

m o n o c r o m o®

NOME
NAME

Semiconductor

COGNOME
SURNAME

MATERIA
SUBJECT

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CLASS

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physics. bone. hu /

1 class, 1 topic on oral exam
2 questions

semiconductors (SC): material whose conductivity can be affected by:

- temperature
- doping (adele's alab) Stegos (new silicon some!)
 - intentional
 - unintentional (includes impurities)
- external voltage
 - drain (self pers.)
 - gate (self pers.)



V_{SD}
 V_{GD}

G: gate

- another semiconductor nearby
diffusion, charge transfer



charge diffusion

defection layer: initiated with junction: element

- light: photoconductivity



conductivity affected by light
sensors, photovoltaic effects (PV)

- magnetism (spintronics, magnetic SC-s)

Mn: GaAs

MRAM
non-volatile memory

metals conductivity does not change significantly with illumination (except low temp.)

SCs properties are good and bad (some)

SC materials

- BULK**
- IV group: C, Si, Ge, Sn (carbon is an insulator)
↑ as different allotropes: diamond, graphite, graphene, CNTs, fullerene
 - IV group compounds: SiC (same structure as diamond)
 - III-V group compounds: GaAs, AlP, InSb and various combinations (arsenide)
 - I-VI group compounds: ZnS, ZnSe, ZnO, PbS₂, FeS₂

Bulk SCs: diamond structure

Low-dimensional SCs: 1D: CNTs, nanowires, GaAs (we won't talk about these) 2D: graphene, transition metal dichalcogenite MoS₂

Molecular SCs: C₆₀

diamond: SC or insulator?
 $E_g = 6 \text{ eV}$ band gap
SC

How?

Si₃N₄ $E_g = 4 \text{ eV}$
insulator

diamond can be metal?

B: C (boron doped diamond)
4% → superconductor (metal)

most innovation are happening ⁱⁿ at the industry, physical principles are not changing, device performance is increasing (Moose-law?)

Early History of SCs (dates are not asked on the exam)

Fundamental effects:

- 1833: Faraday: AgS heated $\rightarrow R$ decreases
 distance sensitivity
- 1839: Becquerel: photovoltaic effect
- 1873: Smith: photoconductivity Se (light $\rightarrow R$ decreases)
- 1874: Braun: rectification (eggenitalitas) in metal-sulfides
- Schuster: rectification in CuO
 (looks like a II-VI SC)

1878: Hall-effect

1900: Baedeker: inverse sign Hall-effect in AuI

Hall-constant: $R_H = \frac{1}{ne}$

$n = \frac{\text{number of } e^-}{\text{cm}^3}$ charge carrier
 has a sign
 $-$: -c.c.
 $+$: +c.c.

1910: Weiss: Halbleiter (origin of the name)
 semi-conductor (metals with strange behaviour)

1928-38: Quantum theory of SC
 Bloch, Schottky, Matt

1940: Bardeen (2 Nobel-prizes, only one): non-reproducing lab. results
 are due to about $< 1 \mu\text{m}$ uniformity
 nobody could make SCs intentionally

1 ppm: ~~part per million~~ too pure technological limitation

ppm: part/million (10^6)

ppb: part/billion (10^9)

often today: 10^{-12} - 10^{-15}

Technology:

1880: Bell: voice transfer with Se, piezoelectricity
 (not very efficient)

1883: Fitts: first selenium:  Se thin layer of gold (transparent) metal

1904: J.C. Bose: sensitive radiodetector (rectifying device)
 (EM radiation, demodulation, AM radio)

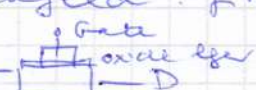
point contact diode:  Ph₃2 galena

1906: Round: first LED

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

1922: Loew: ZnO $\rightarrow$ amplifier (first)

1926: Lilienfeld: first FET (field effect transistor)
 (difficult to make)

 Gate oxide layer Source Drain

where I_{DS} depends on V_{GS}

1941: Ohl: first Si p-n junction

1947: Bardeen-Brattmann-Schocley: bipolar junction transistor
 $\rightarrow$ revolutionised the industry

Nobel prizes

1956: transistor

1973: Esaki: greater tunnel-diode

1985: von Klitzing: quantised Hall-effect

2000: Alferov, Kroemer, Kuly: SC laser IC: integrated circuits

2007 Fast, Grunberg GMR: giant-magnetoresistance
 2009 Boyle, Smith CCD
 2010 Geim, Novoselov graphene
 2014 Aresari, Amano, Nakanuma blue LED (GaN high quality)
 each challenge

Position of SC physics

prerequisite: quantum mechanics, solid state physics, statistical physics, material sciences (optics)

gives us: electronics, spintronics, laser optics/physics

ongoing research: fundamental directions: new materials, low-dimensional SC, optical like excitons
 fundamental phenomena: quantum Hall-effect, structural, QHE, FQHE

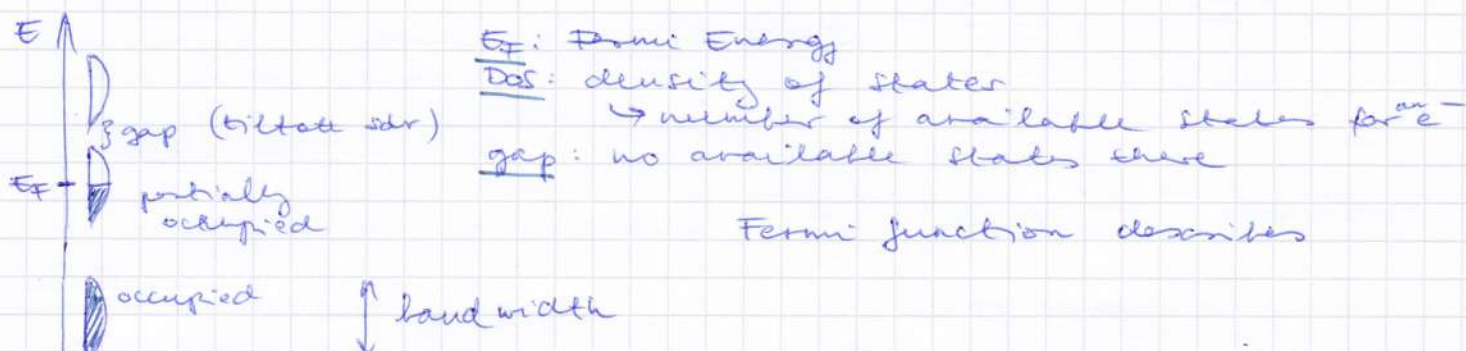
applied research: new devices (HEMT)
 /high efficiency transistors/
Size: smaller, speed: faster, power: decreases, consumption

Resistivity:

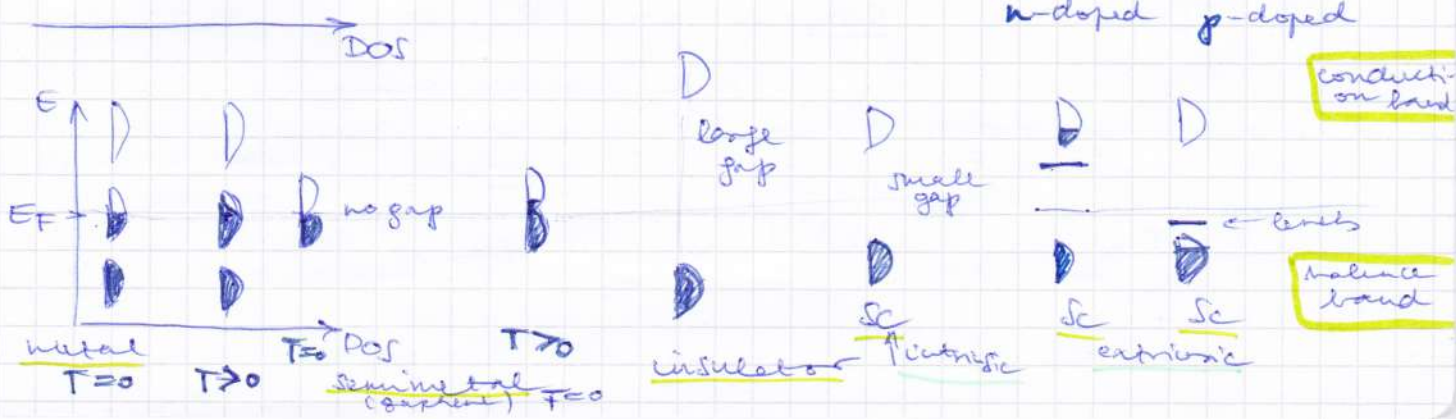


Size of the Universe: 10^{27} m
 Size of nucleus: 10^{-15} m femto
 42 orders of magnitude

Band Structure of Semiconductors (generic overview)



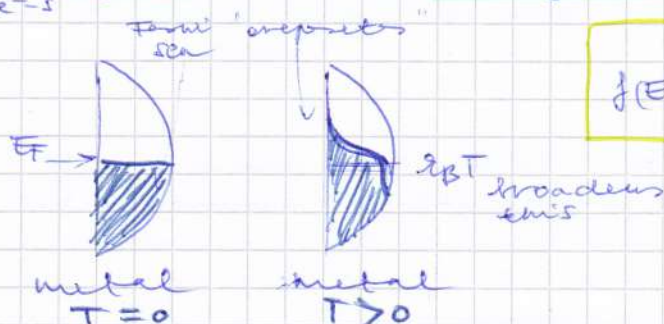
metal $T=0$
~~insulator~~



Fermi energy $\longleftrightarrow$ chemical potential

E_F
 $T=0$ property
 cut-off E
 of e^- s

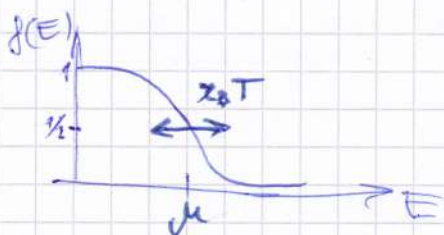
final temperature quantity
 average E of particles



$$f(E) = \frac{1}{1 + e^{\frac{E - \mu}{2kT}}}$$

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

$$\mu \neq E_F$$



$$\frac{1}{1 + e^{\frac{E - \mu}{2kT}}}$$

At $T=0 \Rightarrow E < \mu \Rightarrow f(E) = 1$
 $E > \mu \Rightarrow f(E) = 0$

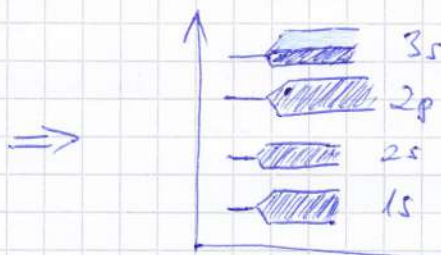
becomes the
step function
 (Heaviside)

$2kT$ at $T=300\text{ K} \rightarrow 26\text{ meV}$
 (broadening is not very large) bands $\sim \text{eV}$

Na (sodium): $1s^2 2s^2 2p^6 3s^1$



atom



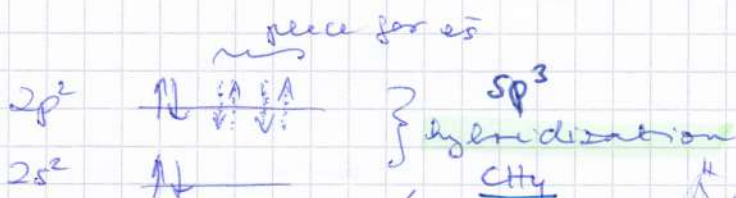
metal

Pauli principle $\rightarrow$ degeneracy is lifted
 $\rightarrow$ (e^- do not want to be at the same level, energy)

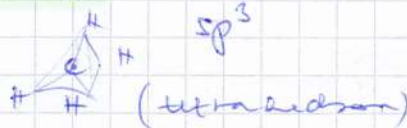
Diamond
 $1s^2 2s^2 2p^2$

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

same band both



in order to
 gain E



needs: s and three p orbitals

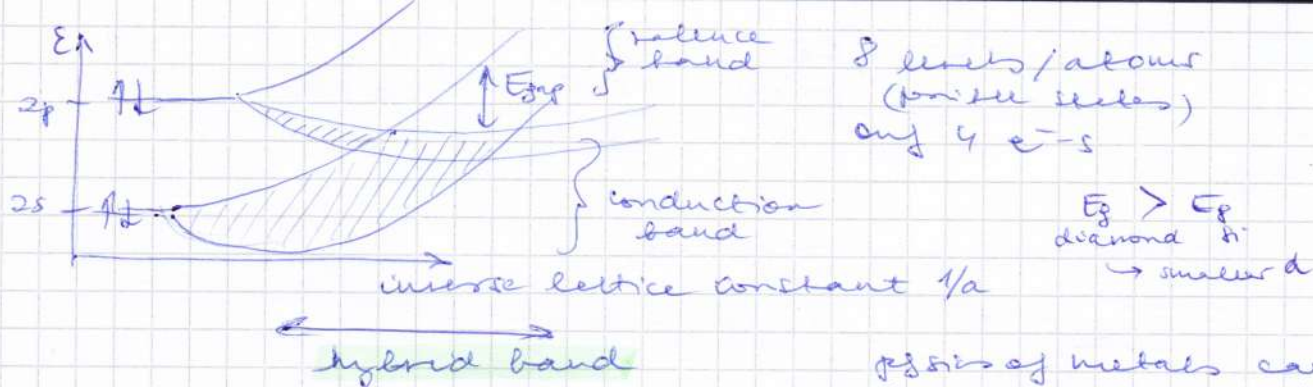
(IV elements)



anti-bonding orbital



bonding orbital



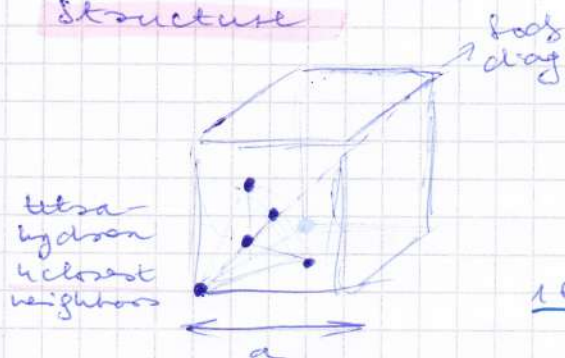
8 levels/atoms (atomic states) only 4 e^- s

which of metals cannot be completely used (due to hybridization)

diamond structure is a consequence of hybridization

structure $\rightarrow$ hybrid? or hybrid $\rightarrow$ structure (?) which dictates which (?)

Structure



diamond structure

Bravais-lattice

FCC: face centered cubic

basis: $(0,0,0)$
 $(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})a$
 1 type of atom

moved by a quarter of body diag

case of GaAs $\rightarrow$

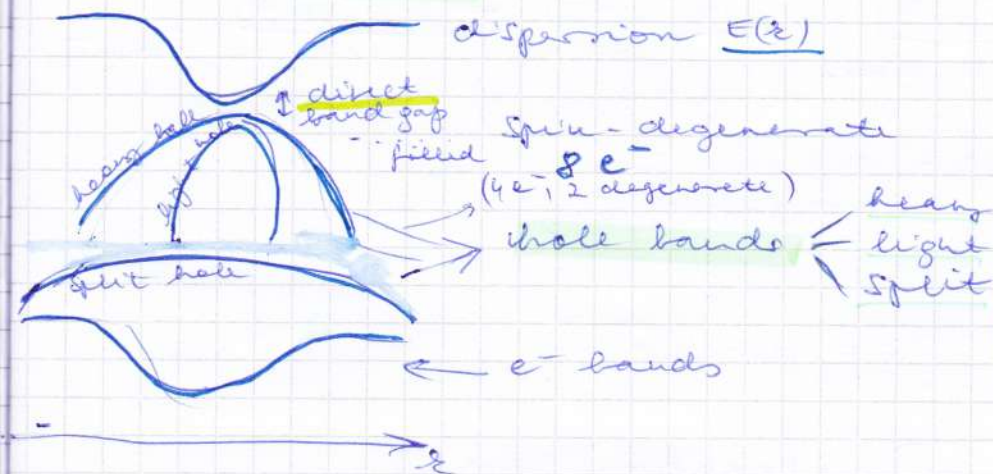
basis: $(0,0,0)$ Ga
 $(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})a$ As
 2 type of atoms

alloy: no underlying structure

name of structure: zincblende (2 type microstructure)

Band Structure GaAs

dispersion $E(k)$

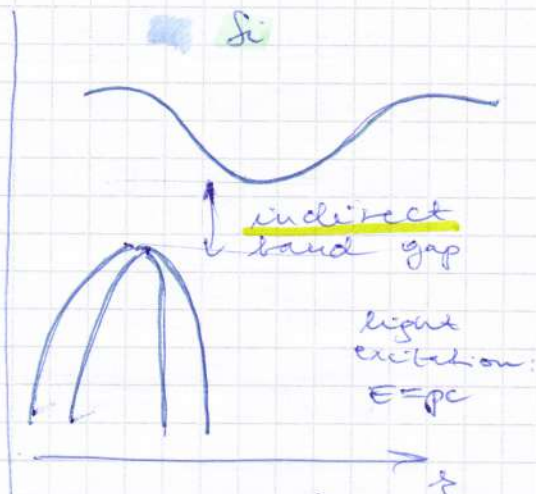


can absorb or emit light
 $\rightarrow$ can make a laser, LED

valid for GaAs unit, not individually (atoms)
 $\rightarrow$ double atom basis

8 e^- basis based bandstr
 (number of levels?)

correlation $\sim$ effective mass



$$p_{light} = \frac{E}{c} = \frac{hw}{c} \text{ (small)}$$

light cannot give or take large momentum
 cannot emit or absorb light ($\neq$ change)

Si:
 (2 atom basis)
 GaAs

Band gap:	C	Si	Ge	GaAs	AlAs
	5 eV	1.1 eV	0.7 eV	1.5 eV	2.2 eV

smaller $\Rightarrow$ gap larger

general consequences for technology

$E_{\text{ins}}: 2 \text{ eV}$ $E_{\text{ge}}: < 1 \text{ eV}$ light detecting

for high power transistor Si or AlAs or C
(high E, high T)

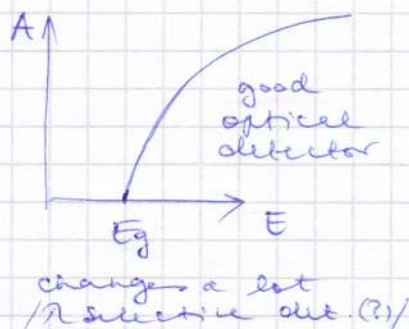
larger gap $\rightarrow$ T does not influence it like smaller gap materials

