Varghа Noémi

2018.
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Physics of Semiconductors

Simon Ferenc

password for online materials : felvezetok

Semiconductor :

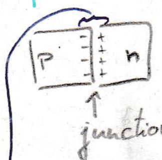
*A material whose conductivity depends strongly on the

~ temperature
~ doping (adalékolás)
~ external bias (drain, gating) (kapuzás) (nyelő elektróda)

impurities
no dependance ($j = \sigma E$)
} metals

~ a nearby semiconductor
- diffusion
- charge transfer

ex. pn diode



junction (átmenet)

depletion layer (no free charge carriers)

~ light (sensor!)
~ magnetic field (magnetism)

ex. spintronics
magnetic sc. ($Ga_x Mn_{1-x} As$)
MRAM (magnetic random access memory)

Semiconducting materials

- IV group ($2s^2 2p^2$) : C, Si, Ge, Sn (tin)
- compounds of IV group : SiC (siliconcarbate) / szilícium - karbid
- III-V group : GaAs, GaN, AlP, InSb (indiumantimonite) (antimón), BN
- II-VI group : ZnS, ZnSe, ZnO, CuO, PbS_2, PbSe, FeS_2

low-dimensional SC

- 1D : carbon nanotubes
  nanowires (GaAs, InP)
- 2D : graphene, *transition metal dichalcogenides (MoS_2, $MoSe_2$, WS_2) (thungstan)
- molecular, organic sc : C_{60}

1*

Early history of SC

- 1833 Faraday : AgS – resistivity drops at high T
- 1839 Becquerel : photovoltaic effect (solar cell) — light → charge
- 1873 Smith : photoconductivity → σ → I — σ changed by light; light
- 1874 Braun : rectification (egyenirányítás) in metal-sulfides → □ → $I > 0$; ← □ ← $I = 0$

  Schuster : CuO
- 1878 Hall-effect
- 1900 Baedeker : CuI, Hall-effect with opposite sign

  Hall-constant $R_H = \frac{1}{n \cdot e}$ ← elementary charge > 0

  $n < 0$ for electrons
  $n > 0$ for holes
- 1910 Weiss : Halbleiter (semi conductor)
- 1926 – 1938 quantum theory of semiconductors

  Bloch, Schottky, Mott
- 1940 Bardeen : non-reproducing results come from contaminants below 1ppm (10^{-6} purity)

  today : 10^{-12}

Devices

- 1880 Bell : voice transmission with Se (piezoelectric property)
- 1883 Fritts : first solar cell — Au electrode (so thin that transparent); Se; metal
- 1904 J.C. Bose : sensitive radio detector — metal needle (spring); PbS_2 (galena) } sc – metal contact

  tune it by pushing the spring
- 1906 Round : first LED → p n → I
- 1920 CuO + Se rectifier
- 1922 Losev : ZnO amplifier
- 1926 Lilienfeld : FET (field effect transistor)
- 1941 Ohl : 1st Si pn junction
- 1947 Bardeen, Brattain, Schockley : 1st transistor

Nobel prizes

- 1956 transistor
- 1973 Esaki, Graver : tunnel diode
- 1985 von Klitzing : QHE (quantum Hall-effect)
- 2000 Alferov, Krolmer
  ↳ SC laser
  hibly -> IC
- 2007 Fert, Grünberg : GMR (giant magneto resistance)
- 2009 Boyl, Smith : CCD (charge coupled device)
- 2010 Geim, Novesolov : graphene
- 2014 Akasaki, Amano, Nakamura : blue LED (GaN)

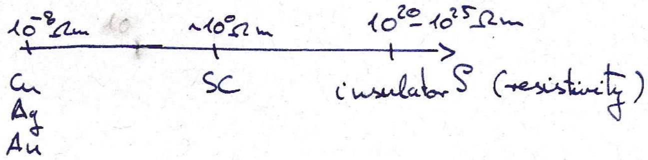
Position of SC physics

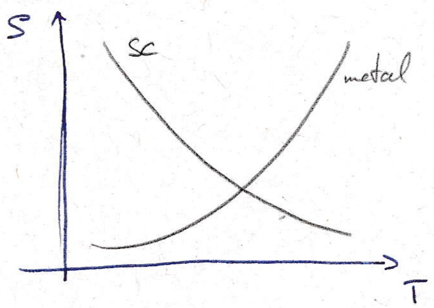
- we need : quantum mechanics
  solid state physics
  statistical physics
  material sciences
  (optics)
- SC physics leads to : electronics
  spintronics
  laser optics
  laser physics
- researches : fundamental (new materials, new low-D materials, excitons)
  demonstration of fundamental physics
  (B-E condensate, QHE, FQHE)
  applied research (new devices HEMT)
  (high e⁻ mobility transistor)

-> smaller size, lower energy consumption

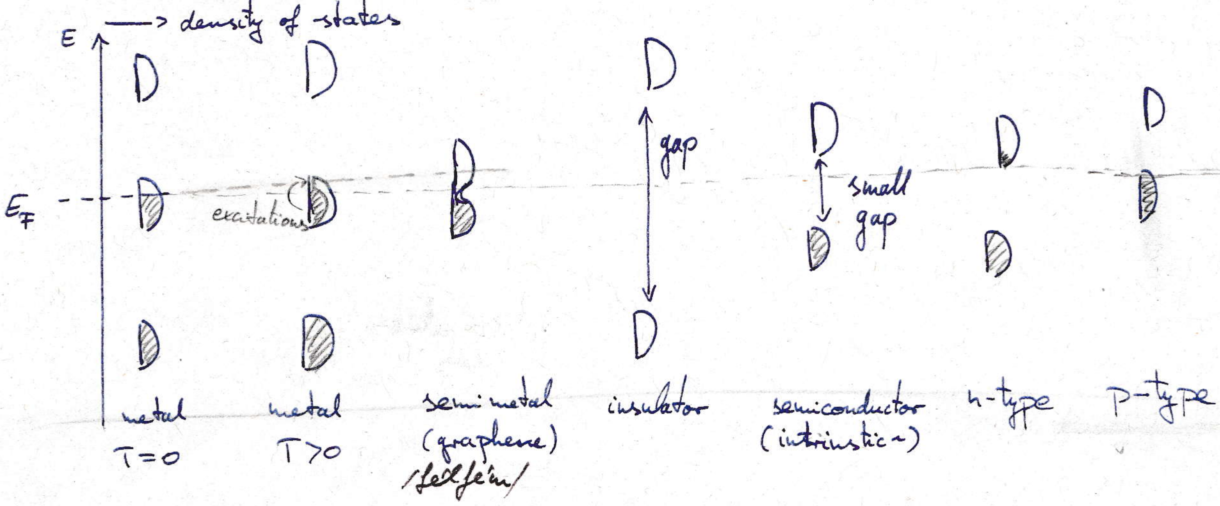
*/

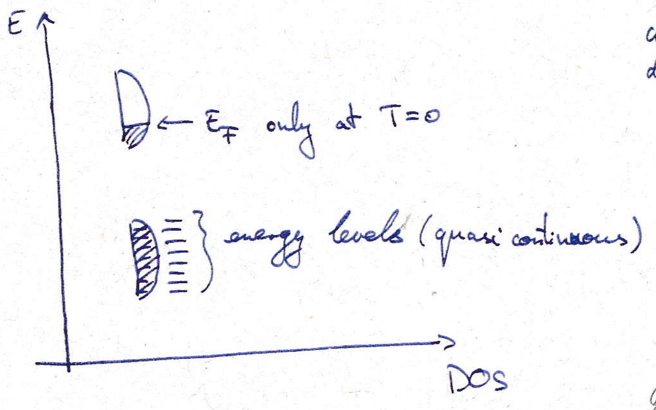
Physical properties of SC

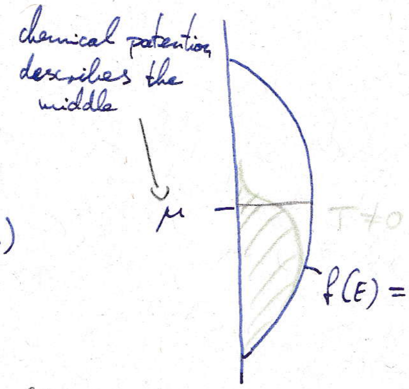




Band structure







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

Kémiai pot.: az az energia szint, ahol $\frac{1}{2}$ a betöltöttség

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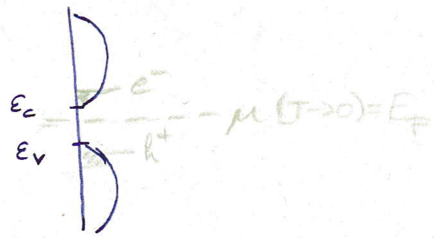
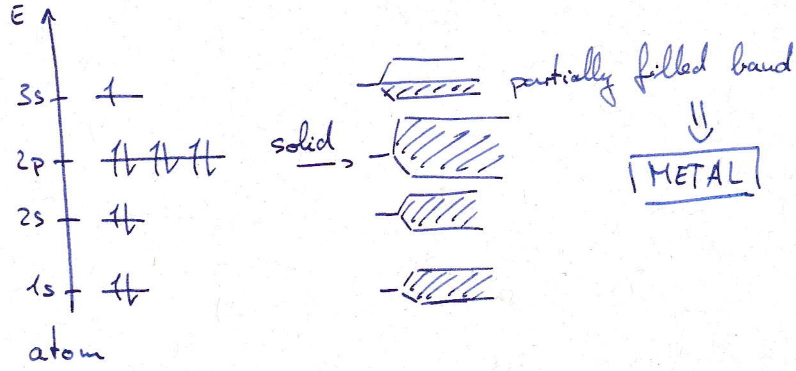
intrinsic SC

