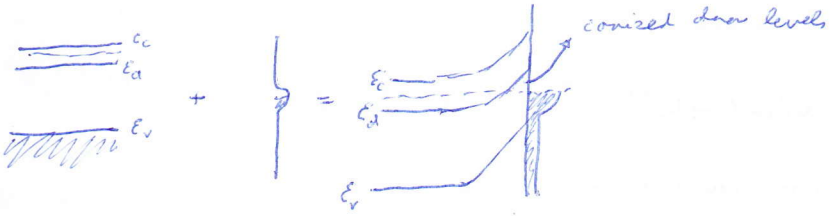
Schottky barrier, surface states

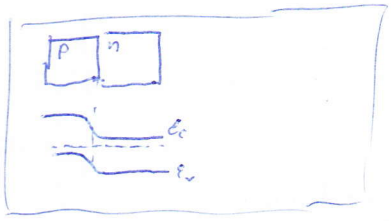


sp^3 hybrid states are in the middle of the gap

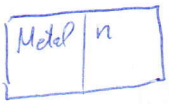


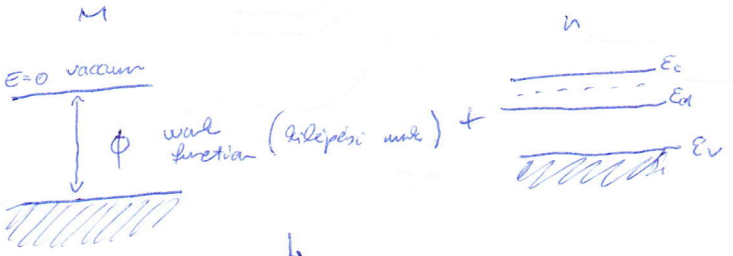
surface of n-type SC

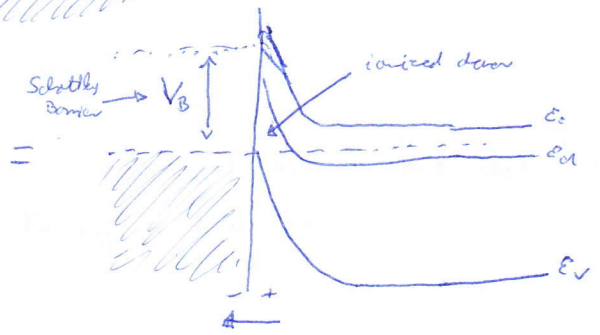




Schottky barrier

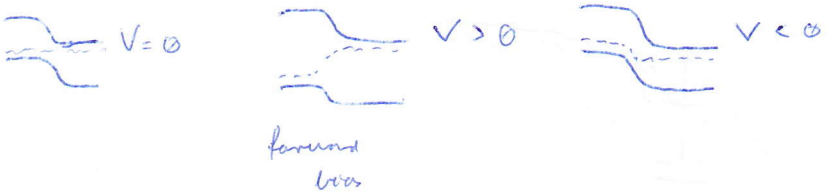




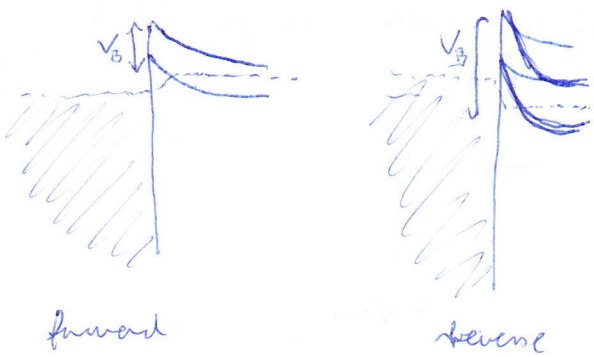


resembles p n

remember



Schottky-diode under bias



forward

V_B smaller

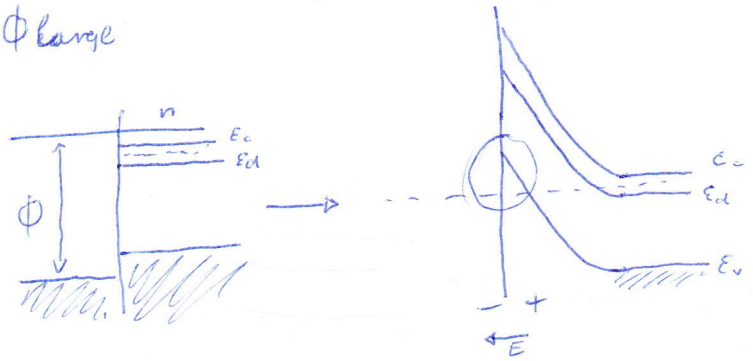
reverse

V_B larger

Advantages of Schottky devices

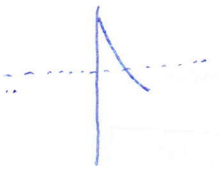
- tunable barrier due to Φ (different metal)
- V_B can be small → small power consumption
- no minority c-cs → faster devices (no recombination effects)