Optical properties:

metal



SC



Charge carriers in SCs

n : concentration of c.c.s

in a metal

$$n = 10^{22} \frac{1}{\text{cm}^3}$$

Ge (300K)

$$n = 2 \cdot 10^{13} \frac{1}{\text{cm}^3}$$

$\rightarrow$ low amount at room T

Drude-model: conductivity $\leftrightarrow n$

$ma = \mp = qE$ plus a viscous force (drag-force)

$$ma = qE - Kv$$

stationary solution: ($a=0$)

$$0 = qE - Kv$$

we introduce:

$$\frac{K}{m} = \frac{1}{\tau}$$

relaxation time

$$ma = qE - Kv \Rightarrow a = \frac{qE}{m} - \frac{K}{m} v$$

$$\left[\frac{K}{m} \right] = \frac{1}{s}$$

phenomenological model

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

$$\tau = 10^{-17} - 10^{-15} \text{ sec typically}$$

$$v_{\text{drift}} \approx 10^{-4} \dots 10^1 \frac{\text{m}}{\text{s}}$$

$v_{\text{signal}} \approx \text{speed of light}$

current density:

$$j = n \cdot e \cdot v_D$$

$j \propto n$

$$[j] = \frac{C}{m^2 s} = (n e v_D) = \frac{1 C m}{s m^2} = \frac{A}{m^2}$$

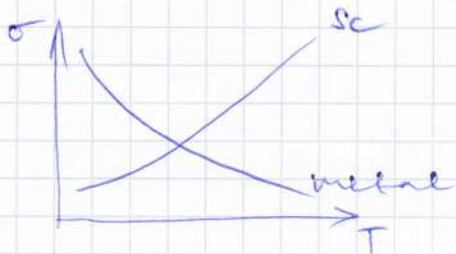
$$j = \sigma E$$

differential Ohm's law

$$j = n e v_D = \underbrace{n e^2 \tau}_{\sigma} E \Rightarrow$$

$$\sigma = \frac{n e^2 \tau}{m}$$

conductivity $\left[\frac{1}{\Omega m} \right]$



metal: $n \approx \text{const.}$

σ is dominated by τ shortening (ρ increases)

sc: n is ~~not~~ independent on T strongly
 ΔT dominates σ

Solid state physics session

1 dimensional ^{free} e^- gas (particle in the box)

$$\psi(x) = \frac{1}{\sqrt{L}} e^{i k x}$$

plane wave (wave function)

$$p = \hbar k$$

canonical impulse

crystal momentum

Energy dispersion

$$E(k) = \frac{\hbar^2 k^2}{2m}$$

(Sch.-eq.)
 $H\psi = E\psi$

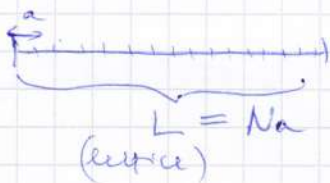
$$H\psi = E\psi$$

free: $V=0$ (no potential)

$$-\frac{\hbar^2}{2m} \Delta \psi = E\psi$$

In a solid k is quantized by periodic boundary conditions.

math tool to make soly problems easier.



$$\psi(0) = \psi\left(\frac{Na}{L}\right)$$

single valued

$$\hookrightarrow e^{i k L} = 1$$

$$\Rightarrow kL = 2\pi n$$

$$n \in 0, \dots, N-1$$

or $n \in -\frac{N}{2}, \dots, +\frac{N}{2}+1$

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

1D

allowed k states

$$\text{spacing: } \frac{2\pi}{L}$$

$$[k] = \frac{1}{m}$$

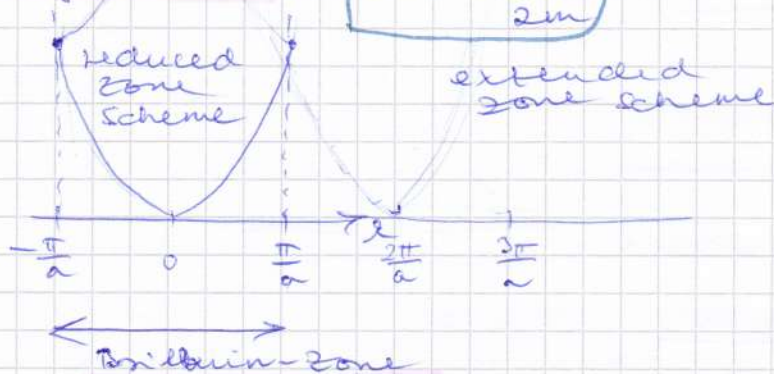
quasi-continuous (small spaces)



N pos. (states)

Dispersion:

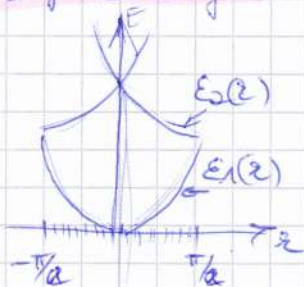
$$E(k) = \frac{\hbar^2 k^2}{2m}$$



We want sp. practical: e.g. compute the n (charge carriers)

Charge carriers in SCs

1D free e^- gas



$E_n(k)$
↑
band index

$$E(k) = \frac{\hbar^2 k^2}{2m}$$

quadratic band dispersion

periodic boundary conditions:

$$k = \frac{2\pi}{L} n \quad n = -\frac{N}{2} \dots \frac{N}{2} \quad \Delta k = \frac{2\pi}{L} \text{ separation } L \text{ (quantization)}$$

$$(m^*)^{-1} = \frac{1}{\hbar^2} \frac{\partial^2 E(k)}{\partial k^2}$$

band effective mass (cc-s mass is different from -) (result of the lattice)

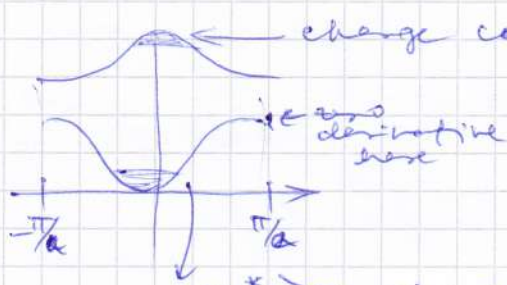
$$v = \frac{1}{\hbar} \frac{\partial E(k)}{\partial k} \text{ velocity of } e^-$$

$$\text{for 1D: } \frac{\hbar k}{m} = v \quad p = \hbar k \quad \left[\frac{q_s}{m} \right] = \left[\frac{q_s \hbar^2}{m^2} \right]$$

for free e^- gas: $(m^*)^{-1} = \frac{1}{m} \rightarrow \boxed{m^* = m}$ in this case

$F_{ext} = \hbar k$ (next lecture: + periodic potential)
(external forces) ↑ crystal momentum

1D free e^- gas + periodic potential



charge carriers $m^* < 0$ charge carriers are holes (negative mass(?))

$m_a = \mp$
negative the force $\rightarrow m$

$m^* > 0$ charge carriers: e^-

GaAs $\downarrow$ e^- band m_c

hole → depending on the curvature m^*
heavy hole band
light hole band

typical values:

$$m_e^* = 0.1 \dots 0.5 m_0$$

electrons

$$m_h^* = -1 \dots -3 m_0 \text{ (heavier)}$$

holes

Density of States

→ central notion

DOS in k -space:

$$(1D) \Delta k = \frac{2\pi}{L};$$

$$D(k) = \frac{L}{2\pi}$$

dimensions of m

density for $\frac{1}{m}$ (?)

$$\text{number of atoms: } N = \int_{-\pi/a}^{\pi/a} D(k) dk = \int_{-\pi/a}^{\pi/a} \frac{L}{2\pi} dk = \frac{L}{2\pi} \frac{2\pi}{a} = \frac{L}{a} = N$$

Statistics

density function

e.g. Gauss

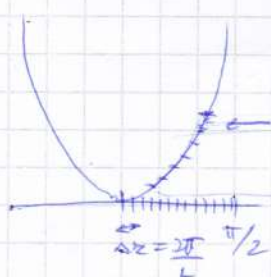
$$\langle x \rangle = \int_{-\infty}^{\infty} x f(x) dx //$$

$$(2D) D(k) = \frac{A}{(2\pi)^2}$$

$$(3D) D(k) = \frac{V}{(2\pi)^3}$$

plus: $\times 2$ for spin degeneracy

Go from $D(k) \rightarrow D(E)$ (better to work in E -space)



← usually

← E spacing here



divergent $D(E)$

$$(1D) D(k) dk = D(E) dE \leftarrow \text{preservation of states or def. of } D(E)$$

$$D(k) \frac{dk}{dE} = D(E) = D(k) \left(\frac{dE}{dk} \right)^{-1}$$

// $\frac{dk}{dE} = \left(\frac{dE}{dk} \right)^{-1}$; derivative of inverse function

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

$$\text{e.g.: } y = x^2 \rightarrow x = \sqrt{y} \quad \frac{dx}{dy} = 2x \quad (\sqrt{y})' = \frac{1}{2\sqrt{y}} = \frac{1}{2x} //$$

$$(1D) \left(\frac{dE}{dk} \right) = \frac{\hbar^2 k}{m^*}$$

$$D(E) = \frac{L}{2\pi} \cdot 2 \cdot \frac{m^*}{\hbar^2 k} = \frac{L m^*}{\pi \hbar^2 k}$$

$$E = \frac{\hbar^2 k^2}{2m^*} \quad k = \sqrt{\frac{E 2m^*}{\hbar^2}}$$

$$\xrightarrow{k \rightarrow E} = \frac{L m^*}{\pi \hbar^2} \sqrt{\frac{\hbar^2}{E 2m^*}} = \frac{L m^*}{\pi \hbar^2 \sqrt{E 2m^*}}$$

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

$$(2D) D(k) \cdot 2\pi k dk = D(E) dE$$

elementary surface in 2D

$$\Rightarrow \frac{2A}{4\pi^2} \cdot 2\pi \cdot \frac{m^*}{\hbar^2} = D(E) = \frac{A m^*}{\pi^2 \hbar^2}$$

constant, no singularity!

(3D) $D(E) 4\pi r^2 dr = D(E) dE$

$D(E) = \frac{V}{4\pi^3} \cdot 4\pi r^2 \frac{m^*}{\hbar^2 r} = \frac{V}{2\pi^2} \sqrt{E} \left(\frac{2m^*}{\hbar^2} \right)^{3/2}$

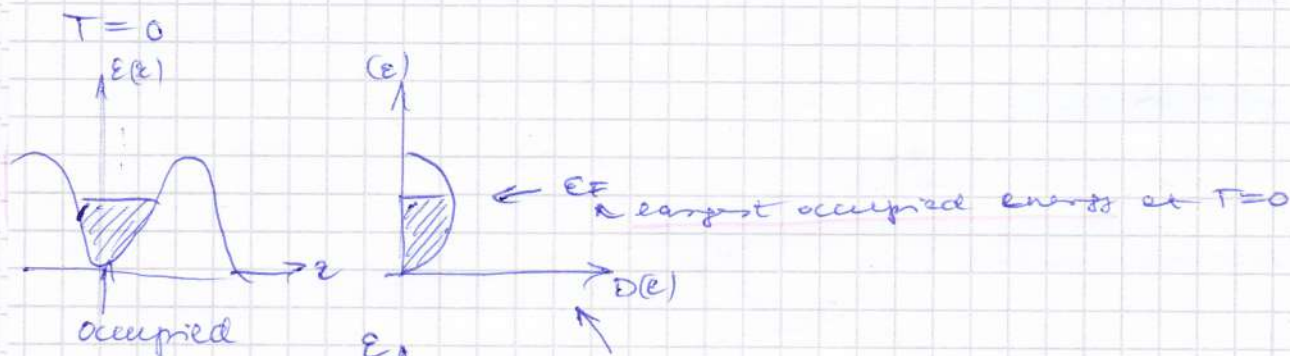
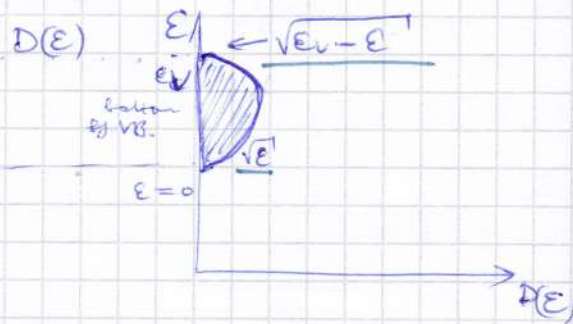
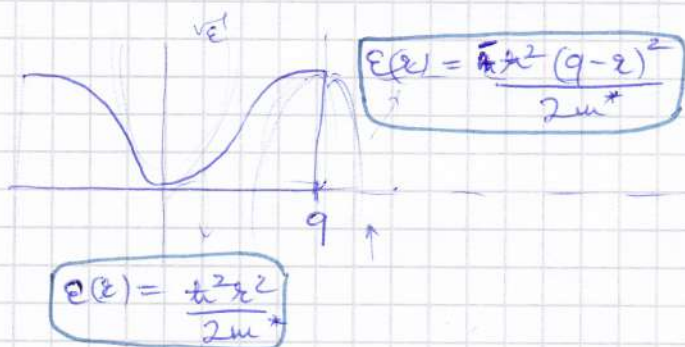
linear in E
 $D(E) \sim r \sim \sqrt{E}$

$D(E)$:

(1D) $\sim \frac{1}{\sqrt{E}}$ (2D) const (3D) $\sim \sqrt{E}$

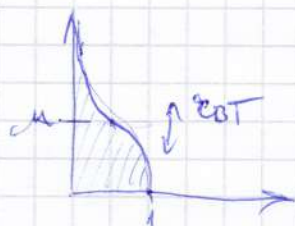
← important!

Occupation of bands in 3D



at $T=0$ $\mu = E_F$

$T > 0$



E_F only makes sense at $T=0$

$\lim_{T \rightarrow 0} f(E) = E_F$

Number of CCs

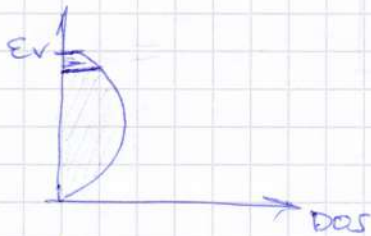
$N_c = nV = \int D(E) f(E) dE$

n : density of e^-
 N_c : number of CCs in CB

we use this equation it describes everything
 $f(E)$: quantum statistics of e^-

$D(E)$: contains the system specific information

Top of the VB

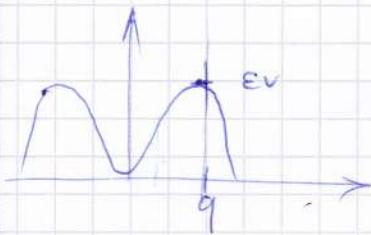


$$D_v(E) = \frac{V}{(2\pi)^3} \left(\frac{2m_v^*}{\hbar^2} \right)^{3/2} (E_v - E)^{1/2}$$

valence

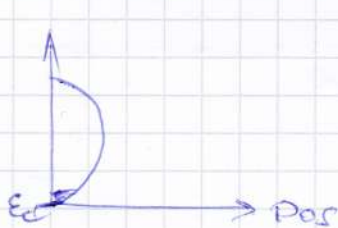
$$E(E) = E_v - \frac{\hbar^2(q - \xi)^2}{2m_v^*}$$

measure ξ back from E_v



(1 ppm doping makes Se semi-metal)

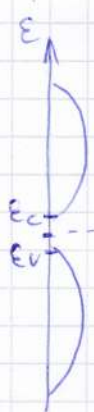
Bottom of CB



$$E_c + (?) \frac{\hbar^2(q + \xi)^2}{2m_c^*} (?)$$

$$E(\xi) = \frac{\hbar^2 \xi^2}{2m_c^*}$$

$$D_c(E) = \frac{V}{(2\pi)^3} \left(\frac{2m_c^*}{\hbar^2} \right)^{3/2} (E - E_c)^{1/2}$$



$$f(E) = \frac{1}{1 + e^{\beta(E - \mu)}} \approx e^{-(E - \mu)/\beta}$$

$$\mu \approx \frac{E_c + E_v}{2}$$

average
E of electrons
/chem. pot/

$$|E - \mu| \leq \frac{1}{2} E_g$$

$$E_c - E_v = E_g \quad \text{and} \quad E_g \gg k_B T$$

1-2 eV 28 meV

density of e^- : $n = \frac{1}{V} \int_{E_c}^{\infty} D_c(E) f(E) dE$

density of h^+ : $p = \frac{1}{V} \int_{-\infty}^{E_v} D_v(E) f(E) dE$

$$n \sim \int_{E_c}^{\infty} \sqrt{E - E_c} e^{-(E - \mu)/\beta} dE = \int_0^{\infty} \underbrace{\sqrt{x}}_{\frac{\sqrt{\pi}}{2}} e^{-x} \underbrace{\beta^{-3/2}}_{\text{const}} e^{-(E_c - \mu)/\beta} dx \Rightarrow$$

$(E - E_c)/\beta = x$

$$n = 2 \left(\frac{m_c^* k_B T}{2\pi \hbar^2} \right)^{3/2} e^{-\frac{(E_c - \mu)}{k_B T}}$$

$$p = 2 \left(\frac{m_v^* k_B T}{2\pi \hbar^2} \right)^{3/2} e^{-\frac{(\mu - E_v)}{k_B T}}$$

if I know $\mu \rightarrow n, p$ can be given

Conservation of charge (μ is unknown)

$n = p$ solve the equations for μ :

$$\mu = \frac{1}{2} (E_c + E_v) + \frac{3}{4} k_B T \ln \left(\frac{m_v^*}{m_c^*} \right)$$

μ is in the middle of the gap small / slow function

$$n \text{ in Na} : n \sim 10^{21} - 10^{22} \frac{1}{\text{cm}^3}$$

calculate n in a SC

$$n_c = 2 \left(\frac{k_B T}{2\pi \hbar^2} \right)^{3/2} (m_e^* m_v^*)^{3/4} e^{-\frac{E_g}{2k_B T}} = \frac{1}{10} \left(\frac{10^{-20}}{10^{-68}} \right)^{3/2} (10^{-21})^3 \cdot \frac{e^{-40}}{10^{-20}} \approx 10^{10}$$

substituting back μ

intrinsic SC $\rightarrow$

charge carriers in intrinsic SC

$$\text{DOS} : D(E)$$

$$n = \frac{1}{V} \int D(E) f(E) dE \text{ in 3D } D(E) \sim \sqrt{E}$$

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

$n \cdot p = n_i^2(T)$ $\rightarrow$ T dependent constant
always valid not only for intrinsic also for extrinsic : **LAW OF MASS ACTION**

$$c = \frac{[\text{OH}^-][\text{H}^+]}{[\text{H}_2\text{O}]} = 10^{-14} \quad \text{pH} = \frac{[\text{H}^+]}{[\text{H}_2\text{O}]}$$



recombination can happen

Mobility vs. charge concentration

$$\text{Drude} : m a = -eE - \hbar v \rightarrow a = -\frac{eE}{m} - \frac{\hbar v}{m}$$

$$\text{stationary} : 0 = -eE - \hbar v$$

e : elementary charge $>$

$$j = \sigma E \quad j = ne v_D \quad ; \quad \boxed{\frac{|v_D|}{E} = \mu} : \text{mobility}$$