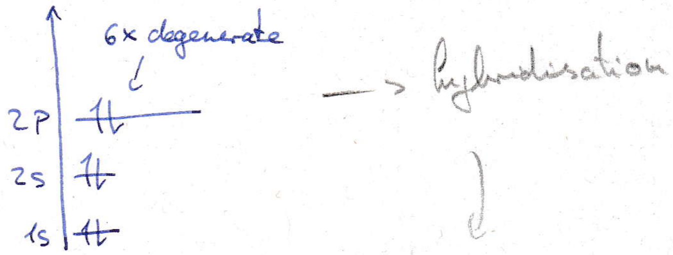


Band structure of SC (in bulk materials)

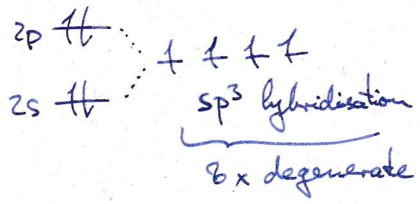
- $Na: 1s^2 2s^2 2p^6 3s^1$

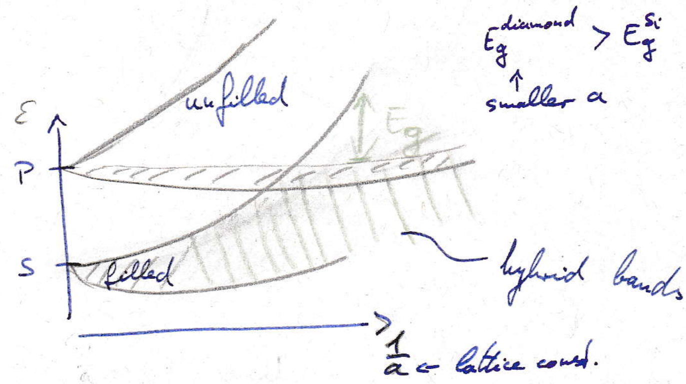


- IV elements, eg. C: $1s^2 2s^2 2p^2$



remark: hybridisation



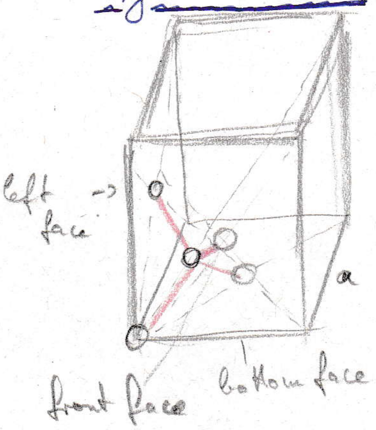


⇓

Crystal structure : diamond lattice
ZnS (zinc-blende lattice) eg. GaAs

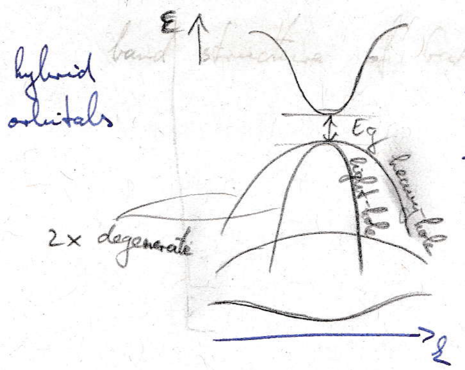
fcc Bravais lattice + 2 atom basis: $(0,0,0)$; $\frac{1}{4}(a,a,a)$

→ tetrahedron
sp^3 orbitals repel each other

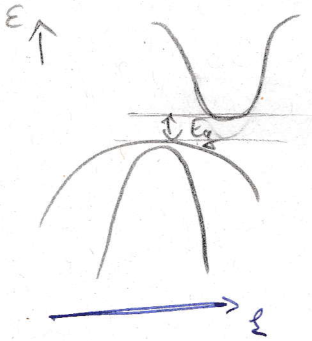


ZnS eg. GaAs   Ga (0,0,0)
As (1,1,1) $\frac{a}{4}$

Band structure



GaAs



Si

↑ empty
↓ filled

- direct gap

indirect gap -> there is momentum change

⚠ energy & momentum conservation have to be satisfied

optical transition
$E = pc$ p is small for light

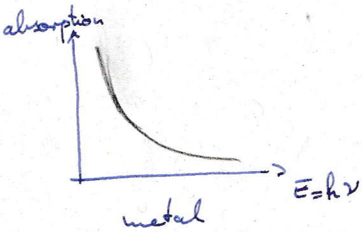
- good for LED or laser

∅ light emission

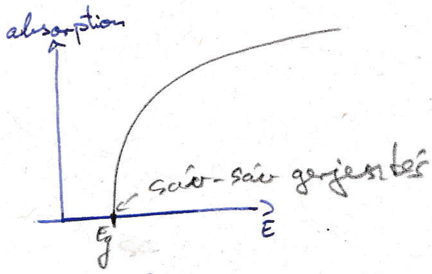
- GaAs: 8 valence e^-/unit cell
  4 bands, 2x degeneration (spin)
- curviture of the bands are in relation with the effective mass

	C	Si	Ge	GaAs	AlAs
E_g(eV)	5	1,1	0,7	1,5	2,2

Optical properties



metal



i-SC

Charge carriers in SC

room temperature ~25-25eV

Th.: density of (negative) charge carriers

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

Ge (300K) $n = 2 \cdot 10^{13} \frac{1}{cm^3}$

1 ppm n doping gives $n = 2 \cdot 10^{19} \frac{1}{cm^3}$ <- 6 orders of magnitude
($10^6 : 1$)

Drude-modell

- $ma = F = qE$

stationary case

$ma = 0 = F = qE - \underbrace{\mathcal{L} v}$
viscose interaction to slow down e^- (if not: accelerated until ∞)

$\hookrightarrow a = \frac{qE}{m} - \frac{\mathcal{L}}{m} v \qquad \left[\frac{\mathcal{L}}{m}\right] = \frac{1}{s}$

- $\frac{\mathcal{L}}{m} = \frac{1}{\tau}$ $\quad \tau$: relaxation time

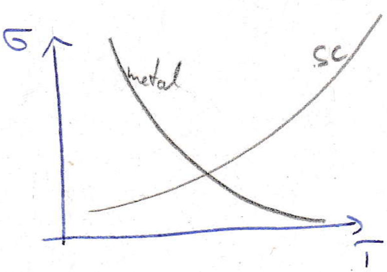
- $qE = \frac{vm}{\tau} \rightarrow \boxed{v_D = \frac{qE\tau}{m}}$ drift-velocity $\rightarrow$ in a metal $\boxed{v_D = \frac{qE\tau}{m^*}}$ $\leftarrow$ effective band mass

- $v_D = \mu E \qquad v_D \ll 1\frac{m}{s}$
  mobility $\qquad [\mu] = \frac{cm^2}{sV} \qquad 1-10^6$

- current density
  $j = nqv \qquad [j] = \frac{A}{m^2} \qquad \left([nqv] = \frac{1}{m^3} A s \frac{m}{s} = \frac{A}{m^2} ✓\right)$

  $\boxed{j = nev_D = \frac{ne^2\tau}{m^*} E}$ differential Ohm's law $\hookrightarrow \boxed{j = \sigma E}$ $\Big\}\ \sigma = \frac{ne^2\tau}{m^*}$ conductivity

  $\boxed{\mu = \frac{e\tau}{m^*}}$



metal: τ shortening $\equiv$ lowering mobility
SC: T dependance on n that is more important than τ shortening

Solid state physics revisit

- 1D e^--gas $\quad \Psi(\xi, x) = \frac{1}{\sqrt{L}} e^{i\xi x}$ $\quad$ plane-waves

- $p = \hbar \xi$
  $\uparrow$ canonical momentum, ξ: crystal momentum

- $\varepsilon(\xi) = \frac{\hbar^2 \xi^2}{2m}$ (from time dependant Schrö.)