Φ large



zoomed in:

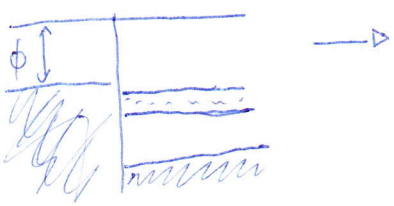
hole c-cs

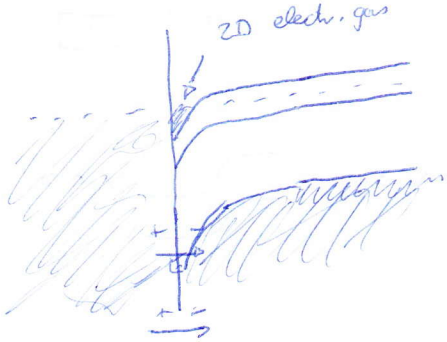


so-called "inversion layer"

inversion layer: 2D hole gas: p-type charge carriers in a n-type SC

When Φ is small:

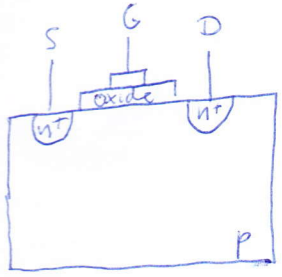




"Accumulation layer" → ohmic contact

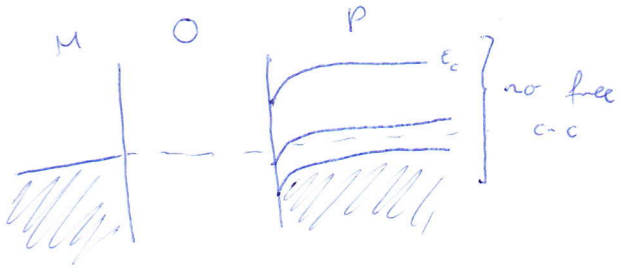
here $n >> n_d$

MOSFET: (Metal-oxide-semiconductor FET)

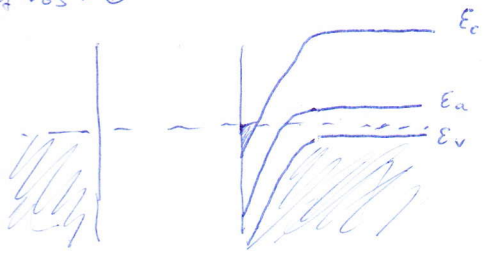


$V_{GS} > 0$ → n-channel forms
I_{SD} is finite

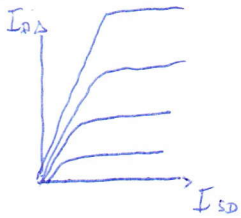
$V_{GS} < 0$ → p channel forms
$I_{SD} = 0$



if $V_{GS} > 0$



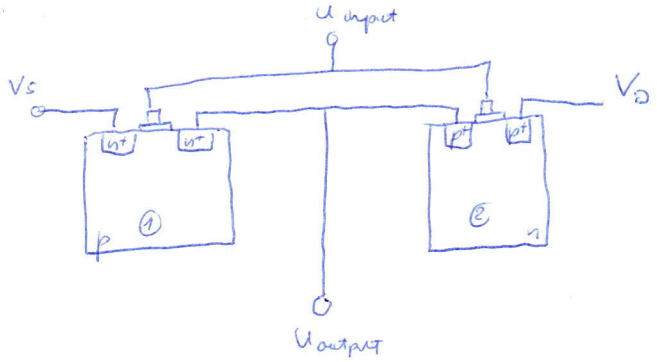
CMOS: (Complementary MOS)



logical 1: large I_D

logical 0: small I_D

every transistor has 1mA



if $U_{input} > 0$ → ① open, ② closed → $U_{out} = V_S$

if $U_{input} < 0$ → ② closed, ① open → $U_{out} = V_D$

always $I_{SD} \approx 0$ except for switching

of V_S = low U_{output} } not gate
V_D = high U_{output}