Electrons	Electrons	Holes + charge	Drift velocity $0 = eE$
Drift velocity	$v_{De} = -\frac{eE\tau_e}{m_e^*}$	$v_{Dh} = \frac{eE\tau_h}{m_h^*}$	
current density conductivity	$j_c = ne v_{De} - ne v_{De}$	$j_h = pe v_{Dh}$	
conductivity $j = \sigma E$ positive for both	$\sigma_e = \frac{ne^2\tau_e}{m_e^*}$	$\sigma_h = \frac{pe^2\tau_h}{m_h^*}$	
mobility	$\mu_e = \frac{v_{De}}{E} = \frac{e\tau_e}{m_e^*}$	$\mu_h = \frac{v_{Dh}}{E} = \frac{e\tau_h}{m_h^*}$	
Full conductivity: e^- & h^+ current are additive $\sigma = ne\mu_e + pe\mu_h$			

HEMT: high e^- -mobility transistor
 → revolutionized analogue electronics

$$[\mu] = \frac{m}{s} \frac{m}{V} = \frac{m^2}{Vs} \Rightarrow \frac{cm^2}{Vs} \text{ are used in literature / why(3) /}$$

typical values: ("the larger the better")

Si $\mu_e = 1000 \frac{cm^2}{Vs}$ ← e^- -phonon scattering

$\mu_h = 100 \frac{cm^2}{Vs}$ ← intra-band scattering → V_c
 μ_h

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

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

(better transistor, than Si)

poly-Si: in solar cells $\mu \approx 1 \frac{cm^2}{Vs}$

Cu $\mu = 0,1 \frac{cm^2}{Vs}$

graphene $\mu \approx 2 \text{ million } \frac{cm^2}{Vs}$

needed to revolutionize modern electronics

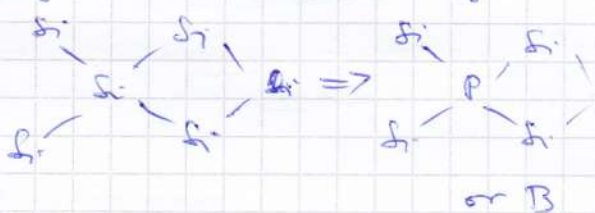
quantum reasons

$\frac{1}{2} m v_F^2 = kT_{\text{opt}}$ large electric fields
 millions
 → falls apart /

Doping

Replacing some atoms by heteroatoms

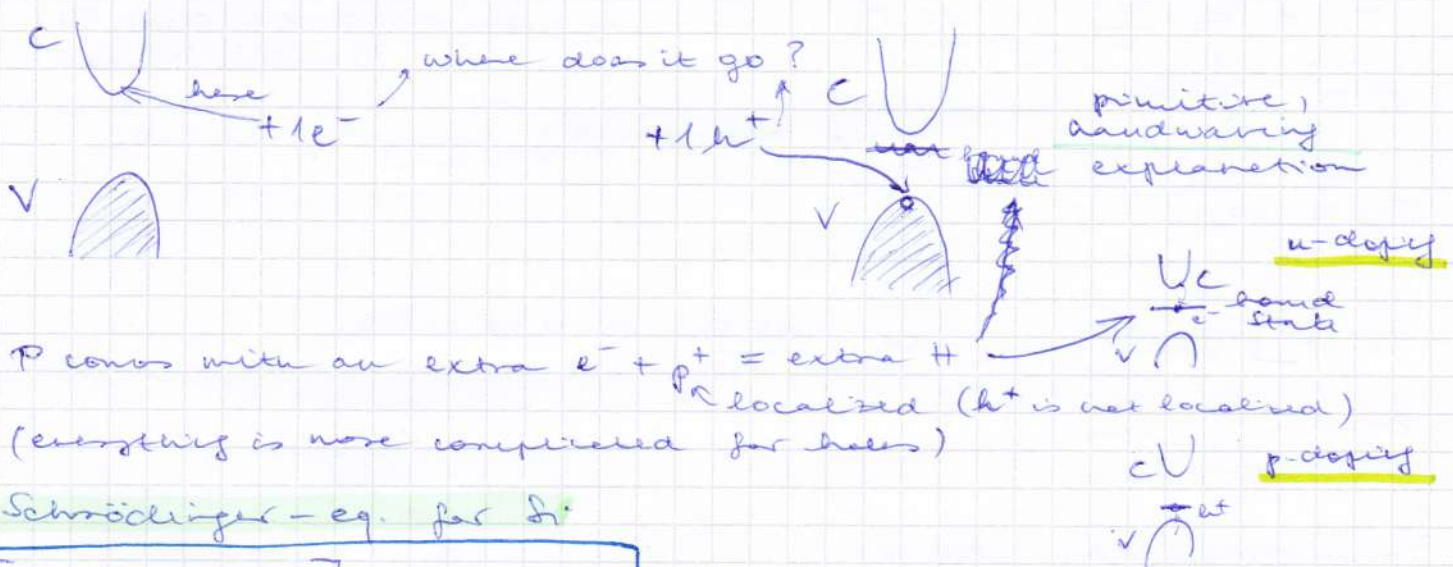
e.g.:



III. B:Si or
 V. P:Si
 AB:Si p-dopant
 AS:Si n-dopant

handwriting explanation
 live in high-school
 ($\pm e^-$)

Band picture



P comes with an extra $e^- + p^+ = \text{extra } H$
 (everything is more complicated for holes)
 localized (h^+ is not localized)

Schrödinger - eq. for Si

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

kinetic atomic potentials

We have the solution! (assuming)

+1 Si replaced by P → same Sch.-eq. + Sch.-eq. for H

H-atom, Bohr-model : good for H ground and excited states, $L = n\hbar$

$$\frac{mv^2}{r} = \frac{1}{4\pi\epsilon_0} \frac{e^2}{r^2} \quad \& \quad L = mvr = n\hbar \Rightarrow r = \frac{1}{4\pi\epsilon_0} \frac{e^2}{mv^2}$$

$$n\hbar = \frac{1}{4\pi\epsilon_0} \frac{e^2}{v} \Rightarrow v = \frac{e^2}{4\pi\epsilon_0 n\hbar}$$

introduce : $\alpha = \frac{1}{137} \approx \frac{e^2}{4\pi\epsilon_0 \hbar c}$
fine structure constant

$$r = \alpha \frac{\hbar}{m v}$$

$$r_n = \frac{1}{4\pi\epsilon_0} \frac{e^2 n^2}{m \alpha^2 c^2} = \frac{e^2}{4\pi\epsilon_0 \hbar c} \frac{\hbar}{m c} \frac{n^2}{\alpha^2} = \frac{n^2 \hbar}{m c \alpha}$$

$$r_n = a_B n^2$$

introduce : $a_B = \frac{\hbar}{m c \alpha} \approx 0.5 \text{ \AA} = 5 \cdot 10^{-11} \text{ m}$
Bohr radius

$$\frac{4\pi\epsilon_0 \hbar^2}{8 m e^2} = \left[\frac{\hbar}{m c \alpha} \right]$$

Binding energy :

$$E_n = \frac{1}{2} m v_n^2 - \frac{1}{4\pi\epsilon_0} \frac{e^2}{r_n} = \frac{1}{2} m \frac{\alpha^2 c^2}{n^2} - \frac{\hbar c}{a_B n^2} = - \frac{1}{2} \frac{m c^2 \alpha^2}{n^2} \approx - \frac{13.6 \text{ eV}}{n^2}$$

$$E_1 = -13.6 \text{ eV} \quad (\text{H: first E level})$$

In a SC :

$m \rightarrow m^*$ $m^* = 0.1 \dots 1 m$ (changes the qualities of the lattice)

$E_0 \rightarrow E_0 + E_r$ extra $e^- + p^+$ Coulomb potential is screened
 $E_r(r) = 11.9$ (from other e^-) $\alpha \rightarrow \frac{\alpha}{\epsilon_r}$

Bohr radius of a dopant

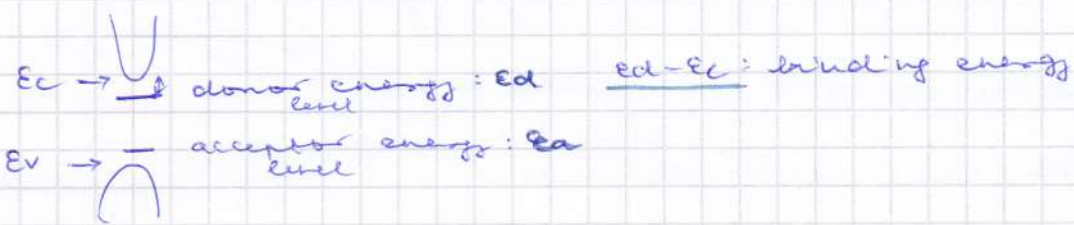
$$a_B^* = \frac{m}{m^*} \epsilon_r a_B \approx 100 a_B ; a_B^* \gg a_B$$

looks like H but much larger radius

binding energy $E_1^* = E_1 \cdot \frac{m^*}{m} \frac{1}{\epsilon_r^2} \ll E_1$; typically $E_1^* = 0.0001 \dots 0.001 E_1$
-13.6 eV 10 meV .. 100 meV

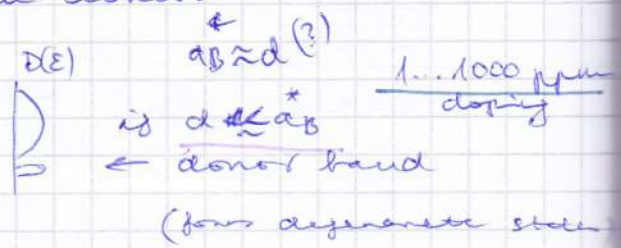
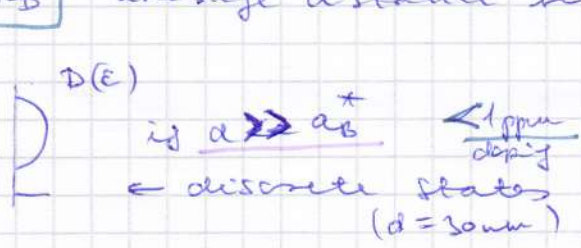
these are mostly accurate values (correct)

Typically :



Donor density : n_D

$$d = \frac{1}{\sqrt{n_D}}$$
 average distance between donors



1..1000 ppm doping

$d \ll a_B^*(\epsilon)$
 $d \approx a_B^*$
 $\leftarrow$ degenerate SC (looks like a metal)
 typically occurs at a few % doping
 > 1000 ppm doping
 / can make an SC fully conducting /

Doping vs charge carriers concentration

V — E_c
 — E_d
 $\wedge$ — E_v
 intrinsic SC $\mu \approx \frac{1}{2}(E_c + E_v)$
 extrinsic SC
 eg. n-doped $\mu \approx \frac{1}{2}(E_c + E_d)$ $\leftarrow$ derivation is complicated (Sb from II. bar)

$\langle n \rangle$: expectation value of e^- occupation (in general)

$$\langle n \rangle = \frac{\sum_i n_i e^{-(E_i - \mu)\beta}}{Z}$$

$$Z = \sum_i e^{-(E_i - \mu)\beta}$$

$$\beta = \frac{1}{k_B T}$$

grand canonical ensemble
(N can change)

partition function

due to Coulomb repulsion (not allowed)

for donor levels: $n = 0, 1, \cancel{2}$
 $\updownarrow$
 double (spin) multiplicity

probability of single occupation:

donor $\uparrow$ statistics

$$f_d(E_d) = \frac{2e^{-(\beta(E_0 + E_d - \mu))}}{e^{-\beta(E_0 + 0)} + 2e^{-(\beta(E_0 + E_d - \mu))}} = *$$

E_0 : ground state E
 $E_0 + E_d$: ground + donor is occupied

$$* = \frac{1}{1 + \frac{1}{2}e^{\beta(E_d - \mu)}} = f_d(E_d) \Leftrightarrow f(E) = \frac{1}{1 + e^{\beta(E - \mu)}}$$

$\uparrow$ consequence of spin degeneracy
 c.f. Fermi func.

probability of ionizing the donor state: ($n=0$)

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

charge carrier concentration in the conduction band

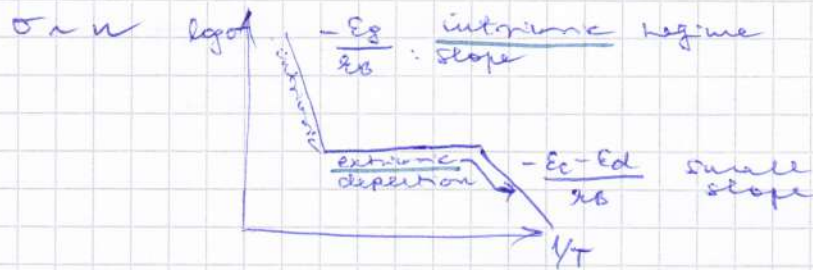
$$n = n_d \cdot \frac{1}{1 + \frac{1}{2}e^{\beta(\mu - E_d)}} \quad ; \quad \mu - E_d = \frac{1}{2}(E_c - E_d) \quad / p: \frac{1}{2}(E_c - E_v) /$$

donor binding E

(1.) $T \rightarrow 0$ $n \approx 0$

(2.) $k_B T \approx E_c - E_d$ donors are ionized $n \approx n_d$; depletion or extrinsic regime

(3.) $k_B T \gg E_c - E_d$ & $k_B T \approx E_g$ intrinsic; band-band excitation



depletion is the relevant in today's technology
 devices work in co and in hot temper
 $\rightarrow$ can control n
 $\rightarrow$ stable: $\sigma = \text{const}$

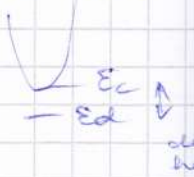
Law of mass action

intrinsic scs $n = p = \sqrt{n_i}$
 $n_i(T) = n_p = n_v n_e = e^{-\frac{E_g}{2k_B T}}$

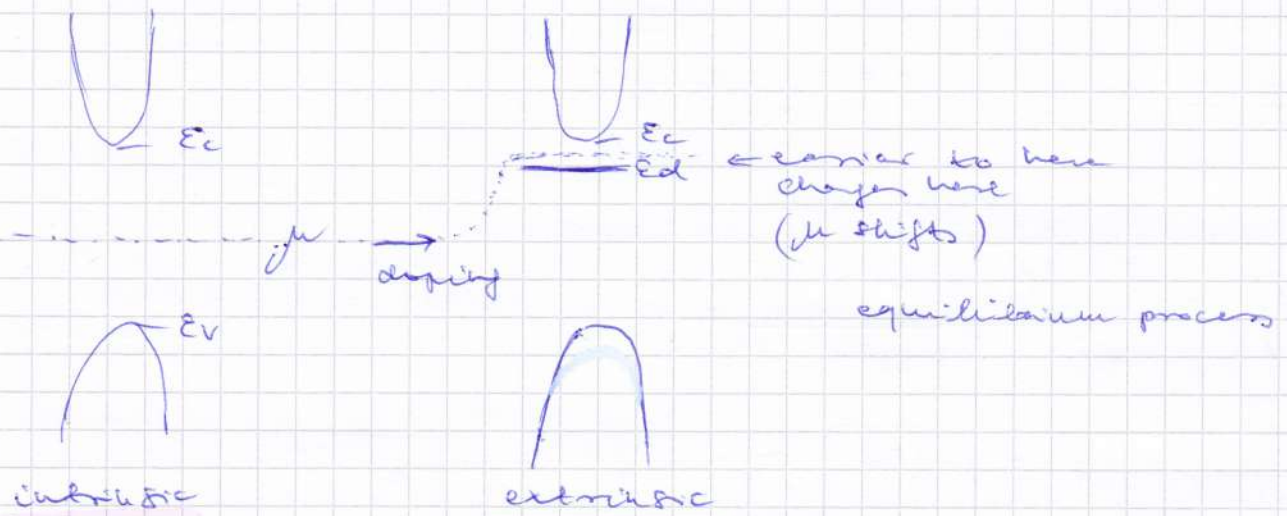
$$n = n_e e^{-\frac{(E_c - \mu)\beta}{2}}$$

$$p = n_v e^{-\frac{(\mu - E_v)\beta}{2}}$$

valid also for doped



Handwaving proof of law of mass action



intrinsic
 $\mu \approx \frac{E_c + E_v}{2}$

$$n = n_e e^{-\frac{(E_c - \mu)\beta}{2}}$$

$$p = n_v e^{-\frac{(\mu - E_v)\beta}{2}}$$

$$n = n_d = n_e e^{-\frac{(E_c - \mu)\beta}{2}}$$

$$p = n_v e^{-\frac{(\mu - E_v)\beta}{2}}$$

$\rightarrow$ goes up
 $\rightarrow$ goes down
 $\Rightarrow$ their product remains same

Band structure calculations in scs

what determines the band structure?