- ξ is given by periodic boundary conditions

- Ψ should be single valued $\Rightarrow e^{i\xi L} = 1$

  $\xi L = 2\pi \cdot n \qquad n \in \mathbb{Z}$ (integer)

  $\xi = \frac{2\pi n}{L}$ and $L = Na$ (N: atoms, a: lattice const.)

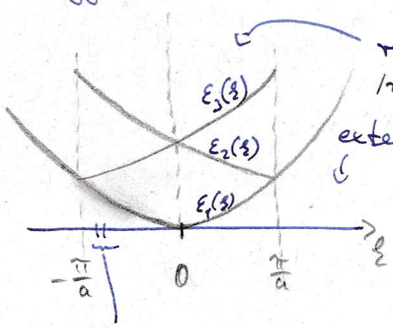
  $\hookrightarrow \xi = \frac{2\pi}{a} \frac{n}{N} \rightarrow N$ different ξ values $\qquad \boxed{\xi_{min} = -\frac{\pi}{a},\ \xi_{max} = \frac{\pi}{a}}$

  $n = 0, \dots, N-1$ or $n = -\frac{N}{2}, \dots, \frac{N-1}{2}$

Energy levels $\quad \varepsilon(k) = \frac{\hbar^2 k^2}{2m}$

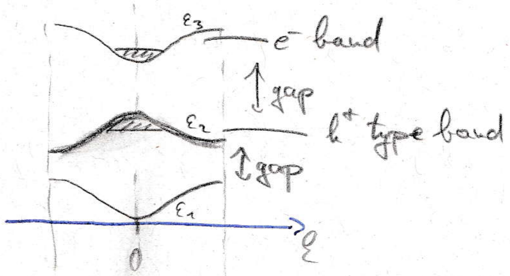
reduced-zone scheme $\left[-\frac{\pi}{a}, \frac{\pi}{a}\right]$
/redukált zóna kép/

extended zone picture



$\left(k = \frac{2\pi}{L} n \Rightarrow\right)$ $\Delta k = \frac{2\pi}{L}$ discretisation of the k place

in presence of a periodic potential



- $v = \frac{1}{\hbar} \frac{\partial \varepsilon(k)}{\partial k} = \frac{p}{m^*}$ and $(m^*)^{-1} = \frac{1}{\hbar^2} \frac{\partial^2 \varepsilon}{\partial k^2}$
- $F = \hbar \dot{k}$
  external forces
- typical values $m_c^* = 0.1 \ldots 0.5\, m_e$
  $m_v^* = -1 \ldots -3\, m_e$

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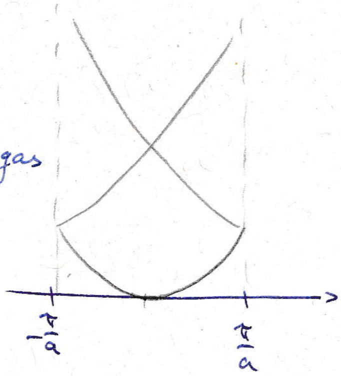
1D

free e^- gas



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

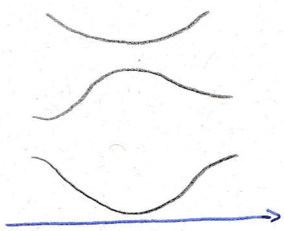
$k = \frac{2\pi}{L} n = \frac{2\pi}{Na} n \qquad n = -\frac{N}{2}, \ldots, \frac{N}{2}$

$v = \frac{1}{\hbar} \frac{\partial \varepsilon}{\partial k} = \frac{p}{m^*}$

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

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

periodic pot.



Density of states $D(k) = \frac{V_d}{(2\pi)^d} \times \underset{\text{spin}}{2}$

1D $\Delta k = \frac{2\pi}{L}$; $D(k) = \frac{L}{2\pi}$; $\int_{-\pi/a}^{\pi/a} \frac{L}{2\pi} dk = N$

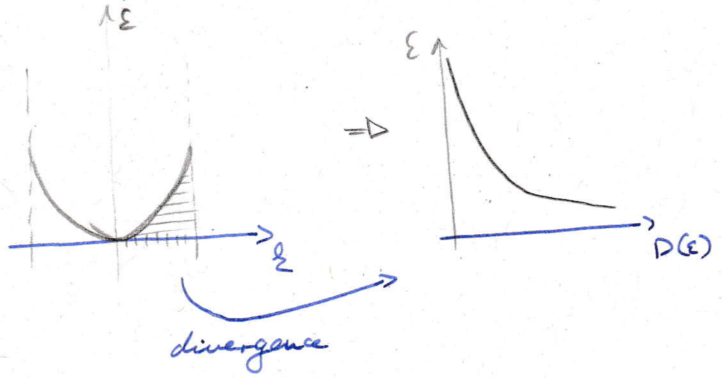
$D(k)$: density of states in k ; N: nb of atoms

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

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

+ spin degeneracy $\Rightarrow$ $D(k) = \frac{A}{2\pi^2}$; $D(k) = \frac{2V}{(2\pi)^3} = \frac{V}{4\pi^3}$

instead of $D(k) \longrightarrow$ we use $D(\varepsilon)$



1D $D(k)\,dk = D(\varepsilon)\,d\varepsilon$ $\qquad \varepsilon = \frac{\hbar^2 k^2}{2m^*} \rightarrow k = \frac{\sqrt{2m^*\varepsilon}}{\hbar}$

$$\frac{L}{2\pi}\,dk = D(\varepsilon)\,d\varepsilon$$

$$\frac{dk}{d\varepsilon} = \left(\frac{d\varepsilon}{dk}\right)^{-1} = \left(\frac{\hbar^2 k}{m^*}\right)^{-1} = \left(\frac{\hbar^2 \sqrt{2m^*\varepsilon}}{\hbar \quad m^*}\right)^{-1} = \frac{\sqrt{m^*}}{\sqrt{2}\,\hbar\,\sqrt{\varepsilon}}$$

$$D(\varepsilon) = \frac{L}{2\pi}\,\frac{\sqrt{m^*}}{\sqrt{2}\,\hbar\sqrt{\varepsilon}} \Rightarrow \boxed{D(\varepsilon) \sim \frac{1}{\sqrt{\varepsilon}}}$$

2D $\boxed{D(\varepsilon) = \text{const}}$

$$\underbrace{D(k)}_{\frac{A}{(2\pi)^2}}\,\underbrace{k\,dk}_{\text{volume}} = D(\varepsilon)\,d\varepsilon \quad \ldots$$

$$\underset{\text{spin}}{2} \cdot \frac{A}{(2\pi)^2} \cdot \overbrace{\frac{\sqrt{2m^*\varepsilon}}{\hbar}}^{k(\varepsilon)} \cdot \overbrace{\frac{\sqrt{m^*}}{\sqrt{2}\,\hbar\,\sqrt{\varepsilon}}}^{\left(\frac{d\varepsilon}{dk}\right)^{-1}} = D(\varepsilon)$$

$$\Rightarrow \boxed{D(\varepsilon) = \frac{A\,m^*}{2\pi^2\hbar^2} = \text{const.}}$$

3D

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

polar coordinates:

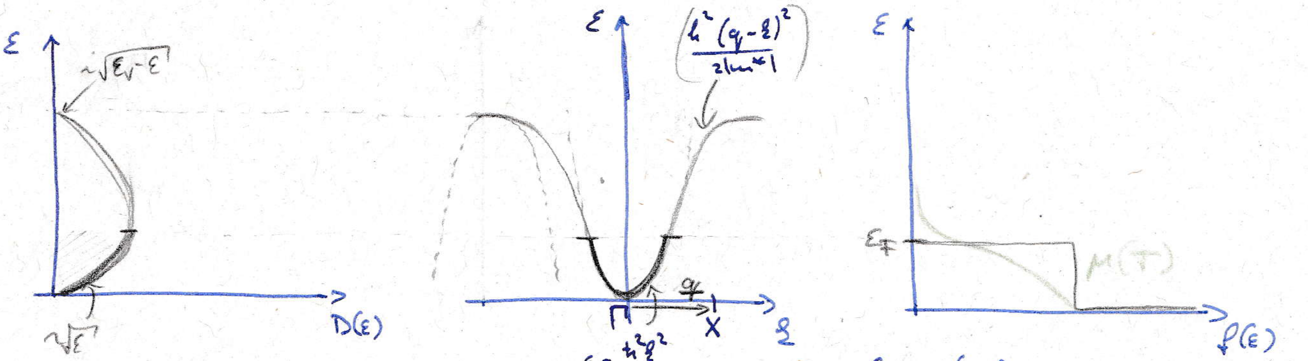
$$\int dV = \int r^2 dr \int_0^{\pi} \sin\vartheta \, d\vartheta \int_0^{2\pi} d\varphi$$

$$D(q)\, 4\pi q^2 \left(\frac{d\varepsilon}{dq}\right)^{-1} = D(\varepsilon)\,, \quad \left(\frac{d\varepsilon}{dq}\right)^{-1} = \left(\frac{\hbar}{m^*}\sqrt{2m^*\varepsilon}\right)^{-1}$$

$$\boxed{D(\varepsilon) = \frac{V}{4\pi^3}\, 4\pi\, \overbrace{\frac{2m^*\varepsilon}{\hbar^2}}^{q^2}\, \overbrace{\frac{m^*}{\hbar}\, \frac{1}{\sqrt{2m^*\varepsilon}}}^{\left(\frac{d\varepsilon}{dq}\right)^{-1}} \sim \sqrt{\varepsilon}} \Rightarrow \text{no singularity in } D(\varepsilon)$$

$$\boxed{D(\varepsilon) = \frac{V}{2\pi^2}\sqrt{\varepsilon}\left(\frac{2m^*}{\hbar^2}\right)^{3/2}}$$

Occupation of bands (3D)



DOS

$\varepsilon = \frac{\hbar^2 q^2}{2m^*}$

dispersion relation

$\varepsilon_F = \mu(T=0)$

F-D statistics

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

Number of charge carriers

$$n = \int_0^{\infty} D(\varepsilon)\, f(\varepsilon)\, d\varepsilon$$

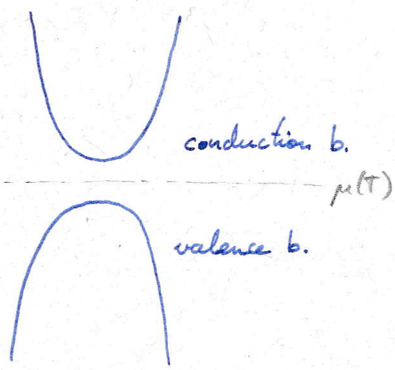
density of nb

describes the system

temperature, quantum statistics, occupation of states

μ(T) ← shows until where bands are charges

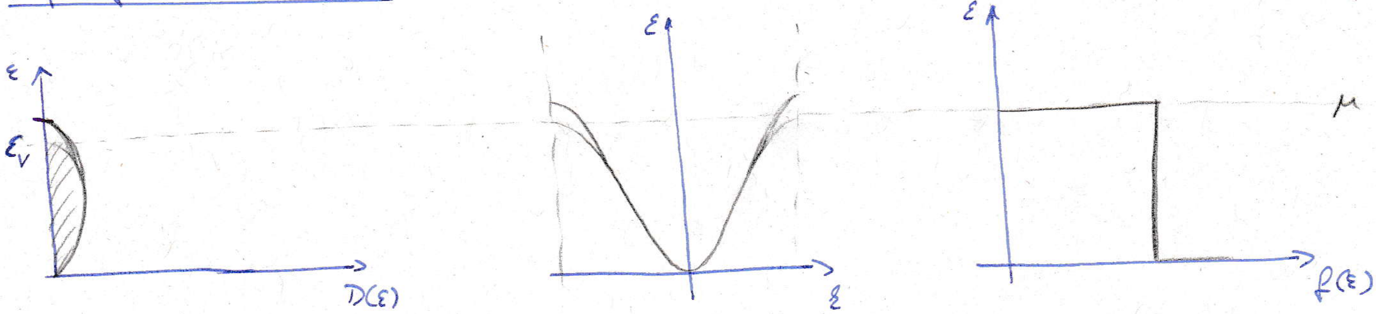
States & charges in SC



if $T \to 0 \Rightarrow \mu(T\to 0)$ makes sense

ε_F is ill-defined (should be at the top of VB but we like to "put" it to μ)

Top of valence band



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

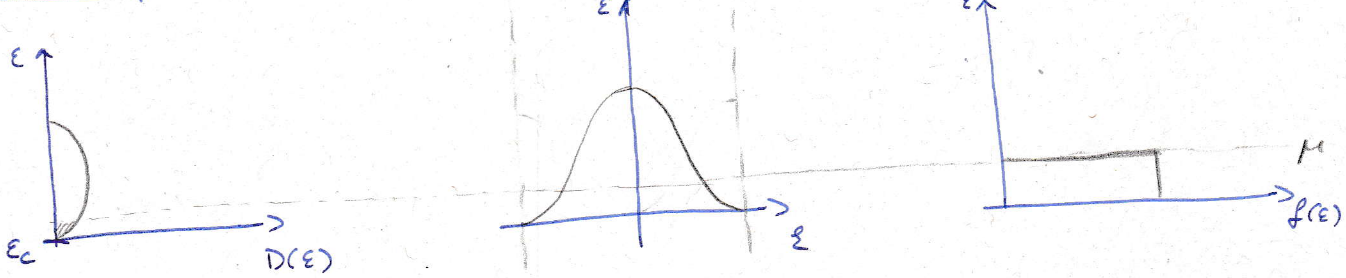
↳ we measure ε from back to ε_V

$$\varepsilon(k) = \varepsilon_V - \frac{\hbar^2(G-k)^2}{2m_V^*}$$

↳ shows that $m_V^* < 0$
VB contains h^+

$\underline{G}$: vector of reciprocal space
$|\underline{G}| = \frac{2\pi}{a}$ in 1D

Bottom of conduction band

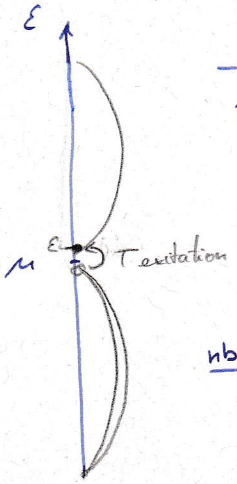


$$D_c(\varepsilon) = \frac{V}{2\pi^2}\left(\frac{2m_c^*}{\hbar^2}\right)^{3/2}\underbrace{\sqrt{\varepsilon-\varepsilon_c}}_{\frac{\partial^2\varepsilon}{\partial k^2} > 0}$$

$$\varepsilon(k) = \frac{\hbar^2 k^2}{2m_c^*}$$

? ↑

$$\varepsilon_c + \frac{\hbar^2(G+k)^2}{2m_c^*}$$



$$\frac{1}{1+e^{\frac{\varepsilon-\mu}{k_BT}}} \approx e^{-\frac{\varepsilon-\mu}{k_BT}}$$

↑ . $\varepsilon-\mu \approx \frac{1}{2}\varepsilon_g$

. $\varepsilon_g >> k_BT$
↑ 1 eV, ↑ 26 meV

__nb of e^-__ in the conduction band

$$n = \int_{\varepsilon_c}^{\infty} D_c(\varepsilon) f(\varepsilon)\, d\varepsilon$$

__nb of h^+__ in the valance band

$$p = \int_0^{\varepsilon_V} D_V(\varepsilon)(1-f(\varepsilon))\, d\varepsilon$$

e.g.

$$n \sim \overset{\text{const.}}{\checkmark} \int_{\mathcal{E}_c}^{\infty} \sqrt{\mathcal{E}_c - \mathcal{E}}\, e^{-\frac{\mathcal{E}-\mu}{k_B T}}\, d\mathcal{E} \underset{\uparrow}{=} \int_0^{\infty} \sqrt{x}\, e^{-x} \frac{1}{\sqrt{\beta}} \cdot \frac{1}{\beta} e^{-\beta(\mathcal{E}_c - \mu)}\, dx = *$$

change of variable: $(\mathcal{E} - \mathcal{E}_c)\beta = \frac{\mathcal{E}-\mathcal{E}_c}{k_B T} = x$

$$* = \frac{1}{(\beta)^{3/2}} e^{-\beta(\mathcal{E}_c - \mu)} \underbrace{\int_0^{\infty} \sqrt{x}\, e^{-x}\, dx}_{\frac{\sqrt{\pi}}{2} \quad \text{const.}}$$

$$\hookrightarrow \begin{cases} n = 2\left(\frac{m_c^* k_B T}{2\pi \hbar^2}\right)^{\frac{3}{2}} e^{\frac{-(\mathcal{E}_c-\mu)}{k_B T}} \cdot V \; ? \\ p = 2\left(\frac{m_V^* k_B T}{2\pi \hbar^2}\right)^{\frac{3}{2}} e^{+\frac{\mathcal{E}_V-\mu}{k_B T}} \cdot V \; ? \end{cases}$$

m_c^*, m_V^* are material dependent

μ is the only unknown variable

conservation of charges: $\underbrace{n = p}_{\mu \text{ can be obtained}}$

$$\Rightarrow \boxed{\mu = \frac{1}{2}(\mathcal{E}_c + \mathcal{E}_V) + \frac{3}{4} k_B T \ln\left(\frac{m_V^*}{m_c^*}\right) \simeq \frac{1}{2}(\mathcal{E}_c + \mathcal{E}_V)} = \mathcal{E}_V + \frac{1}{2}\mathcal{E}_g$$