Importance: understand the conduction properties (μ, E_g)
optical properties (E_g)
intelligent design (band-engineering) (making predictions (designs))

Band structure calculation methods (from scratch to advanced)

- empty lattice model (handwaving model)
 $\rightarrow$ 2-space quantization
 $\downarrow$ All: particle in a box
- quasi-free electron approximation ($\frac{\hbar^2 k^2}{2m} + U(r)$) + periodic potential from atoms
- semi-empirical methods (tight-binding, TB; pseudopotential method)
 $\rightarrow$ fit to experimental properties (μ, E_g) (predicting gap structure)
- ab initio (first principles) DFT
- interacting e models GW

$H\psi = E\psi$ Simple, but the details are complicated

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

$$U(\underline{r}) = \sum U_{at} + \sum U_{ee}$$

atom-ion e⁻ interaction for all e⁻

e⁻ interaction e⁻e⁻ interaction not complications come from here

Simplification: use $1e^- \psi_0$ (wavefunction)

ions fixed

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

1e⁻ wavefunction

In Solids: $U(\underline{r}) = U(\underline{r} + \underline{R})$; $\underline{R}$ ← lattice periodic, $\underline{R}$: lattice vector

Bloch-theorem: $\psi_{\underline{k}}(\underline{r}) = e^{i\underline{k} \cdot \underline{r}} u_{\underline{k}}(\underline{r})$ → plain wave phase factor does not change the system

where $u_{\underline{k}}(\underline{r}) = u_{\underline{k}}(\underline{r} + \underline{R})$: lattice periodic function

$\underline{k}$ are given by the Born-Kohnen periodic boundary conditions

eg. 1D $\dots \dots \dots$ $\underline{R} = \frac{2\pi}{Na} \cdot n$ $n = -\frac{N}{2} \dots \frac{N}{2}$

$\xleftrightarrow{a}$ N

$\underline{k}$: crystal wave number, crystal momentum

the

why? → next lecture

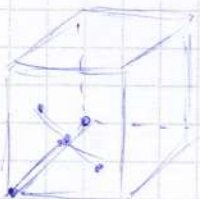
when $\underline{k} = 0 \rightarrow \psi_{\underline{k}=0}(\underline{r}) = u_{\underline{k}=0}(\underline{r})$ same for each lattice site

in 1D when $\underline{k} = \pm \frac{\pi}{a}$; then $+u_{\underline{k}} - u_{\underline{k}} + \dots + - \dots$

wavefunction alternates $\xleftrightarrow{a}$

Structure and $\underline{k}$ -space

Real space:



$\underline{k}$ -space

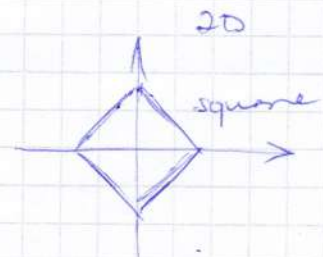


First Brillouin-zone (W-S-cells)

of course on all sides

diamond structure

FCC + 2 atom basis
at $(0,0,0)$; $(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})a$



for 3D we'd need 4D to draw

Distinguished points in $\underline{k}$ -space:

- Γ : Brillouin zone center $(0,0,0)$
- L : middle of the hexagon
- X : middle of the square
- K : midpoint of 2 touching hexagons

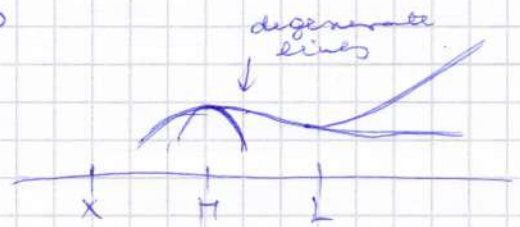
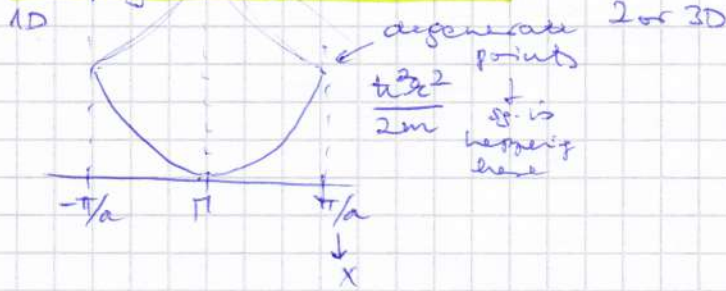
notations
valid for diamond st.
(changes for diff. conc.)

Distinguished directions:

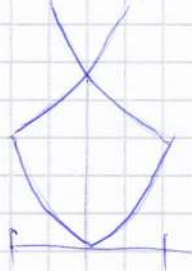
- 100 $\Gamma \xrightarrow{\Delta} X$: Δ line
- 111 $\Gamma \xrightarrow{\Lambda} L$: Λ line
- 110 $\Gamma \xrightarrow{\Sigma} K$: Σ line

Spaghetti diagrams

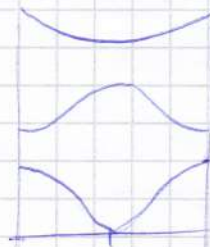
Empty lattice model:



Quasi-free electron approximation



+ $U(x)$
potential



degeneracy lifts with
 (perturbation?)

$$\Delta E = 2|U(G-G')|$$

$$\psi_k(x) = \frac{1}{\sqrt{V}} e^{ikx} \rightarrow \text{waves}$$

$$H = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + U(x) \leftarrow \text{Solve } E_k$$

$$E_k = \frac{\hbar^2 k^2}{2m}$$

$$H \psi_k = E_k \psi_k$$

$$E_k = E_k + \langle \psi_k | U(x) | \psi_k \rangle$$

good far away from degenerate points
 non-degenerate part. calc

Degenerate part. calc.

$$H = \begin{pmatrix} U_{11} & U_{12} \\ U_{21} & U_{22} \end{pmatrix} = \begin{pmatrix} \frac{\hbar^2 k^2}{2m} & U \\ U^* & \frac{\hbar^2 k^2}{2m} \end{pmatrix}$$

Hamiltonian matrix

$$U_{11} = \langle \psi_{1k} | U | \psi_{1k} \rangle$$

$$U_{12} = \langle \psi_{1k} | U | \psi_{2k} \rangle$$



$$U = \int e^{-ikr} U(r) e^{ikr} dr = U(G)$$

where $V = \int e^{-ikr} U(r) e^{ikr} dr$

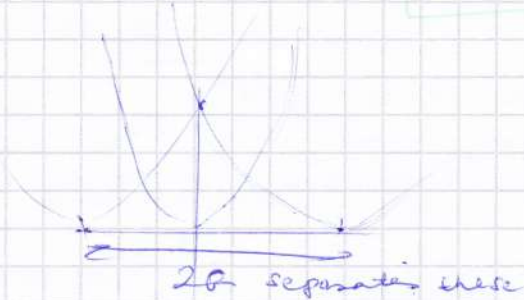
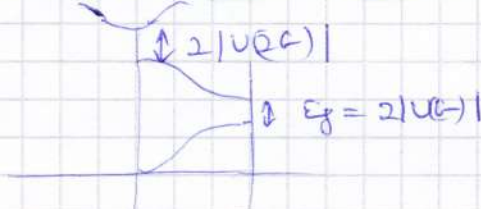
$$\psi_1 = \frac{1}{\sqrt{V}} e^{ikx}$$

$$\psi_2 = \frac{1}{\sqrt{V}} e^{i(k+G)x}$$

$$E_k = \frac{\hbar^2 (k+G)^2}{2m}$$

$U(G)$: Fourier $\int$ of U

Solutions at degeneracy



Tight-binding approximation

$$1D, 1 \text{ atom lattice } H \psi = E \psi; H = -\frac{\hbar^2}{2m} \Delta + U(r)$$

$$U(r) = \sum_R V_{\text{atom}}(r-R)$$

sum of atomic potentials

assuming atomic solution is known
 $H_{\text{at}} \psi_a = E_a \psi_a$

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

(neglects e-e interactions)

Ansatz ("trial"):

$$\psi_k(x) = \frac{1}{\sqrt{N}} \sum_n e^{ikna} \psi_a(r-na)$$

it satisfies the Bloch thm.

shorthand:

$$\Psi_{\alpha}(\underline{r}) = \sum_n e^{i k n a} \underbrace{|n\rangle}_{\Psi_{\alpha}(\underline{r}-n\mathbf{a})}$$

substitute into Sch. eq.:

$$H\Psi = \sum_n e^{i k n a} \left[-\frac{\hbar^2}{2m} \Delta + \sum_{n'} V_{\text{atom}}(\underline{r}-n'\mathbf{a}) \right] |n\rangle = E \sum_n e^{i k n a} |n\rangle$$

project, multiply

$$\langle n'' | \text{ left } \rightarrow \langle n'' | n \rangle = \delta_{n''n}$$

(?)

wavefunctions are orthogonal

$$\sum_{n' \neq n} V_{\text{atom}}(\underline{r}-n'\mathbf{a}) + V(\underline{r}-n\mathbf{a})$$

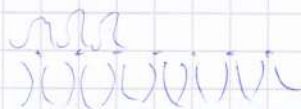
on-site potential

$$\sum_n e^{i k n a} \left[E_a \delta_{n''n} + \sum_{n' \neq n} \langle n'' | V_{\text{atom}}(\underline{r}-n'\mathbf{a}) | n \rangle \right] = E \sum_n e^{i k n a} \underbrace{\langle n'' | n \rangle}_{\delta_{n''n}}$$

Result:

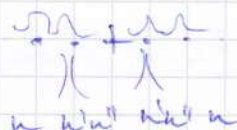
$$E(k) = E_a + \sum_{n' \neq n} e^{i k (n'-n)a} \langle n'' | V_{\text{atom}}(\underline{r}-n'\mathbf{a}) | n \rangle$$

seeing graphically



orbitals
potentials

from the sum: nearest neighbor
tight-binding



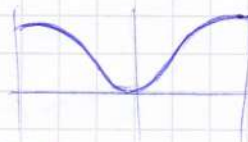
Let's denote:

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

negative $V < 0$ (conduction interaction)

$$E(k) = E_a + \underbrace{(e^{i k a} + e^{-i k a})}_{2 \cos(ka)} \cdot (-|t|)$$

$$E(k) = E_a - 2|t| \cos(ka)$$



Band Structure calculations II

Definition: $H\Psi = E\Psi$ $H: -\frac{\hbar^2}{2m} \Delta + U(\underline{r})$ $U(\underline{r}) = \sum_n V_{\text{atom}}(\underline{r}-n\mathbf{a})$

$$H_{\text{atom}} \Psi_a = E_a \Psi_a$$

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

Ansatz:

$$\Psi_{\alpha}(\underline{r}) = \frac{1}{\sqrt{N}} \sum_n e^{i k n a} \Psi_a(\underline{r}-n\mathbf{a}) \quad (\text{satisfies Bloch-theorem})$$

new notation

$$\Psi_{\alpha}(\underline{r}) = \sum_n e^{i k n a} |n\rangle; \quad \langle n' | n \rangle = \delta_{n'n}$$

$$\int d^3r \Psi_a^*(\underline{r}-n'\mathbf{a}) \Psi_a(\underline{r}-n\mathbf{a})$$

plug into $H\Psi = E\Psi$

$$H\Psi = \sum_n e^{i k n a} \left[-\frac{\hbar^2}{2m} \Delta + \sum_{n'} V_{\text{atom}}(\underline{r}-n'\mathbf{a}) \right] |n\rangle = E(k) \sum_n e^{i k n a} |n\rangle \quad \left/ \begin{array}{l} \langle n' | \\ \text{project} \end{array} \right.$$

$$\sum_{n'} V_{\text{atom}}(\underline{r}-n'\mathbf{a}) = \underbrace{V_{\text{atom}}(\underline{r}-n\mathbf{a})}_{\text{on-site pot.}} + \sum_{n' \neq n} V_{\text{atom}}(\underline{r}-n'\mathbf{a})$$

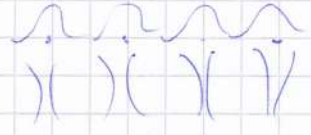
$$\sum_n e^{i n r a} \left[\sum_a \delta_{n a} + \sum_{n' \neq n} \langle n' | V_{\text{atom}}(r - n'a) | n \rangle \right] = E_0 \sum_n e^{i n r a}$$

$$E(z) = E_a + \sum_{n \neq n'} e^{i (n - n') z a} \langle n' | V_{\text{atom}}(r - n'a) | n \rangle$$

Exact Mad
equation

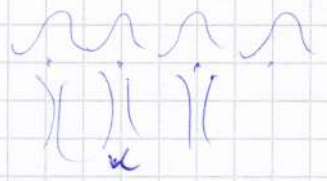
Approximations

(1) Nearest neighbor tight-binding - NNTB



$\psi_a(r - n'a)$ s-type
 $V_{\text{atom}}(r - n'a)$ Coulomb-pot.

NNTB:



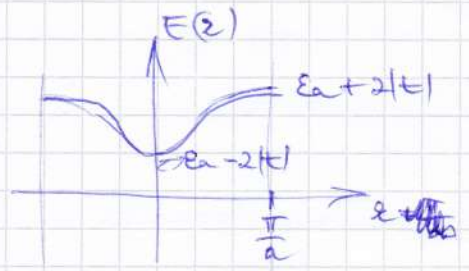
$\Rightarrow$ Approx. $\psi_{n-1} + \psi_{n+1}$ and
 $n' = n'' = n-1$ $n' = n'' = n+1$

keeping where
 $n' = n \pm 1$

$$\begin{aligned} \langle n-1 | V_{\text{atom}}(r - (n-1)a) | n \rangle &= \langle n+1 | V_{\text{atom}}(r - (n+1)a) | n \rangle \\ &= \int \psi_a^*(r - (n-1)a) V(r - (n-1)a) \psi_a(r - na) d^3r \\ &= -|t|; \quad |t| > 0 \end{aligned}$$

t: overlap integral

NNTB: $E(z) = E_a + \left(\frac{e^{i z a} + e^{-i z a}}{2 \cos(z a)} \right) \cdot (-2) \cdot |t|$
 $n'' - n = \pm 1$



(0?)
 $n^* > 1 \rightarrow$ positive curvature

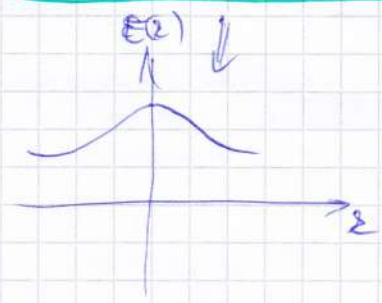
 $\leftrightarrow$ ss σ type overlap
 $\oplus \cdot \oplus \cdot \ominus = \ominus$

p-type orbital: pp σ



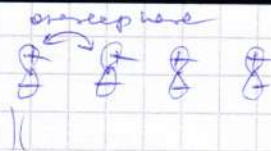
orbitals have a sign
sign of overlap is positive
 $\ominus \oplus \cdot \ominus = \oplus$ (?)

$$E(z) = E_a + 2|t| \cos(z a)$$



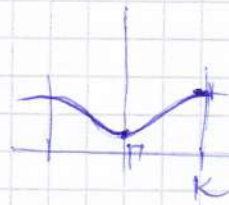
hole type band: $n^* < 0$
(at zero the curvature is $\ominus$)

pp II tight binding



graphene (is like this)

one step is $\ominus$
 $\oplus + \ominus = \ominus$



in graphene interesting things happen here
 Tight-Binding approx. describes it pretty well (quite)

2nd nearest neighbor TB
 (2nd NNTB)



$(e^{i2ka} + e^{-i2ka}) |t'|$ 2nd NNTB

$E(k) = E_a - 2|t| \cos(ka) - 2|t'| \cos(2ka)$

double periodicity
 ↓
 double wiggles

how many TB terms is enough to describe the system?
 (I can consider many terms, as much as I want)
 further I go, the more wiggles I have

TB is semi-empirical:

- PFT band-structure + fitting with TB parameters ($|t|$) (gives numbers)
- fit $|t|$'s from experiment like E_g or m^*

example: effective mass $(m^*)^{-1} = \frac{1}{\hbar^2} \frac{\partial^2 E(k)}{\partial k^2}$

$E(k) = E_a - 2|t| \cos(ka) = E_a - 2|t| \left[1 - \frac{k^2 a^2}{2} \right] \rightarrow (m^*)^{-1} = \frac{2|t|a^2}{\hbar^2}$

$\cos ka \approx 1 - \frac{k^2 a^2}{2}$ (Taylor series)

dim: $[t] = \mathcal{J}(\text{energy})$, $[(m^*)^{-1}] = \frac{\mathcal{J} m^2}{\mathcal{J} s^2} = \frac{m^2}{\mathcal{J} s^2} = \frac{1}{\mathcal{J} g}$ (indeed)

t changes exponentially with a
 constraining $a \rightarrow$ c.c.s get lighter ($\rightarrow$ faster, better)

2D TB Approximation



$E(k) = E_a - 2|t| \cos(k_x a) - 2|t'| \cos(k_y a)$
 $E(k_x, k_y)$

" $s-p$ model" (new topic, new for everyone)

- good semi-empirical model near band extreme $\leftrightarrow$ ideal for important steps in SC
- gives clear results for transport, optics and magnetic properties

$H\psi = E\psi$ we want to solve this still
 solution obeys the Bloch-therm.!

$\psi_{n,k}(r) = e^{i k r} u_{n,k}(r)$
 n : band index $u_{n,k}(r)$: lattice periodic function

$\underline{k}$: crystal momentum, generally

$$\hbar \underline{k} = \underline{F} \tau$$

← external forces

(separation of ext and int. forces is possible)

$$\underline{p} = \hbar \nabla$$

canonical imp

$\hbar \underline{k} \neq \underline{p}$ except for plane

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

↓
periodic
pot.

Substitute: $\Psi_{nk}(\underline{r})$ into $H\Psi$:

$$\Delta \Psi_{nk}(\underline{r}) = (\hbar \nabla)^2 \Psi_{nk}(\underline{r}) + 2i\hbar \nabla \cdot \underline{k} \Psi_{nk}(\underline{r}) + e^{i\hbar \underline{k} \cdot \underline{r}} \Delta \Psi_{nk}(\underline{r})$$

$$\Delta \Psi_{nk} = (i\hbar)^2 \Psi_{nk}(\underline{r}) + 2i\hbar e^{i\hbar \underline{k} \cdot \underline{r}} \nabla \cdot \underline{k} \Psi_{nk}(\underline{r}) + e^{i\hbar \underline{k} \cdot \underline{r}} \Delta \Psi_{nk}(\underline{r}) \rightarrow \text{into } H\Psi$$

$$\left[\frac{\hbar^2 \underline{k}^2}{2m} - \frac{i\hbar^2 \underline{k} \cdot \nabla}{m} - \frac{\hbar^2 \Delta}{2m} + V(\underline{r}) \right] \Psi_{nk}(\underline{r}) = E_{nk} \Psi_{nk}(\underline{r})$$

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

$$\left[\frac{\hbar^2 \underline{k}^2}{2m} + \frac{\hbar \underline{k} \cdot \underline{p}}{m} + \frac{p^2}{2m} + V(\underline{r}) \right] \Psi_{nk}(\underline{r}) = E_{nk} \Psi_{nk}(\underline{r})$$

So far exact!

$\underline{k} \cdot \underline{p}$ approx.: consider solution of Sch. near band - edge where $\underline{k} = 0$ (like Γ)

$$\text{then } \left[\frac{p^2}{2m} + V(\underline{r}) \right] \Psi_{n0}(\underline{r}) = E_{n0} \Psi_{n0}(\underline{r}) \quad \text{Sch. eq. at the center}$$

+ consider $\frac{\hbar^2 \underline{k}^2}{2m} + \frac{\hbar \underline{k} \cdot \underline{p}}{m}$ as perturbation! works if small

2nd order perturbation theory

Suppose:

$H|u\rangle = E_u|u\rangle$ is solved

$|u\rangle$ is a set of orthonormal wavefunctions

$$\langle u'|u\rangle = \delta_{u'u}$$

$(H+V)\psi = E\psi$ what is E and ψ ?

$$\text{Ansatz: } E_u = E_{u0} + \langle u|V|u\rangle + \sum_{u' \neq u} \frac{\langle u'|V|u\rangle \langle u|V|u'\rangle}{E_{u'} - E_u} \quad \text{(1st order w/ u)} \quad \text{(we can ignore...)} \quad \text{2nd order}$$

$$\psi_u = |u\rangle + \sum_{u' \neq u} \frac{\langle u'|V|u\rangle}{E_{u'} - E_u} |u'\rangle$$

my basis: $\Psi_{nk}(\underline{r})$

Result:

$$\Psi_{nk}(\underline{r}) = \Psi_{n0}(\underline{r}) + \sum_{u' \neq u} \frac{\hbar}{m} \frac{\langle u'| \frac{\underline{k} \cdot \underline{p}}{m} | u \rangle}{E_{u'} - E_{u0}} | \Psi_{n0} \rangle$$

$$\langle \Psi_{n0} | \left[\frac{\hbar^2 \underline{k}^2}{2m} + \frac{\hbar \underline{k} \cdot \underline{p}}{m} \right] | \Psi_{n0} \rangle$$

1st term: it's nothing but

$$\frac{\hbar^2 \underline{k}^2}{2m} \langle \Psi_{n0} | \Psi_{n0} \rangle = 0 \text{ but useful}$$

Sch. eq.: substitute $\Phi(\underline{r})$ in here

$$(*) \sum_{\underline{n}} \Psi_{\underline{n}}(\underline{r}) [E_{\underline{n}}(\underline{r}) - E + V(\underline{r})] F_{\underline{n}}(\underline{r}) = 0 \quad \text{no longer a differential eq.}$$

$\Psi_{\underline{n}}(\underline{r})$ forms an orthonormal set of functions

$$\int \Psi_{\underline{n}}^*(\underline{r}) \Psi_{\underline{m}}(\underline{r}) d^3r = \delta_{\underline{n}, \underline{m}} = \delta_{\underline{n}} \delta_{\underline{m}} \quad \leftarrow$$

we $\int \Psi_{\underline{n}}^*(\underline{r})$ the $(*)$ equation $\langle \Psi_{\underline{n}}(\underline{r}) |$ $\langle \Psi_{\underline{n}'} | \Psi_{\underline{n}} \rangle = \delta_{\underline{n}, \underline{n}'}$

$$\Rightarrow (*) \sum_{\underline{n}} [E_{\underline{n}}(\underline{r}) - E] \delta_{\underline{n}, \underline{n}'} + \langle \Psi_{\underline{n}'} | V(\underline{r}) | \Psi_{\underline{n}} \rangle F_{\underline{n}}(\underline{r}) = 0 \quad \text{sum over } \underline{n}$$

$$\langle \Psi_{\underline{n}'} | V(\underline{r}) | \Psi_{\underline{n}} \rangle = \int \Psi_{\underline{n}'}^*(\underline{r}) \Psi_{\underline{n}}(\underline{r}) \cdot e^{i(\underline{k}-\underline{k}')\cdot\underline{r}} \cdot V(\underline{r}) d^3r$$

fast varying (if $\underline{k} \neq \underline{k}'$) $\uparrow$ slowly varying $\leftarrow$ diff. with $\underline{k}$ approximated

separation: if functions are different in properties

$$\langle \Psi_{\underline{n}'} | V(\underline{r}) | \Psi_{\underline{n}} \rangle \approx \underbrace{\int \Psi_{\underline{n}'}^*(\underline{r}) \Psi_{\underline{n}}(\underline{r}) d^3r}_{\text{Bloch's theorem sgs: } \delta_{\underline{n}, \underline{n}'} \delta_{\underline{k}, \underline{k}'}} \cdot \underbrace{\int e^{i(\underline{k}-\underline{k}')\cdot\underline{r}} V(\underline{r}) d^3r}_{(FT)}$$

Substitute back to $(**) eq.$

$$\sum_{\underline{n}} [E_{\underline{n}}(\underline{r}) - E] \delta_{\underline{n}, \underline{n}'} + V(\underline{k}-\underline{k}') F_{\underline{n}}(\underline{r}) = 0$$

This is a Sch. eq. for $F_{\underline{n}}(\underline{r})$

Example:

plane wave solution + effective mass approximation

$$E_{\underline{n}}(\underline{r}) = E_c + \frac{\hbar^2 \underline{k}^2}{2m_e^*} \quad \text{with this we get the EFA equation as:}$$

(known solution)

$$\frac{\hbar^2 \underline{k}^2}{2m_e^*} F_c(\underline{r}) + \sum_{\underline{n}} V(\underline{k}-\underline{k}') F_c(\underline{r}) = (E - E_c) F_c(\underline{r})$$

$\uparrow$ band index

EFA for conduction band

$\leftarrow$ set of linear equations

We approximate canonical impulse with:

$$-i\hbar \nabla \equiv \underline{k} \quad (\text{is valid for plane waves})$$

the Schrödinger equation for $F_c(\underline{r})$:

$$\left[\frac{\hbar^2 \nabla^2}{2m_e^*} + E_c + V(\underline{r}) \right] F_c(\underline{r}) = E F_c(\underline{r}) \quad \text{sch. eq. for } F_c(\underline{r}) \text{ function}$$

FT. both sides: $F_c(\underline{r}) \rightarrow F_c(\underline{k})$

$$FT(f(\underline{r})) = \int e^{i\underline{k}\cdot\underline{r}} f(\underline{r}) d^3r = \int_0^{2\pi} \int_0^{2\pi} \int_0^{2\pi} e^{i\underline{k}\cdot\underline{r}} f(\underline{r}) d^3r = \int_0^{2\pi} \int_0^{2\pi} \int_0^{2\pi} e^{i\underline{k}\cdot\underline{r}} f(\underline{r}) d^3r$$

$$FT(V(\underline{r}) F_c(\underline{r})) = \int V(\underline{k}-\underline{k}') F_c(\underline{k}') d^3k' \quad \leftarrow \text{convolution}$$

Substituting it back gives:

$$\frac{\hbar^2 \underline{k}^2}{2m_e^*} F_c(\underline{k}) + \sum_{\underline{k}'} V(\underline{k}-\underline{k}') F_c(\underline{k}') = (E - E_c) F_c(\underline{k})$$

Exam: Sch. for plane waves is valid

Semiempirical method as it needs E_c and m_e^* as input

Example: extra charge (doping)

charge density: $n_e(r) = \frac{\int |\psi(r)|^2 \rho(r)}{\int |\psi(r)|^2 \rho(r)}$ ← probabilistic interpretation
Bohr / Fermi fr.

$$n(r) \stackrel{\text{EFA}}{=} \sum_i |\psi_i(r)|^2 \rho(r) \stackrel{\text{original}}{=} n_{\text{co}} \cdot \sum_i F_i(r) \rho(r)$$

e.g. n doped Si, P: Si



(EFA) everything is self-consistent
 works well if $\frac{a_p^*}{d} \gg 1$
(Bohr) atomic distance

Transport phenomena in Sc

current: j
 thermal current: j_Q
 magnetoresistance:
 frequency dependent conductivity
 Seebeck-effect, Peltier-effect

size (length) scales

— cc. length $\xrightarrow{\text{diffusion}}$ charge is created, annihilates
 typically: $10 \mu\text{m} - 1 \text{cm}$ (Solar cells)

Diffusion:
 ↓ propagation in material is diffusive

mean-free-path: $l = v_F \tau$
Fermi velocity momentum scales by time relaxation time
 τ_c : cc. lifetime: $\tau_c(\text{Si}) = 10 \text{ps} - 10 \text{ns}$

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

diffusion current diffusion constant; $D \approx \frac{1}{3} \cdot v_F^2 \tau \approx \frac{1}{3} v_F \cdot l$

$l < d_F < 0.5 < d_c$

charge carrier diffusion length: $d_c = \sqrt{D \tau_c}$; solution of diffusion eq.

spin diffusion length; τ_s : spin lifetime

$$\tau_s = 1 \text{ns} - 1 \mu\text{s}$$

$$d_s = \sqrt{D \tau_s}$$

typical values:
 1... 100 μm



phase coherence length: 100 nm ... 1 μm



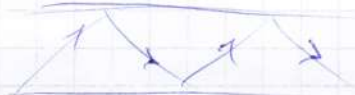
e^- propagates as a plane wave

wave scatters coherently on an impurity

important for: wave localization
ballistic transport
 optical analogy of ballistic transport:
 optical fibre

Momentum relaxation time: $10^{-13} - 10^{-15}$

mean-free path 1 nm ... 100 nm $l = v_F \tau$
 ↓ Ohm's law (diffusion + drift)



no attenuation
 always phase coherent

mesoscopic physics → 100 nm - 1 μm → Landauer-Buttiker formalism: (Ohm's law may not work below a given length scale)

Transport in SCs

Diffusion $\rightarrow$ ohm's law

Free electrons (Sommerfeld model)

quantum no. $\rightarrow$ periodic b.c.
 $\rightarrow$ periodic boundary condition

velocity $v = \frac{1}{\hbar} \frac{\partial E}{\partial k} = \frac{\hbar k}{m}$

Energy dispersion $E(k) = \frac{\hbar^2 k^2}{2m}$

wave fn (ψ) $\psi_k(r) = \frac{1}{\sqrt{V}} e^{ikr}$

effective mass $m^* = m$

Block - electrons

$k \in$ periodic b.c. + n : band index

$$v(k) = \frac{1}{\hbar} \frac{\partial E_n}{\partial k} = \frac{1}{\hbar} \nabla_k E_n(k)$$

$$E_n(k) = E_n(k+G); G \in \text{reciprocal lattice}$$

$$\psi_{nk} = e^{ikr} u_{nk}(r); \text{ where } u_{nk}(r) = u_{n,k+G}(r+R)$$

$$(m^*)^{-1} = \frac{1}{\hbar} \frac{\partial^2 E}{\partial k^2}$$

$$m^* \text{ tensor: } m_{ij}^{-1} = \frac{1}{\hbar^2} \frac{\partial^2 E}{\partial k_i \partial k_j}$$

Remarks:

Drude - model: $ma = -eE - \frac{\hbar}{\tau} v$
 $\uparrow$ damping, viscous force constant
 $m \dot{v} = -eE - \frac{m}{\tau} v \rightarrow \sigma = \frac{ne^2 \tau}{m}$

resistivity is due to collisions with ions, viscous environment

Block - model: motion of e^- in a perfect lattice (ions at equilibrium position)

$$\sigma = \infty$$

$$\tau = \infty$$

$$\text{velocity of } e^- : v(k) = \text{const.}$$

imperfections, lattice vibrations: ~~phonons~~
 $\rightarrow$ ion motion

Canonical vs Crystal momentum (impulse)

conservation of momentum $\rightarrow$ result of translational invariance

In a crystal we have a discrete translational invariance

$$r \rightarrow r + R \quad \text{R: lattice vector}$$

$\rightarrow$ crystal momentum is conserved: $\hbar k$

Forces:

$$F_{\text{ext}} = \hbar \dot{k}$$

$\leftarrow$ periodic potential is transformed out from the problem! (eg. $-eE$, bohrer...)

Price paid: $u_{nk}(r)$ are not nice

canonical impulse $\neq$ crystal momentum $\rightarrow p \neq \hbar k$

$$\text{canonical impulse: } p = \frac{\hbar}{i} \nabla; p \psi_{nk}(r) = \frac{\hbar}{i} \nabla (e^{ikr} u_{nk}(r)) = \hbar k \psi_{nk}(r) + \hbar \nabla u_{nk}(r)$$

Block - fms are no eigenstates of canonical impulse $[p, h] \neq 0$

contribution of a closed e^- band to conduction

$$j = -e \int \frac{d^3k}{4\pi^3} \frac{1}{\hbar} \frac{\partial E}{\partial k} v(k) f(k) = -e \int \underbrace{D(k)}_{\text{DOS}} \underbrace{f(k)}_{\text{Fermi-fn. (occupation fn.)}} \underbrace{v(k)}_{\text{group velocity}} d^3k$$

at $T=0$ $v(k) = \frac{1}{\hbar} \frac{\partial E}{\partial k}$ $E = E(k)$

j for a closed band : ~~not zero~~ $= 0$

$$j = -e \int \frac{d^3k}{4\pi^3} \frac{1}{\hbar} \frac{\partial E}{\partial k} = 0$$

closed band

Strong statement (Aschcroft - Mermin book)

(no conduction in closed bands) / bandwaving arguments / (sponge tilting demonstration)

$$\int \frac{d^3k}{4\pi^3} \frac{\partial E}{\partial k} = 0$$

symmetric domain $\leftarrow$ odd fn.

concept of holes :

$$0 = \int \frac{d^3k}{4\pi^3} v(k) = \int \frac{d^3k}{4\pi^3} v(k)_{\text{states below } E} + \int \frac{d^3k}{4\pi^3} v(k)_{\text{states above } E}$$

closed band $\uparrow$ states below E $\downarrow$ states above E



$$-e \int \frac{d^3k}{4\pi^3} v(k)_{\text{states below } E} = +e \int \frac{d^3k}{4\pi^3} v(k)_{\text{states above } E}$$

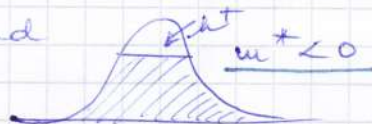
electron conduction



hole conduction

as if te c.c.s were present

hole is just a concept band



$$m^* = \frac{\hbar^2}{m a^2}$$

Boltzmann - equation

We describe the system with particle distribution function.

$f(k, r, t)$ distribution function simplest form :

measurable quantities :

$$j = -e \int \frac{d^3k}{4\pi^3} v(k) f(k)$$

$\uparrow$ external forces affect the distribution

$$f_0(E(k), r, t) = \frac{1}{e^{\frac{E(k) - E_F}{k_B T}} + 1}$$

(for fermions)

stationary $\rightarrow$ no (t, r)

$$\frac{\hbar}{m} \nabla \cdot \nabla \psi = 0$$

Boltzmann:

$$\frac{df}{dt} = \frac{\partial f}{\partial t} + \underline{\dot{x}} \cdot \underline{\nabla_x} f + \underline{\dot{r}} \cdot \underline{\nabla_r} f = \left. \frac{\partial f}{\partial t} \right|_{\text{collision term}}$$

(no general solution)

collision term $\longleftrightarrow$ Drude-model $m \underline{v} = -e \underline{E} - \frac{m \underline{v}}{\tau}$
 ↑ introduced heuristically ↓ not the collision term collision

$$f(\underbrace{E(\underline{x})}_{1.}, \underbrace{\underline{x}}_{2.}, \underbrace{\underline{r}}_{3.}, \underbrace{t}_{4.}); \quad \frac{df}{dt} \stackrel{\text{chain's rule}}{=} \underbrace{\frac{\partial f}{\partial t}}_{\text{scalar}} + \underbrace{\frac{\partial f}{\partial \underline{x}} \cdot \underline{\dot{x}}}_{\substack{1. \\ \underline{\nabla_x} f}} + \underbrace{\frac{\partial f}{\partial \underline{r}} \cdot \underline{\dot{r}}}_{\substack{2. \\ \underline{\nabla_r} f}} + \underbrace{\frac{\partial f}{\partial E} \cdot \frac{\partial E(\underline{x})}{\partial \underline{x}} \cdot \underline{\dot{x}}}_{\substack{3. \\ 1.}}$$

$$\left[f^0 = \frac{1}{e^{(E - \mu)/kT} + 1} = \frac{1}{e^{x/2} + 1} \text{ additional terms: } \frac{\partial f}{\partial x} \frac{\partial x}{\partial \mu} \frac{\partial \mu}{\partial \underline{r}} \cdot \underline{\dot{r}} + \frac{\partial f}{\partial x} \frac{\partial x}{\partial T} \frac{\partial T}{\partial \underline{r}} \cdot \underline{\dot{r}} \right]$$

- $\underline{\dot{x}} \cdot \underline{\nabla_x} f$: force term $\underline{x} \cdot \underline{\dot{x}} = \underline{F}_{\text{ext}} = -e \underline{E} = -e \underline{v} \times \underline{B}$

- $\underline{\dot{r}} \cdot \underline{\nabla_r} f$: diffusion term (we neglect it)

Assume force term only

$$\frac{\partial f}{\partial t} + \frac{1}{\tau} \underline{F}_{\text{ext}} \cdot \frac{\partial f}{\partial \underline{x}} = \left. \frac{\partial f}{\partial t} \right|_{\text{collision term}} = -\frac{g(\underline{x}, t)}{\tau}$$

relaxation time approximation

$$f(\underline{x}, t) = f^0(\underline{x}, t) + g(\underline{x}, t)$$

eg. distribution difference in equilibrium

τ -relaxation time

scattering probability per unit time from $\underline{x} \rightarrow \underline{x}'$;
 usually: $\tau = \tau(\underline{x})$

τ is the same as τ in the Drude-model

Assume: $\underline{F}_{\text{ext}} = 0$ relaxation approximation ($\tau = \text{const}$)

$$\left[\frac{\partial f}{\partial t} = \frac{\partial f^0}{\partial t} + \frac{\partial g(\underline{x}, t)}{\partial t} = -\frac{g(\underline{x}, t)}{\tau} \right] \rightarrow g(t) = g(t=0) e^{-t/\tau}$$

origin of the name: relaxation time

f : distribution fun.

$$f^0(\underline{x}) = \frac{1}{e^{\frac{E(\underline{x}) - \mu}{kT}} + 1}$$

$f(\underline{x}, \underline{r}, t)$

$$\frac{\partial f}{\partial t} = \frac{\partial f}{\partial t} + \underbrace{\underline{\dot{x}} \cdot \underline{\nabla_x} f}_{\text{force}} + \underbrace{\underline{\dot{r}} \cdot \underline{\nabla_r} f}_{\text{diffusion}} = \left. \frac{\partial f}{\partial t} \right|_{\text{coll.}}$$

Stationary case: $\frac{\partial f}{\partial t} = 0$ plus DC electric field $\underline{F}_{\text{ext}} = -e \underline{E}$

neglect diffusion term: $\underline{\nabla_r} f = 0$

$$\text{force term: } \underline{\nabla_x} f = \frac{\partial f}{\partial x} = \frac{\partial f}{\partial E} \cdot \frac{\partial E(\underline{x})}{\partial \underline{x}}$$

$$\underline{v}(\underline{x}) = \frac{1}{\hbar} \frac{\partial E(\underline{x})}{\partial \underline{k}}$$

$$\Rightarrow \nabla_x f = \frac{\partial f}{\partial E} \hbar v(x)$$

$$\underline{x} = \frac{1}{\hbar} \text{Foot}$$

Substitute back to Boltzmann - eq. :

$$-\frac{eE}{\hbar} \frac{\partial f}{\partial E} \hbar v(x) = -\frac{g(x,t)}{\tau}$$

Solution for g : $g(x,t) = \frac{\partial f}{\partial E} \cdot eE \cdot v(x) \cdot \tau$

Final result: $f(x,t) = f^0(x) + \frac{\partial f^0}{\partial E} \cdot eE \cdot v(x) \tau$

looks like a linearization

approx: $\frac{\partial f}{\partial E} \approx \frac{\partial f^0}{\partial E}$

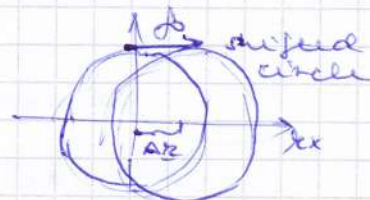
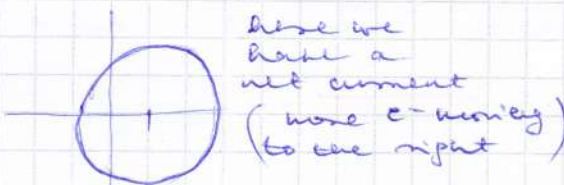
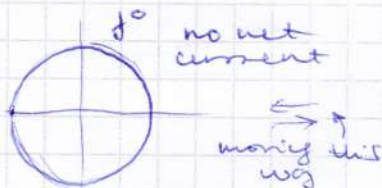
consider:

$$f^0\left(x + \frac{eEx}{\hbar}\right) \approx f^0(x) + \frac{eEx}{\hbar} \cdot \frac{\partial f^0}{\partial E} \cdot \frac{\partial E}{\partial x} = f^0(x) + eEx \frac{\partial f^0}{\partial E} v(x)$$

$$f(x+dx) = f(x) + dx \frac{\partial f}{\partial x} + o(dx^2)$$

perturbed distribution function looks like as if it was shifted in x -space by $\Delta x = -\frac{eEx}{\hbar}$ (parallel to E)

net current:



net drift velocity from Boltzmann - eq.