$\boxed{n = p = \sqrt{np}}$ ← valid for | intrinsic
mass law action / law of mass action | extrinsic ($n_i^2 = np$) — for free charge carriers

tömeghatás törvénye

substitute μ into n, p → $n = p = 2\left(\frac{k_B T}{2\pi\hbar^2}\right)^{\frac{3}{2}} (m_c^* m_V^*)^{3/4} \underline{e^{-\frac{\mathcal{E}_g}{k_B T}}} \cdot V$

$\int D(\mathcal{E})\, d\mathcal{E}$ = pieces ⇒ $[D(\mathcal{E})] = \frac{1}{eV}$

$$D(\mathcal{E}) = \frac{V}{2\pi^2}\left(\frac{2m^*}{\hbar^2}\right)^{3/2} \sqrt{\mathcal{E}} \qquad [D(\mathcal{E})] = m^3 \left(\frac{\cancel{kg}}{\cancel{m^2 J s^2}}\right)^{3/2} \sqrt{J} = \frac{1}{J}$$

e.g. charge carrier concentration in Na

$n_{Na} \sim 10^{21} - 10^{22} \frac{1}{cm^3}$

$$\frac{n_{SC}}{V} \underset{\uparrow}{=} 2\left(\frac{k_B T}{2\pi\hbar^2}\right)^{\frac{3}{2}} (m_c^* m_V^*)^{3/2} e^{-\frac{\mathcal{E}_g}{k_B T}} = \frac{1}{10}\left(\frac{10^{-20}}{10^{-68}}\right)^{\frac{3}{2}} (10^{-31})^3 \underbrace{e^{-40}}_{\sim 10^{-20}} \ldots \approx 10^{10} \frac{1}{cm^3}$$

in SC at $T \to \infty$

intrinsic SCs have a low charge carrier concentration ~ 10^{12} x smaller than metals

Mobility versus charge carrier conc.

Drude-modell: $\sigma = \frac{ne^2\tau}{m^*}$ ← momentum scattering time $j = nev_D$ ← drift velocity $\mu = \frac{e\tau}{m^*}$ ← mobility

	e^-	h^+
v_D	$\frac{-eE\tau_e}{m_e^*}$	$\frac{eE\tau_h}{m_h^*}$
σ	$\frac{ne^2\tau_e}{m_e^*}$	$\frac{ne^2\tau_h}{m_h^*}$
$\mu = \frac{\lvert v_D\rvert}{E}$	$\frac{e\tau_e}{m_e^*}$	$\frac{e\tau_h}{m_h^*}$

e^- & h^+ conductivity contribution add together

for both types of charge carriers:

$\boxed{\sigma = ne\mu_e + pe\mu_h}$; $j = \sigma E$

e^- & h^+ direction is opposite but their charge as well

Mobility $[\mu] = \frac{cm^2}{Vs}$

typical values:

- $\mu_e^{Si} \approx 1\,000 \frac{cm^2}{Vs}$, $\mu_h^{Si} \approx 100 \frac{cm^2}{Vs}$
  given by phonons


band-band scattering for holes

- $\mu_e^{GaAs} = 30\,000 \frac{cm^2}{Vs}$, $\mu_h^{GaAs} = 1000 \frac{cm^2}{Vs}$
- $\mu_e^{poly\text{-}Si} \approx 1 \frac{cm^2}{Vs}$ (eg. solar cells)
- organic SCs: $\mu_e \approx 10 \frac{cm^2}{Vs}$
- $\mu_e^{Cu} \approx 0.01 \frac{cm^2}{Vs}$
- $\mu_e^{graphene} = 10^6 \frac{cm^2}{Vs}$ very large => large v_D

BUT! physical limit of v_D: optical phonon emission

$\frac{1}{2} m v_D^2 = \hbar\omega_{opt}$

large lattice vibration => material falls apart

2018. IX.25. 4.hét 4.ea

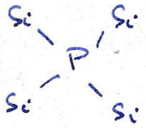
Doping [adalékolás]

3

Heteroatoms in the SC lattice

e.g. B:Si   As:Si -> trivalent (3 vegyértékű) doping => p-type

P:Si   Al:Si -> pentavalent doping => n-type

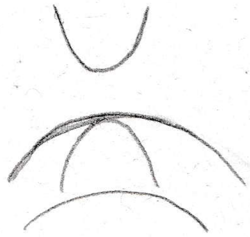


- plus 1e⁻, +1p⁺
- material is neutral (always)
- P ionised -> e⁻ is delocalised

Considering Schrö-equation for bulk Si

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

↑ periodic atomic potential



↓ + 1e⁻, 1p⁺

approximation: exact Si solution + Hydrogen atom

atom ($m_0 \to m^*$, $\varepsilon_0 \to \varepsilon_0 \varepsilon_r$)

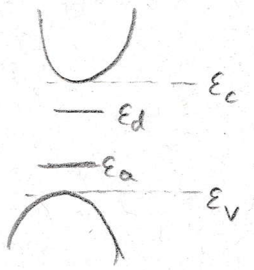
↑ band eff. mass

↑ shielding due to other electrons

handwaving: extra e⁻ would $E_c \to p^+ + e^-$ is measured with respect to E_c

donor level

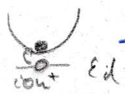
acceptor level



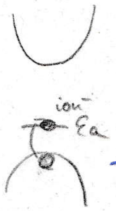
} ~25 meV => termikusan könnyen gerjeszthető

bounded states at $T = 0$ <= adalék atom mellett kötött állapot

exitation ($T \neq 0$):



-> delocalisation of the e⁻



-> delocalisation of the h⁺

Bohr-model jól adja vissza a H atom alap és gerjesztett állapotát de az impulzust nem

centripetal force $m_0 \frac{v^2}{r} = \frac{1}{4\pi\varepsilon_0}\frac{e^2}{r^2}$ coulomb force

$L = n\hbar \to m_0 v r = n\hbar$

$\to r = \frac{1}{4\pi\varepsilon_0}\frac{e^2}{m_0 v^2}$

$\to v = \frac{n\hbar}{m_0 r} = \frac{n\hbar}{\frac{1}{4\pi\varepsilon_0}\frac{e^2}{v^2}} \to \boxed{v_n = \left(\frac{n\hbar\, 4\pi\varepsilon_0}{e^2}\right)^{-1} = \frac{1}{4\pi\varepsilon_0}\frac{e^2}{n\hbar}} =$

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

with $\boxed{\alpha = \frac{1}{4\pi\varepsilon_0}\frac{e^2}{\hbar c}} \approx \frac{1}{137}$ finomszerkezeti állandó

$[\alpha] = \frac{Vm}{As}\frac{A^2s^2}{VAs^2m} = 1$

- $r = \alpha\hbar c\frac{1}{m_0}\frac{n^2}{\alpha^2c^2} = \frac{n^2}{\alpha}\cdot\frac{\hbar}{m_0c} = n^2 a_B$ with $\boxed{a_B = \frac{\hbar}{m_0c}\frac{1}{\alpha}} \approx 0.5 Å = 0.05 nm$ Bohr-radius

$\frac{h}{m_0c} = \lambda_{compton}$

- $\boxed{E_n} = \frac{1}{2}m_0v_n^2 - \frac{1}{4\pi\varepsilon_0}\frac{e^2}{r_n} = \frac{1}{2}\underbrace{m_0\frac{\alpha^2}{n^2}c^2}_{\frac{\alpha^2}{n^2}m_0c^2} - \underbrace{\alpha\hbar c\frac{\alpha}{n^2}\frac{m_0c}{\hbar}}_{\frac{\alpha^2}{n^2}m_0c^2} = \boxed{-\frac{1}{2}\frac{\alpha^2}{n^2}m_0c^2} \approx 13.6 eV$ for H

energy of bound states /kötési energia/

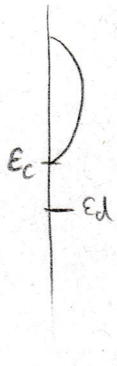
SC:
$m_0 \to m^* = 0.1 \ldots 0.5\, m_0$
$\varepsilon_0 \to \varepsilon_0\varepsilon_r \approx 11\, \varepsilon_r$ for Si
↑ from other e^--s ← e^--k leárnyékolják az atomtörzs Coulomb potenciálját

$\alpha \to \frac{\alpha}{\varepsilon_r}$; $a_B^* = a_B\cdot\underbrace{\varepsilon_r\frac{m_0}{m^*}}$ makes the Bohr-radius larger: 30–100 Å

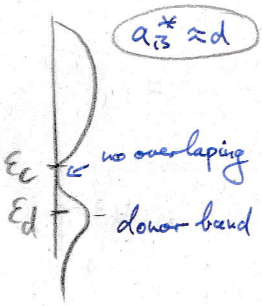
$E_1^* = -\overbrace{13.6 eV}^{E_1}\underbrace{\frac{m^*}{m_0}}_{\frac{1}{10}-\frac{1}{2}}\frac{1}{\varepsilon_r^2}$ → typically $E_1^* \approx 20-100$ meV $\ll E_1 = 13.6$ eV