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

$$v_d = -\frac{eEx}{m^*}$$

← Boltzmann eq.
⇒ same as Drude

Drude:

$$m^* \vec{v} = eE - \hbar \vec{v}$$

$$\vec{v} = \frac{eE}{m^*} - \frac{\vec{v}}{\tau} \Rightarrow \text{stationary: } v_d = -\frac{eEx}{m^*}$$

Drude

Block (Boltzmann eq.)

→ conceptual differences

lot of small moving e^-

$$v = v_d \ll v_F = \left(10^{-5} - 10^{-6} \frac{m}{s}\right) \quad (\text{Fermi-velocity})$$

a few e^- are fast those on the Fermi surface, but they move fast with v_F

$$j = nev_d \quad (\text{net current})$$

$$j = e n_F \frac{m v_d}{m_F}$$

same result, but conceptually different!
QM is right!

→ number of charge carriers

Transport in SCs II.

τ is a principal quantity

low T: impurity

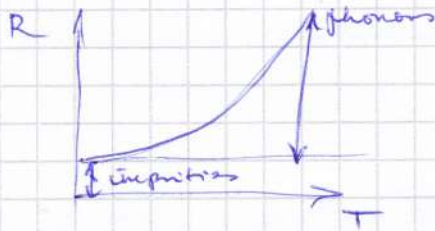
high T: ionized defects

origins: phonons, impurities, defects
 → everything that breaks the perfect lattice (the symmetry)

Matthiessen's rule:

$$\frac{1}{\tau} = \frac{1}{\tau_{e-e}} + \frac{1}{\tau_{e-phonon}} + \frac{1}{\tau_{imp}} + \dots$$

shortest timescale dominates



R : resistivity

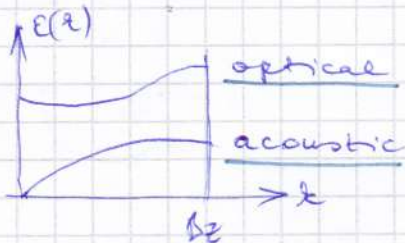
examples:

$$\frac{1}{\tau_{e-e}} \sim T^2; \quad \frac{1}{\tau_{e-ph}} = \begin{cases} \sim T & T > T_{Debye} \\ \sim T^5 & T \ll T_{Debye} \end{cases}$$

$$T > T_{Debye} \\ T \ll T_{Debye}$$

$$(k_B T_D = \hbar \omega_D) \quad (2D)$$

phonon - dispersion



optical : and excited with optical phonons $\left(\frac{\hbar E}{\hbar \omega} \right)$

acoustic : looks like an acoustic ~~osc~~ : $E \sim k$

Debye-model: (acoustic)

DOS(phonon)



Debye - Einstein model: acoustic + optic



Ω : phonon dispersion frequency

Eliashberg - formalism: (phonons only)

$$\frac{\hbar}{\tau} = 2\pi k_B T \lambda$$

λ : e-phonon coupling constant typ.: 0.1-1

scattering rate

τ is always around $10^{-13} - 10^{-15}$ second
 only valid if T is large

$$\lambda = 2 \int \frac{d\Omega}{\Omega} \Omega^2 F(\Omega); \quad \frac{\Omega^2 F(\Omega)}{\downarrow \text{DOS}} : \text{notation: how strong e- are coupled to phonons}$$

if T is small

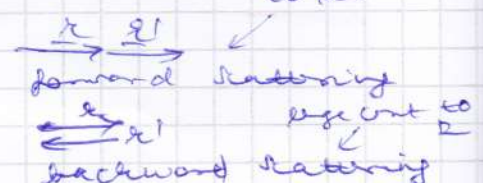
$\Omega^2 F(\Omega)$ contains the so-called $\frac{1 - \cos k \cdot k'}{\Omega}$ term:



or



no contribution to R



R : resistivity

$$\frac{v}{v_0} = \frac{e}{2\pi} \frac{2\pi}{\lambda'} \rightarrow \frac{e}{\lambda'}$$

$$v=0 \rightarrow 1 - \cos \theta = 0 \quad (\text{does nothing})$$

$$v=\pi \rightarrow 1 - \cos \theta = 2$$

Bloch-Grüneisen-law : (acoustic, isotropic phonons)

Debye model with a single T_D

explicit, analytic solution

$$\frac{\kappa}{\tau} = 2\pi \lambda k_B T \int_0^{T_D/T} \left(\frac{dQ}{d\omega} \right) \left(\frac{\hbar \omega / k_B T}{\sinh(\hbar \omega / 2 k_B T)} \right)^2$$

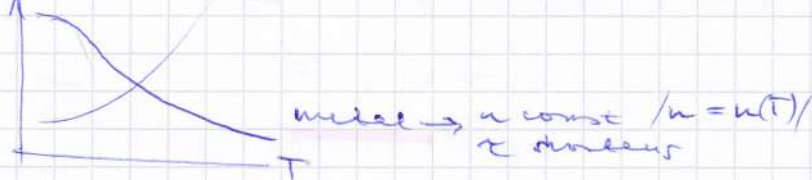
↑
high T
constant

$$\left. \begin{array}{l} 1 \text{ if } T \rightarrow \infty \\ \sim 10^4 \text{ if } T \rightarrow 0 \end{array} \right\}$$



in SCs: $\sigma = \frac{ne^2 \tau}{m^*} = \xi$

$\xi \rightarrow n(T)$ prevails



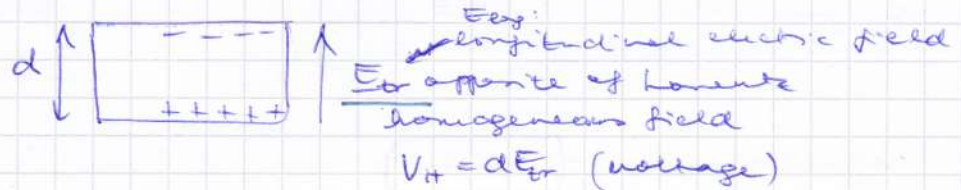
Magnetotransport

Hall-effect :
applying Drude-model

$$\underline{F} = q \underline{v} \times \underline{B} \quad \downarrow \text{Lorentz force}$$



in stationary conditions: internal field builds up to compensate for it



$$N_d = \frac{e E_y \tau}{m^*}$$

$$e E_y = e v_d \cdot B \Rightarrow E_y = N_d B = \frac{e E_{\text{long}} \tau}{m^*} B$$

Hall voltage: $V_H = d N_d \cdot B = \frac{d e E_{\text{long}} \tau B}{m^*}$

define: R_H : Hall resistivity

$$\underline{j} = \sigma \underline{E}, \quad \underline{j} \cdot \underline{B} = 0$$

$$R_H = \frac{E_y}{j_{\text{long}}} = \frac{N_d B}{j_{\text{long}}} = \frac{N_d B}{n e v_d} = \frac{B}{n e}$$

$$[R_H] = \frac{V}{\frac{A}{m^2} \frac{m^3}{As}} = \frac{V}{A} m = \Omega m \quad \checkmark$$

Hall constant: $R \triangleq \frac{R_H}{B} = \frac{1}{n e}$

c.c. - sign sensitive!
(e for n , or $n < p$ for e^- , $n > p$ for e^+)
($n = -10^{23} \frac{1}{cm^3}$)
 $n e + p e$ eg/



large for SC

Q. Hall-effect (quantum) : QHE



Landau levels
level spacing
 $\hbar \omega_B$; $\frac{\hbar}{\tau}$: broadening parameter

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

Zeeman Energy

Cyclotron effect

OB



$$r = \frac{v}{\omega} \quad ; \quad v = \omega r$$

$$m\omega^2 r = qvB$$

$$m\omega^2 r = q\omega r B$$

$$\omega_c = \frac{qB}{m}$$

cyclotron frequency

$\hbar\omega_c$ = level spacing

$$\frac{q\hbar}{m} B$$

$$\mu_B = \frac{e\hbar}{2m}$$

physical meaning:

e^- can close a cyclotron orbit before scattering

QHE appears when:

$$\hbar\omega_c > \frac{\hbar}{\tau} \quad \text{or} \quad \omega_c \tau > 1$$

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

more precisely:

$$\begin{pmatrix} j_x \\ j_y \end{pmatrix} = \begin{pmatrix} \sigma_{xx} & -\sigma_{xy} \\ \sigma_{yx} & \sigma_{xx} \end{pmatrix} \begin{pmatrix} E_x \\ E_y \end{pmatrix}$$

isotropic material

no simple inversion:

$$\rho \neq \frac{1}{\sigma}$$



E_y : builds up (Hall effect)

E_x : applied

$$\rho_{xx} = \frac{\sigma_{xx}}{\sigma_{xx}^2 + \sigma_{xy}^2} = \frac{\mu_x}{\mu_y} = \frac{1}{\mu_y}$$

without derivation

$$\rho_{xx} \propto \frac{1}{\sigma_{xx}} \text{ if } \sigma_{xx} \text{ is small}$$

$$\rho_{xy} = \frac{\sigma_{xy}}{\sigma_{xx}^2 + \sigma_{xy}^2} = \frac{B}{|e|n} \Leftrightarrow \text{Hall resistivity}$$

in practice:

$$n = \frac{1}{|e| \left(\frac{\partial \rho_{xy}}{\partial B} \right)_{B=0}}$$

sign

$$\mu = \frac{\left(\frac{\partial \rho_{xy}}{\partial B} \right)_{B=0}}{\rho_{xx}}$$

carrier mobility

Magnetothermal effects

Boltzmann eq.

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

$f(\vec{r}, \vec{p}, t)$ Experiment shows $\nabla T \rightarrow j$ (Seebeck-effect)

$j \rightarrow j_Q$ (Peltier-effect)
heat current

$\mu(\vec{r}); T(\vec{r}); E(\vec{r}) \leftarrow$ spatial variations

neglect diffusion: $\vec{r} \cdot \nabla_{\vec{r}} f = 0$

$$\frac{df}{dt} = \frac{\partial f}{\partial t} + \vec{v} \cdot \nabla_{\vec{r}} f + \frac{\partial f}{\partial x} \cdot \frac{\partial x}{\partial t} \cdot \frac{\partial T}{\partial x} \cdot \frac{\partial T}{\partial f} \cdot \vec{r} + \frac{\partial f}{\partial x} \frac{\partial x}{\partial \mu} \frac{\partial \mu}{\partial r} \frac{\partial r}{\partial t} + \frac{\partial f}{\partial x} \frac{\partial x}{\partial E} \frac{\partial E}{\partial t} \cdot \vec{r}$$

$$f^0 = \frac{1}{e^{(E-\mu)/kT} + 1} = \frac{1}{e^x + 1}$$

$$\frac{\partial f}{\partial x} \frac{\partial x}{\partial T} \nabla T \cdot \vec{r} + \frac{\partial f}{\partial x} \frac{\partial x}{\partial (E-\mu)} \nabla (E-\mu) \cdot \vec{r} \quad ; \quad \frac{\partial x}{\partial T} = -\frac{x}{T}$$

Collect all terms:

Force term: $\nabla_{\mathbf{r}} f - \dot{\mathbf{r}}$

$$\left[\frac{df}{dt} = \frac{\partial f}{\partial t} + \frac{\partial f}{\partial \mathbf{r}} \cdot \mathbf{v}(\mathbf{r}) \right] \left[T_{\text{ext}} - \nabla \mu + \frac{E(\mathbf{r}) - \mu}{T} (-\nabla T) \right]$$

$\dot{\mathbf{r}} = \frac{F_{\text{ext}}}{\hbar}$ $\nabla_{\mathbf{r}} f = \frac{\partial f}{\partial \mathbf{r}} \frac{\partial \mathbf{r}}{\partial \mathbf{r}} = \frac{\partial f}{\partial \mathbf{r}} \mathbf{v}(\mathbf{r})$

(don't have to remember this!)

$E = E(\mathbf{r}), \quad \mathbf{v}(\mathbf{r}) = \frac{1}{\hbar} \frac{\partial E}{\partial \mathbf{r}}$

reminder: we had: $\frac{df}{dt} = \frac{\partial f}{\partial \mathbf{r}} \cdot \mathbf{v}(\mathbf{r}) \cdot (-e\mathbf{E}) = -\frac{\mathbf{j}}{e}$

Solution: $f = f^0 + eE \mathbf{r} \cdot \mathbf{v}(\mathbf{r}) \cdot \frac{\partial f}{\partial \mathbf{r}}$

stationary solution
why don't we use this one?

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

Particle current

$\mathbf{j}_n = \int \frac{d^3 \mathbf{r}}{4\pi^3} \mathbf{v}(\mathbf{r}) f(\mathbf{r})$

$\mathbf{j} = -e \int \frac{d^3 \mathbf{r}}{4\pi^3} \mathbf{v}(\mathbf{r}) f(\mathbf{r})$ ← electric current

~~particle~~ current (?)

First law of thermodynamics: $dU = \delta Q + \delta W \rightarrow dU = T dS + \mu dN$

$T dS = dU - \mu dN$: $dU \leftrightarrow$ energy current

heat transfer

$\mathbf{j}_E = \int \frac{d^3 \mathbf{r}}{4\pi^3} \mathbf{v}(\mathbf{r}) f(\mathbf{r}) \cdot E(\mathbf{r})$

thermal current: $T dS \rightarrow \mathbf{j}_Q = \int \frac{d^3 \mathbf{r}}{4\pi^3} \mathbf{v}(\mathbf{r}) f(\mathbf{r}) (E - \mu)$

without derivation:

$$\begin{aligned} \mathbf{j} &= k_0 \left(\mathbf{E} + \frac{\nabla \mu}{e} \right) - k_1 \left(-\frac{\nabla T}{T} \right) \\ \mathbf{j}_Q &= -k_1 \left(\mathbf{E} + \frac{\nabla \mu}{e} \right) + k_2 \left(-\frac{\nabla T}{T} \right) \end{aligned}$$

k_1 are integrals of $\mathbf{v}(\mathbf{r}) f(\mathbf{r})$

two k_1 's are the same
cross-coefficients

Onsager-relation (IV law of thermodynamics)
principle of detailed balance

Examples:

(1) Heat conductivity: $\mathbf{j}_Q = -K \nabla T$ Fourier-law

$\mathbf{j} = 0$

$k_0 \left(\mathbf{E} + \frac{\nabla \mu}{e} \right) = k_1 \left(\frac{\nabla T}{T} \right)$

substitute into second

$K = \frac{k_2}{T} - \frac{k_1^2}{k_0 T}$

(2) Seebeck effect $\nabla T \neq 0, \quad \mathbf{E} = 0 \Rightarrow \mathbf{j} \neq 0$ or open circuit $\mathbf{j} = 0$
 $\mathbf{E} \neq 0, \quad \nabla T = 0$

definition of Seebeck-coeff: $\frac{E + \nabla \mu}{e} \triangleq S \nabla T$

gives: $S = -\frac{1}{T} \cdot \frac{k_1}{k_0}$

Seebeck

↑ Seebeck-coeff.

(3) Peltier-effect: $j \neq 0 \rightarrow j_Q \neq 0$ definition of Peltier-coeff
 $\nabla T = 0$
 $\pi = - \frac{K_1}{K_0}$
 $j_Q \Delta = \pi j$

relation between π and $S \rightarrow \pi = ST$ kelvin-relation
 special case of Onsager

(4) Wiedemann-Franz law:

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

↑
for free e's
Lorenz number

what is good electric conductor usually good heat conductor
 ↑ (counter example: diamond)
 not lattice vibrations

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

Thermoelectric-cooler (Peltier)

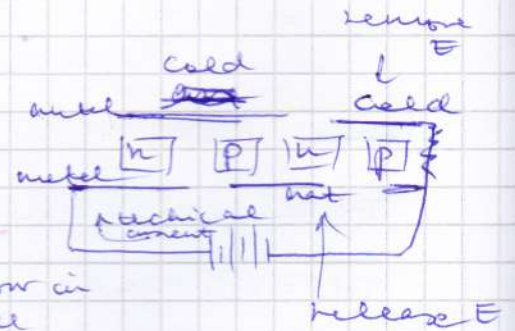


Front
 $\dot{Q}$ leaves

Side
 cold



heat flow in parallel



n-type

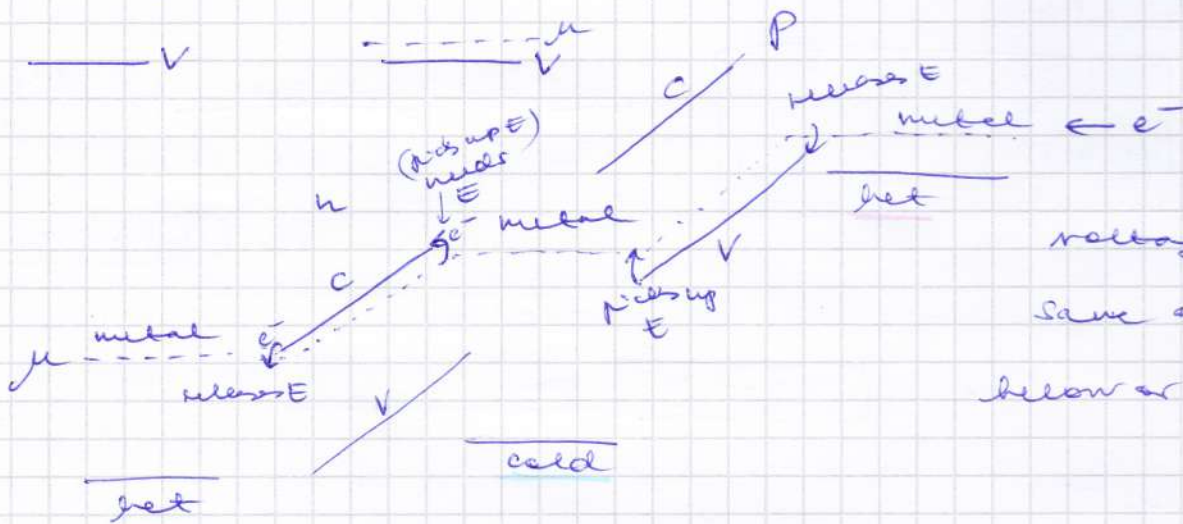
p-type

— c —
 - - - μ

— c —

— V —

— μ —
 — V —

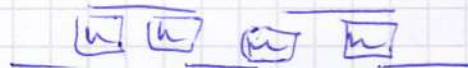
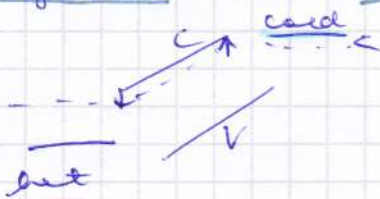


voltage drop $\rightarrow$
 same as separation
 below or above μ

Single n is a Peltier-cooler, but not practical

this wouldn't work

each electrode
 is cold and hot
 at the same time



Diffusion effects in SCs

non-uniform charge distribution $\rightarrow$ form two SCs n & p
 $\rightarrow$ doping homogeneous

Intrinsic SCs

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

don't have to remember this (?)
 depends on T

Law of mass action: (like water pH: dissociates)
 (e^- pairs dissociate, recombine)

$$np = n_i^2(T)$$

Extrinsic SCs

$$n \gg p$$

Intrinsic

$$n \approx p$$

$$v$$

$$v$$

doped: majority carriers
 minority

n -type $n \gg p$ n : maj.
 p : min.
 p -type $p \gg n$ p : maj.
 n : min.

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

e.g. why is $np = n_i^2(T)$ retained
 n doping

$$\frac{n}{n_i} \sim e^{-\beta(E_F - E_i)}$$

n increases by $e^{-\beta(E_F - E_i)}$

p decreases by $e^{-\beta(E_i - E_F)}$

product stays the same

$$n \sim e^{-\beta(E_F - E_i)}$$

$$n \sim e^{-\beta(E_F - E_i)}$$

$$p \sim e^{-\beta(E_i - E_F)}$$

$$p \sim e^{-\beta(E_i - E_F)}$$

a non-equilibrium charge concentration

excitation (by light, injection, thermal excitation)

equilibrium concentration n_0, p_0
 non-equilibrium n, p

$$\frac{n_0 p_0}{n p}$$

recombination rate R_{sp}
 thermal excitation $G_{th} = 2^0$

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

$$U = c[(n - n_0)(p - p_0) + n_0(p - p_0) + p_0(n - n_0)]$$

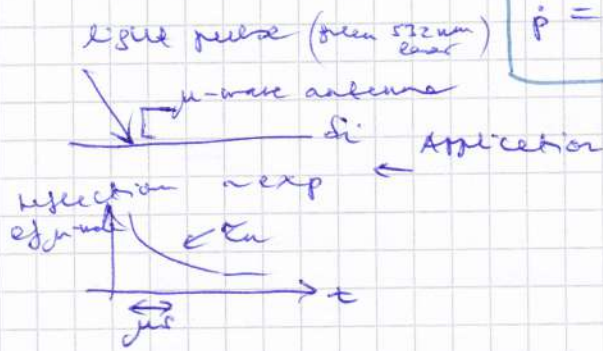
Small, second order
 neglect

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

n -type $n_0 \gg p_0 \rightarrow U \approx c n_0 (p - p_0)$
 p -type $p_0 \gg n_0 \rightarrow U \approx c p_0 (n - n_0)$
 Recombination is given by minority carrier concentration

E.g. $\dot{n} = - (u - u_0)$; $\dot{n} = - \frac{n - n_0}{\tau_n}$
 $\dot{p} = - \frac{p - p_0}{\tau_p}$

τ_n, τ_p : cc lifetime
 ↓
 how long it can survive
 cc recombination time



Recombination :

n-type $n \gg p$
 p-type $p \gg n$

$n \approx n_d$ (donors)
 $p \approx n_a$ (acceptors)

in equilibrium $n_0 p_0 = n_i^2(T)$ always! / Law of mass action

recombination is given by the minority cc.

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

$\frac{\partial p}{\partial t} = - \frac{p - p_0}{\tau_p}$ if $p < p_0$
 $p < n_0$

if $p > p_0 \rightarrow$ annihilation

τ_n, τ_p : cc. lifetime $\tau_n, \tau_p \gg \tau$ up to 1ms

Continuity equation :

$\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{j} = \sigma$
 ↑ source of the liquid
 current

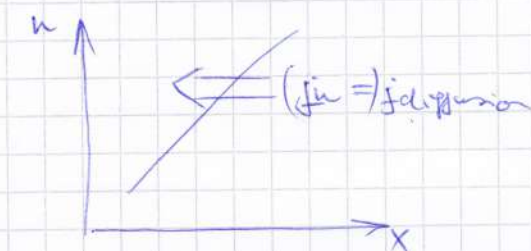
in SC : charge imbalances due to injection

For our case :

n-type $\left\{ \begin{aligned} \frac{\partial n}{\partial t} - \frac{1}{e} \nabla \cdot \mathbf{j}_n &= - \frac{p - p_0}{\tau_p} \\ \frac{\partial p}{\partial t} + \frac{1}{e} \nabla \cdot \mathbf{j}_p &= - \frac{p - p_0}{\tau_p} \end{aligned} \right.$

p-type $\left\{ \begin{aligned} \frac{\partial n}{\partial t} - \frac{1}{e} \nabla \cdot \mathbf{j}_n &= - \frac{n - n_0}{\tau_n} \\ \frac{\partial p}{\partial t} + \frac{1}{e} \nabla \cdot \mathbf{j}_p &= - \frac{n - n_0}{\tau_n} \end{aligned} \right.$

Case of spatial inhomogeneity (stationary)



number of e's witnessed $\rightarrow$ diffusion

diffusion current (particle current)

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

D : diffusion constant

$D \approx v^2 \tau$

in the mean-free path approximation
 τ : momentum scattering time
 v usually v_F (Fermi velocity)

In the presence of an external field $\Rightarrow$ drift current

$$j = n e v_{\text{drift}} = n e \mu E = - n e \mu \nabla V \quad E = -\nabla V$$

Stationary case: $j_{\text{diff}} + j_{\text{drift}} = 0$

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

$$(*) \quad + e D \nabla n - n e \mu \nabla V = 0$$

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

$$\text{few meV's} \quad \text{if } k_B T \ll E - eV - \mu \quad \approx e^{-\frac{(E - eV - \mu)}{k_B T}}$$

with this: $\nabla n = \nabla f = n \frac{e}{k_B T} \cdot \nabla V$ (important)

if $V = V(x)$

Write it back to (*):

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

Einstein-Relation:

$$\mu = \frac{e}{k_B T} D \quad (\text{mobility})$$

special case of fluctuation dissipation theory

Charge inhomogeneity + Stationary condition

example: charge injection

n-type $\&$ inject holes in conduction in 1D

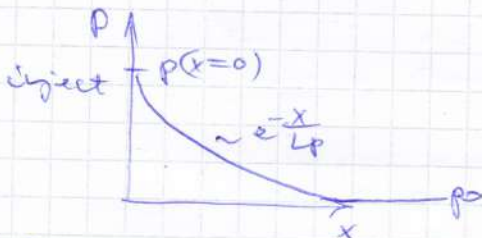
$$\begin{cases} \frac{1}{e} \nabla p = - \frac{p - p_0}{\tau_p} & \text{eq. of continuity} \\ j_p = - e D \nabla p & \frac{\partial p}{\partial x} \text{ in 1D} \end{cases}$$

$$\frac{\partial p}{\partial x^2} = \frac{p - p_0}{\tau_p} \cdot \frac{1}{D} \quad \text{diff. eq.}$$

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

$$\frac{\partial^2 p}{\partial x^2} = a \rightarrow e^{-\frac{x \cdot \sqrt{a}}{L_p}}$$

where $L_p = \sqrt{D \tau_p}$: charge diffusion length. Since $D = \frac{k_B T}{e} \mu$:
(length just with diffusion) $L_p = \sqrt{\tau_p \frac{k_B T}{e} \mu} \rightarrow$ can be up to 1 cm



Semiconductor devices (basics)

$$E_c \text{ --- } E_v \quad E_c \text{ --- } E_v \quad \mu$$

$$E_c \text{ --- } E_v \quad E_c \text{ --- } E_v \quad \mu$$

p-type

n-type

p-n junction



diffusion



When does the diffusion stop?

(V stops it)

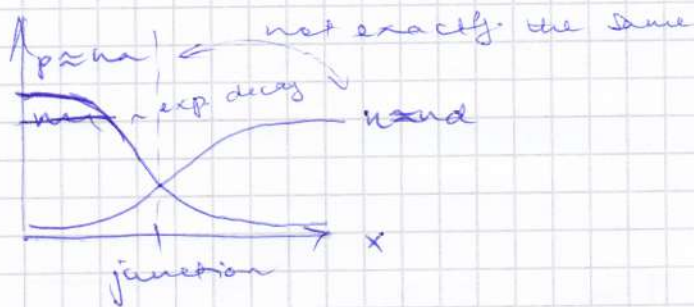
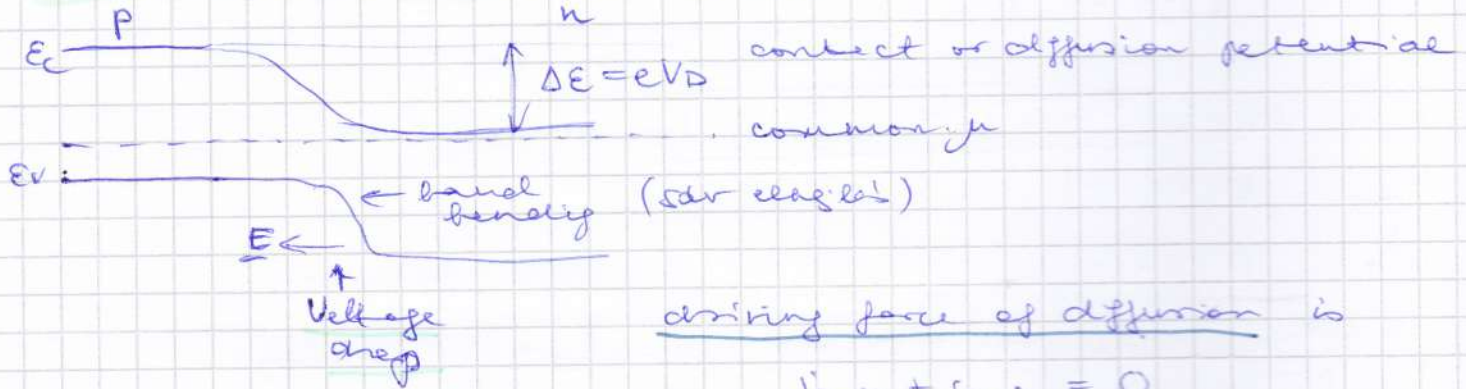
depletion region, no free c.s.
also called: diffusion or contact region



built in electric field



band structure after contact

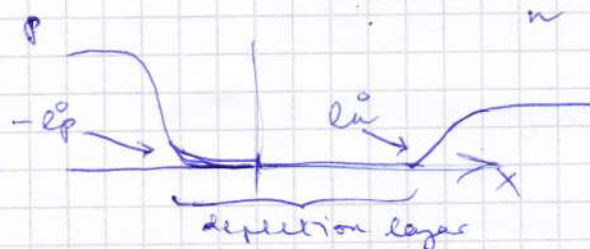


$$j_{\text{diff}} + j_{\text{drift}} = 0$$

$$nq\mu E + eD \frac{dn}{dx} = 0$$

built-in e-field

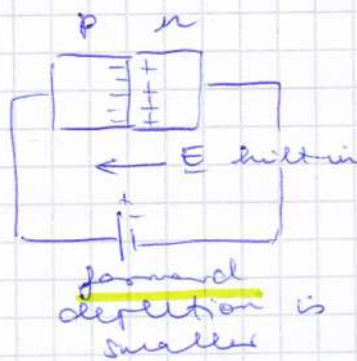
Schottky - approximation



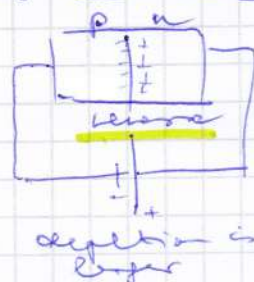
charge neutrality: $p \cdot l_p^0 = n \cdot l_n^0$
 $\Rightarrow = 0 (?)$
 $n \cdot l_p^0 = n \cdot l_n^0$

heavily doped $\rightarrow$ small depl. layer
 lightly doped $\rightarrow$ wide depl. layer

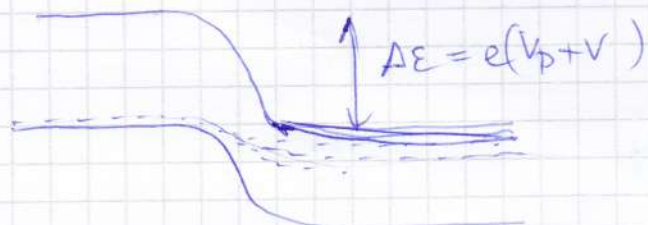
p-n junction + bias



if $E_{\text{ext}} \parallel E_{\text{built-in}} \Rightarrow$ reversed
 if $E_{\text{ext}} \perp E_{\text{built-in}} (?) \Rightarrow$ forward



(pn open, up closed)

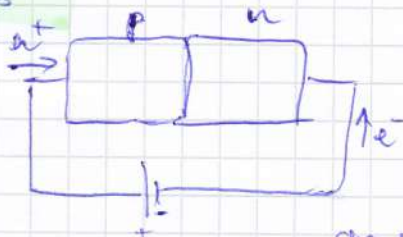


Schottky - formula:

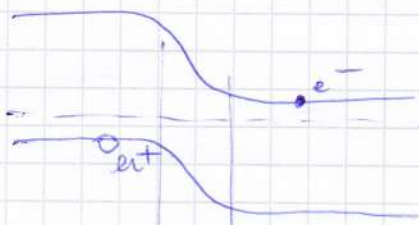
$$I(V) = I_c \left(e^{\frac{eV}{k_B T}} - 1 \right)$$

↑ reverse current

Diode characteristics



charge $\rightarrow$ happy when majority
sad when minority
 $\rightarrow$ recombination

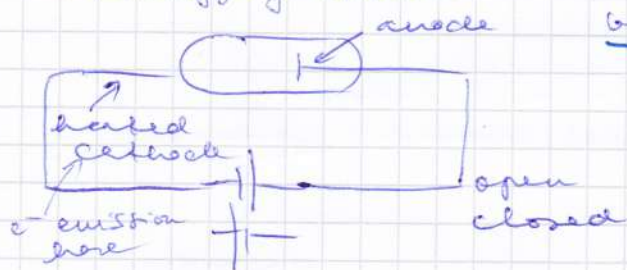


LED: light is emitted

depl. layer $\rightarrow$ charge annihilation is happening

all vacuum tubes

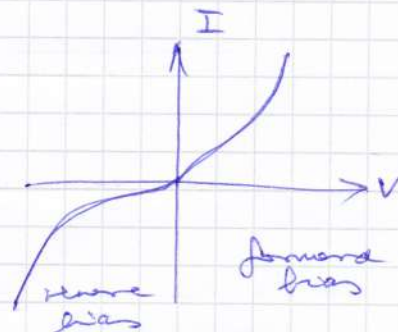
$\rightarrow$ rectifying device



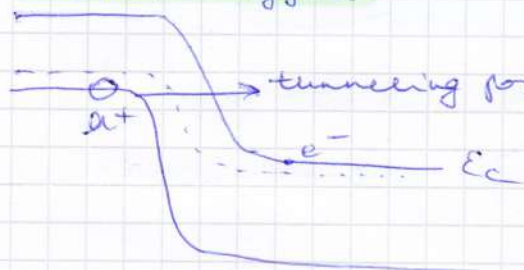
begin of name: diode

avalanche breakdown:

- reverse bias
- minority ccs are accelerated
 $\downarrow$
excite additional minority ccs
- don't like it: destroys the device
- occurs in heavily doped SCs.