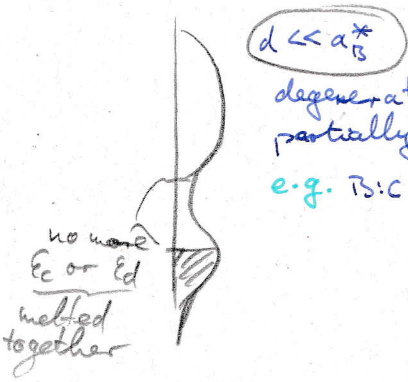
energies form Rydberg series

distance between dopants: $\boxed{d = \frac{1}{\underbrace{n_D^{1/3}}}}$
dopant concentration (for both kinds of dopants)



if $a_B^* \ll d$
⇓
E_d states are localised, non interacting states
1ppm dopants → d = 30nm → non interacting states



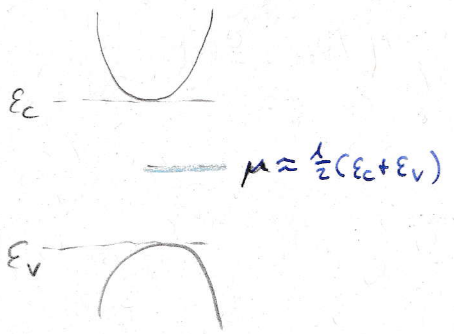


$d \ll a_B^*$

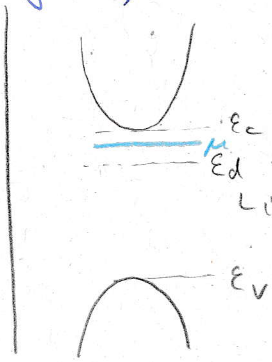
degenerate SC
partially filled band
e.g. B:C - boron doped diamond → metal
$T_c \approx 10K$

Number of charge carriers in doped SC (extrinsic)
/ concentration

μ : chemical potential (Sólyom II)



intuition: $\mu \approx \frac{1}{2}(\varepsilon_c + \varepsilon_d)$



ε_d - highest occupied e^- states
└ individual, non-interacting states

occupation of donor levels

· donor levels form a grand canonical ensemble

$$\langle n \rangle = \frac{\sum n e^{-\beta(\varepsilon_n - n\mu)}}{Z}$$

occupation (excepted value)

$$Z = \sum_n e^{-\beta(\varepsilon_n - n\mu)}$$

[állapotösszeg]
grand canonical ensemble
partition function

possible values of n : $n=0$ — donor ionized
$n=1$ ↑ or ↓ neutral donor
$n=2$ ~~↑↓~~ not possible bcs of Coulomb-interaction

$n=0$ has ε_0 energy
└ energy of ground state

$$\Rightarrow Z = e^{-\beta\varepsilon_0} + 2 e^{-\beta(\varepsilon_0 + \varepsilon_d - \mu)}$$

extra energy of donor states
2 — denegeracy bcs of 2 spin states

$$\langle n \rangle = \frac{2 e^{-\beta(\varepsilon_0 + \varepsilon_d - \mu)}}{e^{-\beta\varepsilon_0} + 2 e^{-\beta(\varepsilon_0 + \varepsilon_d - \mu)}} = \frac{1}{1 + \frac{1}{2} e^{\beta(\varepsilon_d - \mu)}} = f_d$$

└ donor function

⇕

Fermi-function: $\frac{1}{1 + e^{\beta(\varepsilon_d - \mu)}}$

Probability of ionisation

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

!

$\downarrow$ with $\mu \approx \frac{1}{2}(\varepsilon_c+\varepsilon_v)$

/!\ $$\boxed{1-f_d = \frac{1}{1+e^{\frac{\beta}{2}(\varepsilon_c-\varepsilon_d)}}}$$ nb of charge carriers in the conduction band in a doped SC

n: e^- concentration in the conduction band

p: hole concentration in the valence band

N_d: donor atom nb

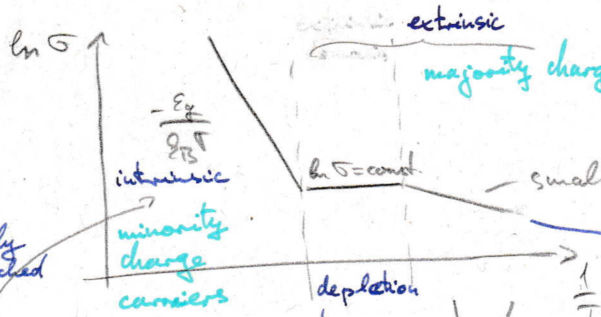
N_a: acceptor atom nb

$$n = \frac{N_d}{V}\,\frac{1}{1+\frac{1}{2}e^{\frac{\varepsilon_c-\varepsilon_d}{2k_BT}}} \to 0$$

$$p = \frac{N_a}{V}\,\frac{1}{1+\frac{1}{2}e^{\frac{\varepsilon_a-\varepsilon_v}{2k_BT}}}$$

Temperature dependance of n

1. $T \to \emptyset \Rightarrow n \to \emptyset$
2. $2k_BT \approx \varepsilon_c - \varepsilon_d \Rightarrow n \approx \frac{N_d}{V} = n_d$ donor density, constant in a relatively large T interval
   ? 26meV 50 .. 100meV
3. $k_BT \approx \varepsilon_g = \varepsilon_c - \varepsilon_v$
   direct band-band excitation like in intrinsic SC



majority charge carriers (e^- for n-doped, h^+ for p-doped)

small slope ~ $\frac{-(\varepsilon_c-\varepsilon_d)}{2k_BT} \leftrightarrow \frac{1}{1+\frac{1}{2}e^{\frac{\varepsilon_c-\varepsilon_d}{2k_BT}}}\Bigg|_{T\to\emptyset} \approx e^{-\frac{\varepsilon_c-\varepsilon_d}{2k_BT}}$

activated charge carriers

usually never reached

1eV ~ 10 000 K

$1{,}38\cdot10^{-23}\,\frac{J}{K} \leftrightarrow 1{,}6\cdot10^{-19}\,As$

depletion
↓
donors are ionised
↓
technological case: we want to use our devices in this region (stable against ΔT)

ε_d

Law of mass action

tömeghatás törvénye

from chemistry
$OH^- \leftrightarrow H_3O^+$ dissociation

For intrinsic SC: $n=p=n_i(T)$ or $np = n_i^2(T)$

$$\left.\begin{aligned} n &= n_c\, e^{-\frac{\varepsilon_c-\mu}{k_BT}} \\ &\text{nb of states in CB} \\ p &= n_v\, e^{-\frac{\mu-\varepsilon_v}{k_BT}} \end{aligned}\right\}\quad np = n_c n_v\, e^{-\frac{\varepsilon_g}{k_BT}} \leftarrow \text{only depends on } T$$

$\boxed{T}$: $np = n_i^2(T)$ is also valid in a doped SC

motivation

- assume it is valid

$np = n_i^2(T)$ e.g. for n-doped $n = n_d$ (in the extrinsic regime: all donors are ionised)

n_d = density of the donors

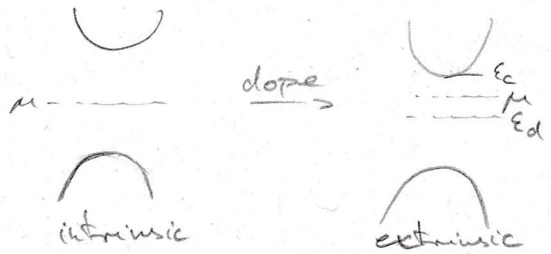
-> p is lowered

$n_d\, p = n_i^2(T) \;\rightarrow\; p = \dfrac{n_i^2(T)}{n_d} \ll n_i(T)$

"e^- eat up h^+"

$n = n_d = n_c\, e^{-\frac{\varepsilon_c - \mu}{k_B T}}$

negative charge density — n; CB density — n_c



$\mu = \frac{1}{2}(\varepsilon_c + \varepsilon_V)$

$n = n_c\, e^{-\frac{\varepsilon_c - \mu}{k_B T}}$

$p = n_v\, e^{-\frac{\mu - \varepsilon_V}{k_B T}}$

μ shift → p drops, n increases } while their product remains const.

2018.
X. 2.
5. hét
5. ea

Band-structure calculation in SC

$\boxed{14}$

Important for:

- conduction properties (m^*, E_g)
- optical properties (E_g)
- intelligent designe, band-gap engineering /smart-engineering

Band-structure calculation models

- empty lattice model (free e^- gas in a lattice) "hand-waving"
- quasi-free e^- approximation
- ↑ semi-empirical method (tight-binding, pseudo potential methods)
- ab-initio (first principles) DFT
- interacting, many e^-, GW

Schrödinger equation (∇ [Del operator])

- $H = -\frac{\hbar^2}{2m}\Delta + U(\underline{r})$ where $U(r) = \underbrace{\sum H_{at}}_{\text{ion-}e^-} + \underbrace{H_{e\text{-}e}}_{e\text{-}e \text{ interaction}}$

simplifications

ion as a fix nucleus, e^- moves around

- -> one electron Hamiltonian

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

$\Psi(r)$: one e^- wavefunction

- in solids $U(\underline{r}) = U(\underline{r}+\underline{R})$ ← periodicity of the lattice
  ↳ lattice vector

síkhullám tag

- Bloch-theorem : $\boxed{\psi_k(\underline{r}) = e^{i\underline{k}\underline{r}} u_k(\underline{r})}$ $u_k(\underline{r}) = u_k(\underline{r}+\underline{R})$
  ↳ all different k gives a different $u_k(\underline{r})$
  megadja a megoldás/hullámfv formáját

-> discret translational symmetry
-> $k \in$ allowed values by the Born-Kármán periodic boundary condition

in 1D
N atoms
$\ldots \quad k = \frac{2\pi}{N a}\cdot n \quad n = -\frac{N}{2} \ldots \frac{N}{2}$
(a)

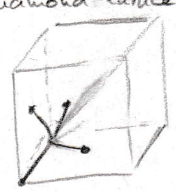
k: crystal wavenb
↳ crystal momentum $\hbar k$

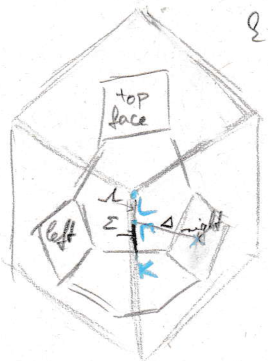
e.g. • $k=\emptyset$ then $e^{ikr}=1$ -> $\psi_{k=0}(\underline{r}) = u_{k=0}(\underline{r})$
constant lattice points (same at each lattice point)

• $k = BZ \overset{1D}{=} \frac{\pi}{a}$ -> $e^{ikr} = \pm 1$ (alternating)
↳ wave func. changes sign between lattice points

Real space and reciprocal space

diamond lattice

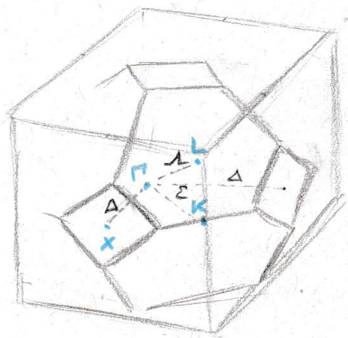


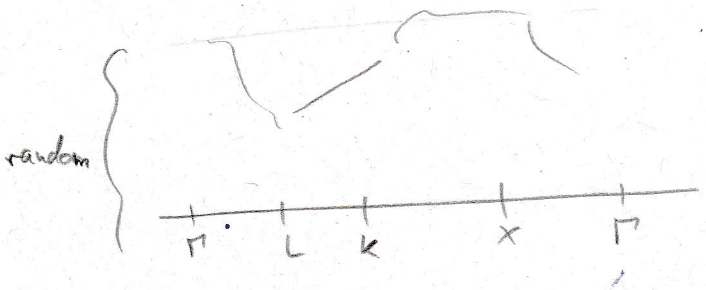


k-space

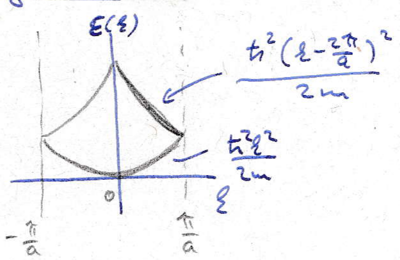
Γ: zone centre $(0,0,0)$
L: middle of hexagon
X: middle of square
K: halving point on two tuching hexagons

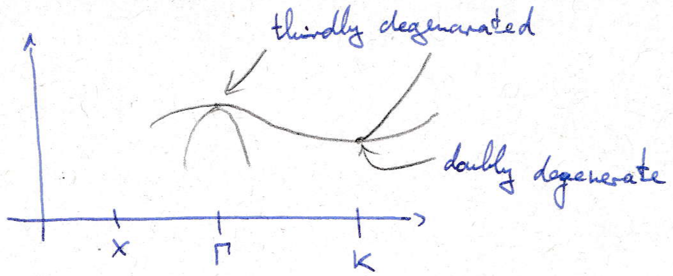
100 direction: $\Gamma \xrightarrow{\Delta} X$, Δ line
111 $\quad \Gamma \xrightarrow{\Lambda} L$, Λ line
110 $\quad \Gamma \xrightarrow{\Sigma} K$, Σ line





Empty lattice





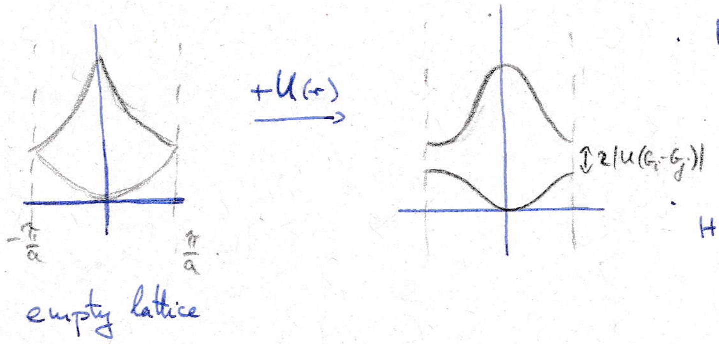
$\boxed{1D}$

single degeneracy

$\boxed{2D/3D}$

degeneracy: parabols (from different directions) are touching

Quasi-free e^- model



· $H\Psi = E\Psi$, $H = -\frac{\hbar^2}{2m}\Delta \to \Psi_k = \frac{1}{\sqrt{V}} e^{ikr}$

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

$\downarrow +U(r)$

· $H = -\frac{\hbar^2}{2m}\Delta + U \to E_k = \varepsilon_k + \underline{\langle \Psi_k | U | \Psi_k \rangle}$

non degenerate perturbation calculation

↳ doesn't work for BZ boundary

Degenerate perturbation calculation for BZ boundary

$$\underset{\text{matrix}}{H} = \begin{pmatrix} U_{11} & U_{12} \\ U_{21} & U_{22} \end{pmatrix} \overset{1^{st}\text{ BZ boundary}}{=} \begin{pmatrix} \frac{\hbar^2 k^2}{2m} & U \\ U^* & \frac{\hbar^2}{2m}\left(\frac{2\pi}{a} - k\right)^2 \end{pmatrix} \to$$

eigenvalues → $2|U|$ gap on BZ boundary

∘ $U_{12} = U_{21}^* = \langle \Psi_{2k} | U | \Psi_{1k} \rangle = \int d^3r\, e^{i(k+G)r}\, U(r)\, e^{-ikr} =$

∘ $U_{11} = \langle \Psi_{1k} | U | \Psi_{1k} \rangle$ $= \int d^3r\, e^{iGr}\, U(r) = U(G)$

Fourier-transformation

↑ also works for k points going away from BZ boundary

↳ gives back the non degenerate p.c.

at the BZ boundary: U has the most effect

Tight-binding model /szoros kötésű közelítés/ (TB)

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

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

R ← lattice vectors

atomokhoz kötött e^--ok különö nagy rácsállandóval (N-szeresen degeneráltak)

↳ rácsállandót csökkentjük

assuming that $H_{at}\, \varphi_a = \varepsilon_a\, \varphi_a$ is known

Ansatz: $\Psi_k(r) = \frac{1}{\sqrt{N}} \sum_n e^{ikna}\, \varphi_a(r - na)$ ← satisfies Bloch theorem

/próba fv/

{ feltéve, hogy a hullámfv-ek közt nincs nagy átfedés shortened notation: $\Psi_k(r) = \sum_n e^{ikna}|n\rangle$

$\uparrow$ e^- shifted to the n^{th} lattice site

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

↳ plug into $H\Psi = E\Psi$ (Hamiltonian)