Zener - effect



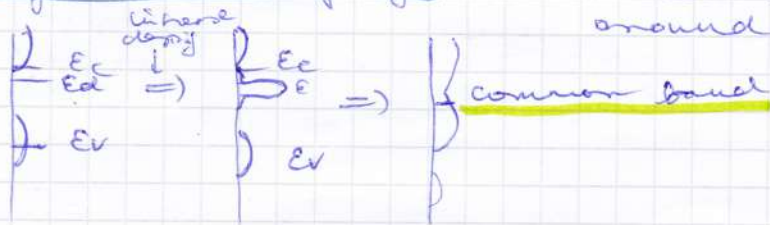
(cannot go the other way)

- thin depletion layer
heavily doped
- reversible: doesn't destroy the device
- similar physics as tunnel-diode

Tunnel diode (Esaki)

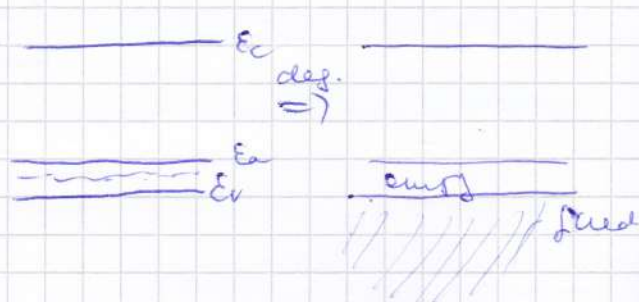
degenerate doping:

it occurs around 1% doping



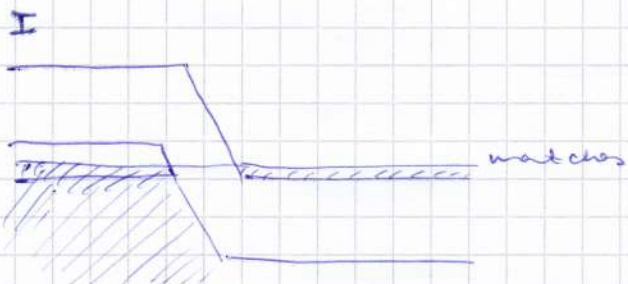


n-type

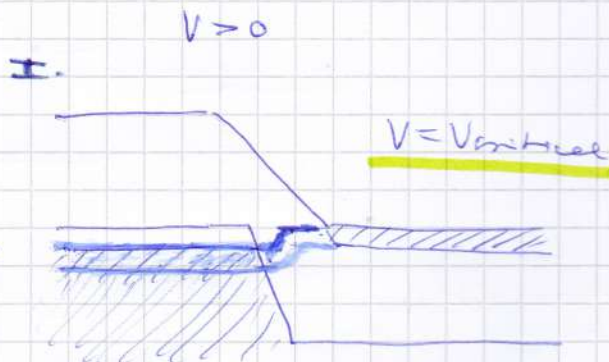


p-type

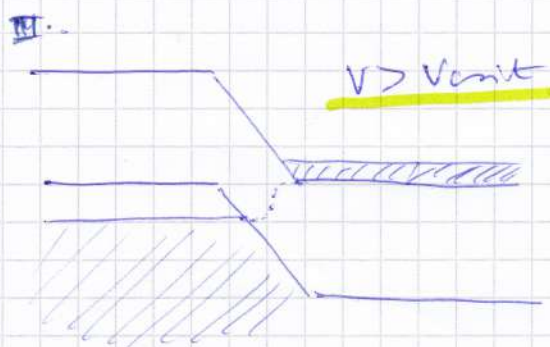
Esaki diode: heavily doped p-n junction



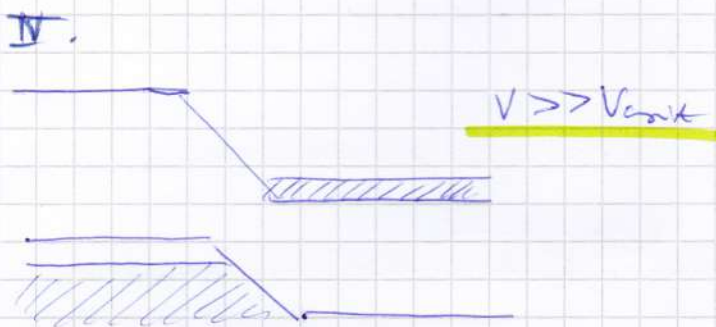
V=0
(0 bias)
tunnel current



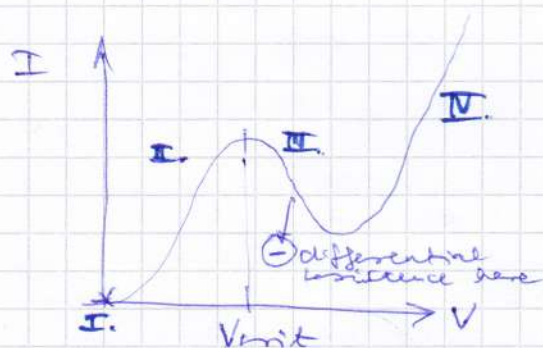
(forward bias)
tunnel current increases



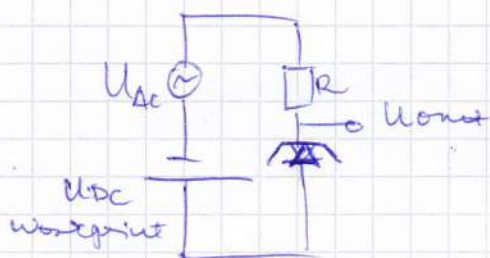
tunnel current drop
V > Vcrit



again current ~~flows~~ just
like in a normal diode



circuit notation:



$$U_{out} = U_{AC} \cdot \frac{-r}{R-r} = U_{AC} \frac{r}{r-R} > U_{AC} \text{ if } \boxed{R < r}$$

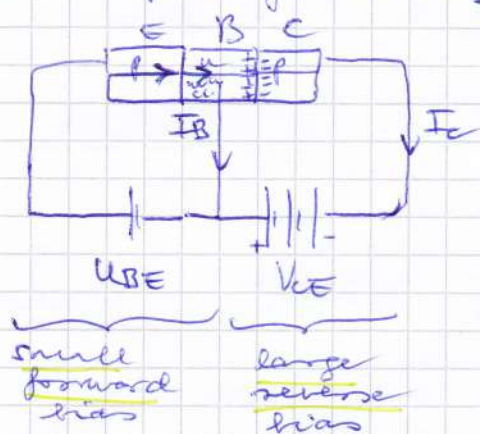
$$-r = \left(\frac{\partial I}{\partial V} \right)^{-1} \Big|_{\text{Esaki at } U_{out}}$$

analogue
amplifier

SC devices

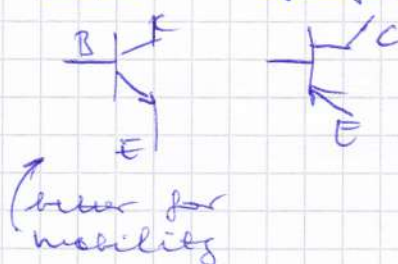
dec 15th
9⁰⁰ - 12⁰⁰
unofficial
exam date
(email)

BJT: bipolar junction transistor



Emitter, Base, Collector
E B C

n-p-n or p-n-p type



BJT $\neq$ up + pn diode

base is thin: $l_B \ll L_{diff}$

smaller than the diffusion length



large E field: sweep the e^- to the collector
minority

BJT: minority carrier device

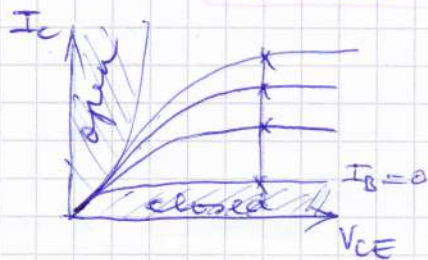
I_C depends on the injected charges (V_{BE}) and is proportional to I_B (not explaining it)

$\rightarrow I_B$ controls I_C ; construction is such that

$$\frac{I_C}{I_B} = \beta = 10 \dots 100$$

current amplification factor

$I_C = I_E - I_B$ - recombination



Working ways:

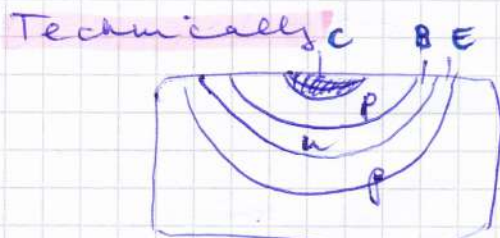
(1) digital device

(ETL, TTL) $\rightarrow$ disappeared (old computers)
ON-OFF: open-closed

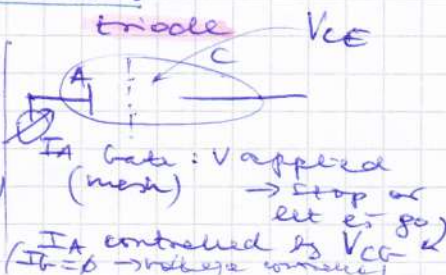
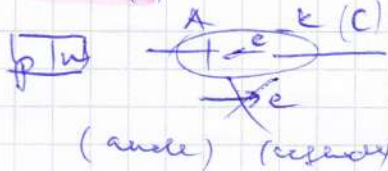
control it with I_B

(2) analogue amplification

$I_C = \beta I_B$ (this is still used)

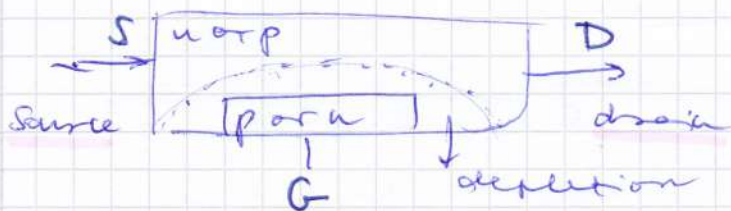


Analogy: vacuum tubes
diode



(anode) (cathode)
Gate: V applied $\rightarrow$ stop or let e^- go
 I_A controlled by V_{CG}
 $I_B = \beta \rightarrow$ voltage controlled

JFET: junction field effect transistor



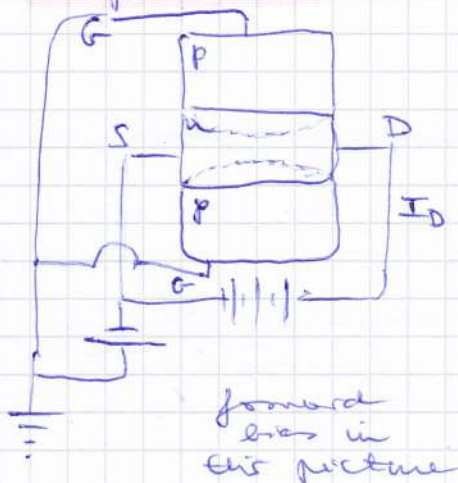
gate source is forward
→ large I_{SD}

gate-source reversed
→ small I_D
(large depletion)

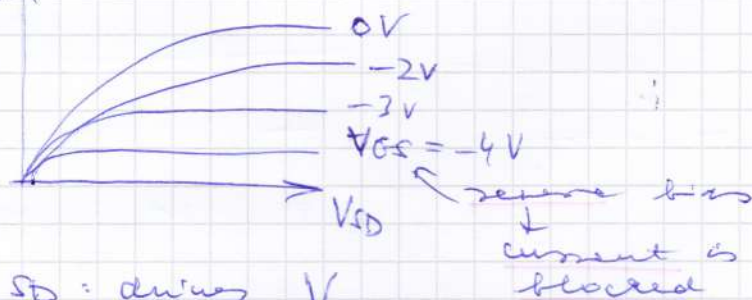
Majority GC. device

↓ in high speed device

in practice:



I_D



V_{DS} : drives V
 V_{GS} : controls

reverse bias
↓
current is blocked

JFET

vs.

BJT

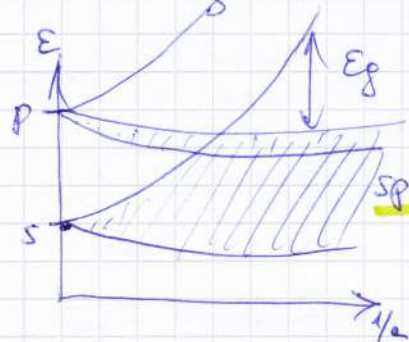
large control
impedance
↓ (1-10 M Ω) ($I_G=0$)

better for digital
and low freq. analogue
amplification

finite control
impedance
(I_B finite)

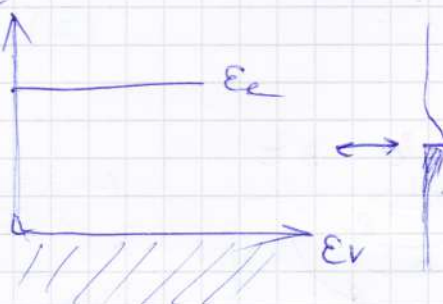
better for high
freq. amplification

Schottky barrier and surface states



bulk
material

⇒ sp^3 hybrid
states are in the middle of the
gap (dangling bonds).

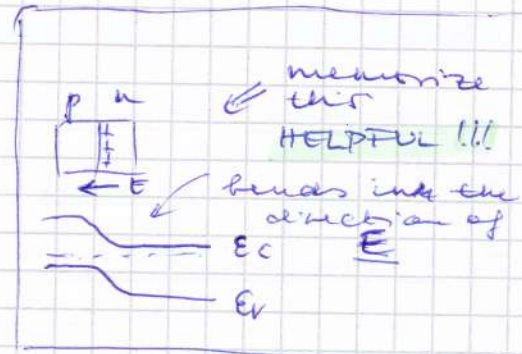
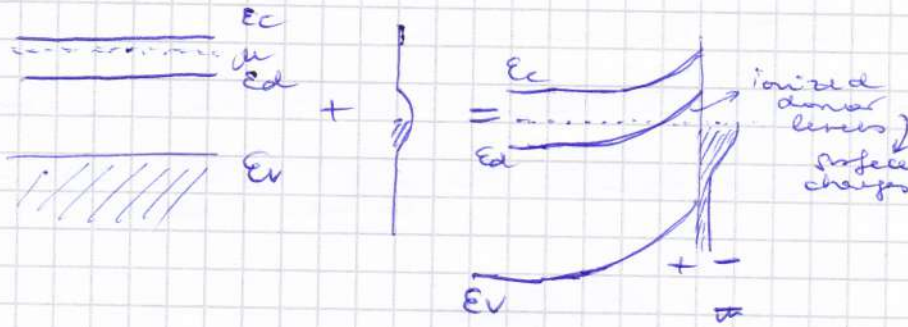


bulk

surface

Shetty requires surface
states, understanding it

Surface of an n-type Sc



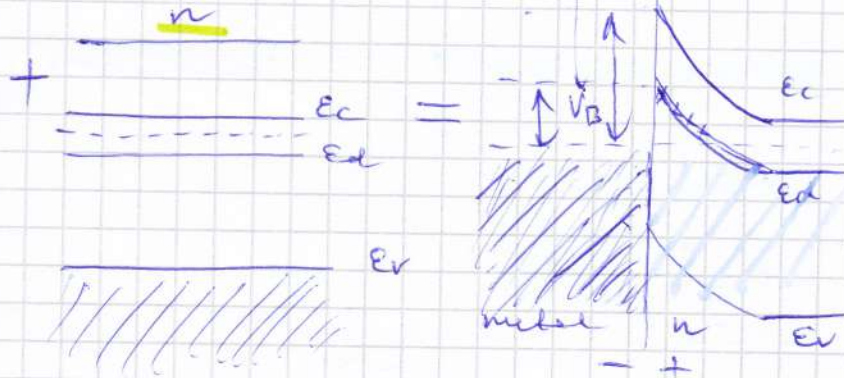
Schottky barrier: metal + Sc



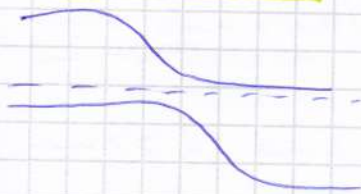
1 type of cc. only

M:

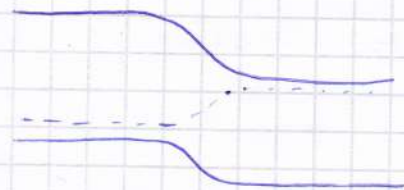
$E=0$ vacuum



reminders:

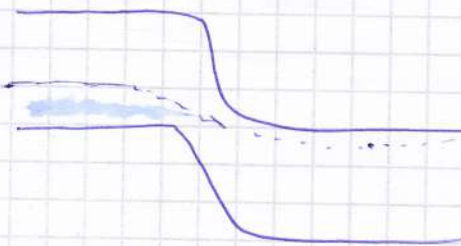


$V \neq 0$



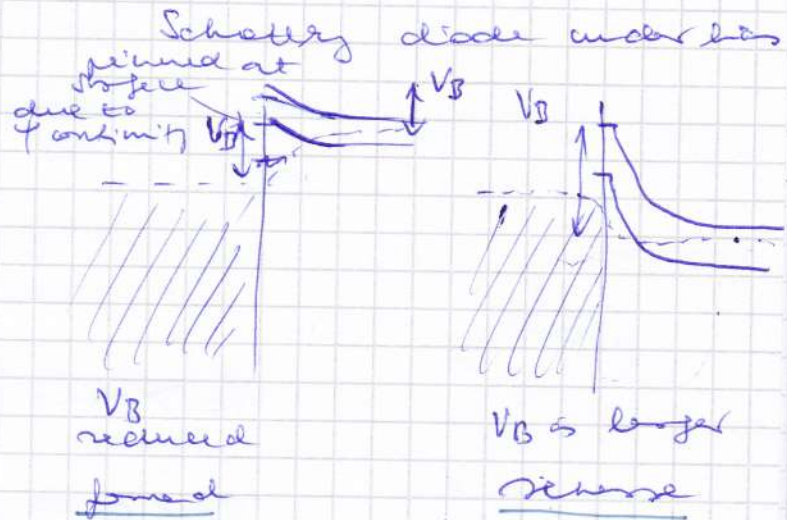
$V > 0$

forward bias
(up)

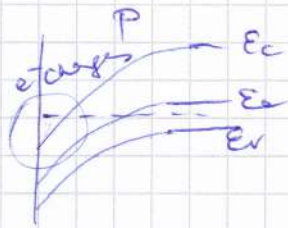
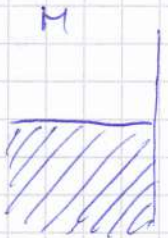


$V < 0$

Reverse bias
(down)

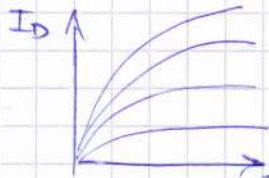


if $V_{GS} > 0$



like the inversion layer
(e⁻s in a p-type)

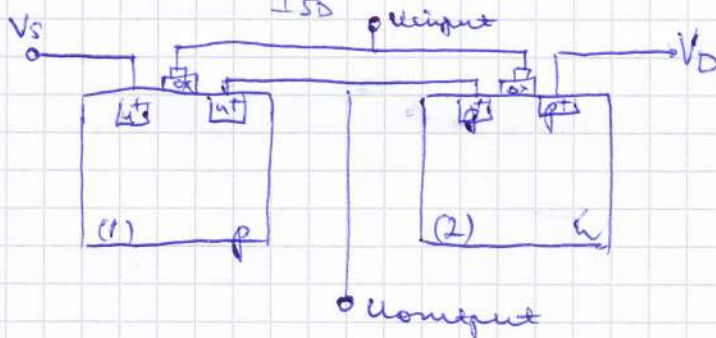
CMOS: Complementary metal-oxide-semiconductor



logical 1: large I_D
logical 0: small I_D

(usually 0 is large)

every transistor has 1 nA



if Uinput > 0

(1) open (2) closed (n-channel) → Uoutput = Vs

if Uinput < 0

(1) closed (2) open (p-channel) → Uoutput = Vd

always $I_{SD} = 0$ except for switching

→ this gives consumption

if Vs = low Uinput

if Vd = high Uinput

} logical NOT gate
you can build up anything from
NOT and OR, XOR, AND
→ to be double operation
(make these in pairs in tech.)

Bring lecture notes!

→ better mark if nice :)