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

$\langle n''| \downarrow$ projection

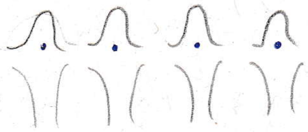
$\rightarrow \langle n''|n\rangle = \delta_{nn''}$

$$\rightarrow \sum_{n'} V_{atom}(r-n'a) = \underbrace{V_{atom}(r-na)}_{\text{on site potential}} + \sum_{n'\neq n} V_{atom}(r-n'a)$$

$$\Rightarrow \sum_n \cancel{e^{ikna}}\left[\varepsilon_a \delta_{nn''} + \sum_{n'\neq n}\langle n''|V_{atom}(r-n'a)|n\rangle\right] = E\sum_n \cancel{e^{ikna}}\,\delta_{nn''}$$

$$\boxed{E(k) = \varepsilon_a + \sum_{n,n'\neq n} e^{ik(n-n'')a}\langle n''|V_{atom}(r-n'a)|n\rangle}$$

no neglection so far



$\varphi_a(r-na)$

$V_{atom}(r-na)$

NNTB (nearest neighbor TB)

these are the only non-vanishing terms

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

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

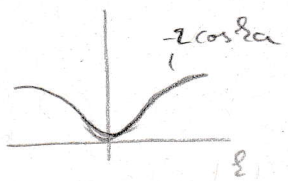
t: overlap integral

$[t] = J$

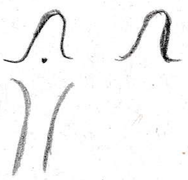
$$\Rightarrow E(k) = \varepsilon_a + (e^{ika} + e^{-ika})|t|(-1) =$$

$$\circ\ -|t| = \int d^3r\, \varphi_a^*(r-a)V(r-a)\varphi_a(r) = \int d^3r\, \varphi_{at}^*(r+a)V(r+a)\varphi_{at}(r)$$

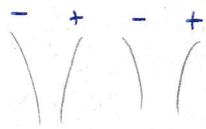
$$= \underline{\underline{\varepsilon_a - 2|t|\cos ka}}$$



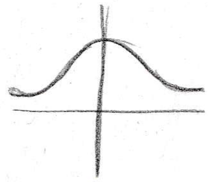
SSσ model



φ_a : p orbital
↳ wave function changes signe

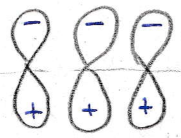


$E(k) = \varepsilon_a + 2|t| \cos ka$



ppσ

TB is semi empirical
- gives the right qualitative k dependance
- t is determined from exp. or DFT



eg. in graphene

ppπ

1D + 2nd NN terms

$$\sum_{n, n' \neq n} e^{ik(n-n'')} \langle n'' | V_{at}(r - n'a) | n \rangle$$

$(e^{i2ka} + e^{-i2ka})|t|$ appears $\rightarrow \cos(2ka)$ higher periodicity

$$E(k) = \varepsilon_a - 2|t_{NN}| \cos(ka) - 2|t_{2^{nd}NN}| \cos(2ka)$$

2D TB

$$E(\underset{(k_x k_y)}{\underline{k}}) = \varepsilon_a - 2|t_a| \cos(k_x a) - 2|t_b| \cos(k_y b)$$

overlaping integral differs in different directions $\rightarrow$ anisotropic band structure

· effective mass in TB : $(m^*)^{-1} = \frac{1}{\hbar^2} \frac{\partial^2 E(k)}{\partial k^2}$, $E(k) = \varepsilon_a - 2|t| \cos(ka) \approx$
$\approx \varepsilon_a - 2|t| \left(1 - \frac{k^2 a^2}{2}\right)$

$\Rightarrow (m^*)^{-1} = \frac{2ta^2}{\hbar^2}$ $\quad [(m^*)^{-1}] = \frac{\cancel{J} m^2}{J^2 s^2} = \frac{s^2}{kg\, m^2}\frac{m^2}{s^2} = \frac{1}{kg}$ ✓

$\underline{k}.\underline{p}$ model [key dot pi] [k-szor p modell]

- good semi-empirical model near band extrema → ideal for SC
- gives result on transport properties, low energy optics, magnetic properties

$H\Psi = E\Psi$ Bloch's functions: $\Psi_{n\underline{k}}(\underline{r}) = \underbrace{e^{i\underline{k}\underline{r}}}_{\text{plain wave}}\ \underbrace{u_{n\underline{k}}(\underline{r})}_{\text{lattice periodic fn}}$

crystal momentum: $\underline{k}$
band index: n

$$H = -\frac{\hbar^2}{2m}\Delta + \underbrace{V(\underline{r})}_{\text{periodic potential}}$$

vector prod. vector scalar

$$\Delta\Psi_{n\underline{k}}(\underline{r}) = (i\underline{k})^2 e^{i\underline{k}\underline{r}} u_{n\underline{k}}(\underline{r}) + 2(i\underline{k})e^{i\underline{k}\underline{r}}\,\underline{\nabla}u_{n\underline{k}}(\underline{r}) + e^{i\underline{k}\underline{r}}\Delta u_{n\underline{k}}(\underline{r})$$

↳ substitution into Schrö.

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

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

operator of the canonical impulse ($\neq \hbar\underline{k}$)

external forces act on the crystal mom.: $\underline{F}_{ext} = \hbar\dot{\underline{k}}$
↳ separation of crystal mom. and canonical impulse

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

$\underline{k}.\underline{p}$ approximation: consider $\underline{k}=\emptyset$ solution near a band extrema (e.g. $\Gamma \Rightarrow \underline{k}=\emptyset$) or we can translate it to $\underline{0}$ from the point in consideration

↳ at $\underline{k}=\emptyset$: $\left[\frac{p^2}{2m} + V(\underline{r})\right]u_{n\emptyset}(\underline{r}) = E_{n\emptyset}\,u_{n\emptyset}(\underline{r})$

we assume that the problem is solved $u_{n\emptyset}$ and $E_{n\emptyset}$ are known that is why semi empiric model

→ $\frac{\hbar^2k^2}{2m} + \frac{\hbar(\underline{k}.\underline{p})}{m}$ is a perturbation

2^{nd} order perturbation theory (for non degenerate case)

$H|n\rangle = \varepsilon_n|n\rangle$; $|n\rangle$ orthonormal basis

$$(H+V)\Psi = E\Psi \quad ; \quad E_n = \varepsilon_n + \langle n|V|n\rangle + \underbrace{\sum_{n'\neq n}\frac{|\langle n'|V|n\rangle|^2}{\varepsilon_{n'}-\varepsilon_n}}_{2^{nd}\text{ order energy correction}}$$

$$\boxed{\Psi_n = |n\rangle + \sum_{n'\neq n}\frac{|\langle n'|V|n\rangle|^2}{\varepsilon_{n'}-\varepsilon_n}|n'\rangle}$$

in our case: $u_{n\underline{k}}(\underline{r}) \overset{\text{Ansatz}}{=} \sum_n c_n(\underline{k})\, u_{n\phi}(\underline{r})$

coefficients

If the point of interest is extremum, there are no linear terms in k.

Results: $u_{nk} = u_{n\phi} + \frac{\hbar}{m} \sum_{n' \neq n} \frac{\langle u_{n\phi} | \underline{k} \cdot \underline{p} | u_{n'\phi} \rangle}{E_n - E_{n'\phi}} | u_{n'\phi} \rangle$

- $\langle u_{n'\phi} | \frac{\hbar^2 k^2}{2m} | u_{n\phi} \rangle = \underbrace{\frac{\hbar^2 k^2}{2m}}_{\text{simple product}} \delta_{n'n} \underset{n' \neq 0}{=} 0$

- energy: $\boxed{E_{nk} = E_{n\phi} + \frac{\hbar^2 k^2}{2m} + \frac{\hbar^2}{m^2} \sum_{n' \neq n} \frac{|\langle u_{n\phi} | \underline{k} \cdot \underline{p} | u_{n'\phi} \rangle|^2}{E_{n\phi} - E_{n'\phi}}}$

  1st order energy correction

- perturbation: $\frac{\hbar^2 k^2}{2m} + \frac{\hbar(\underline{k} \cdot \underline{p})}{m}$ → linear term disappears
- $\langle u_{n'\phi} | \hbar^2 k^2 | u_{n\phi} \rangle \sim \delta_{n'n}$ → quadratic term disappears

curvature

Effective mass approximation

$E_{nk} = E_{n\phi} + \frac{\hbar^2 k^2}{2m^*}$

$m^* > 0$ conduction band
$m^* < 0$ valence band

band edge (E_C or E_V)

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

dominant contribution comes when $E_{n\phi} - E_{n'\phi} = E_{gap}$ only E scale (independent of other parameters) in SC

- $|\langle u_{n\phi} | \underline{k}\underline{p} | u_{n'\phi} \rangle|^2 \frac{1}{k^2} = P^2$ experimentally known: $\frac{2P^2}{m} \approx 20\,eV$ for most IV and III-V SC

↳ $\boxed{\frac{1}{m^*} = \frac{1}{m} + \frac{2P^2}{m E_g}}$ → gives m^* reasonably well for III-V and IV SC

Envelope function approximation (EFA) [burkoló fv közelítés]

- works well in SCs with slowly varying (in space) external fields ($\underline{E}$, $\underline{B}$, doping, heterostruc, band gap engineering) $Ga_{1-x}Al_xAs$

$H_0 \Psi(\underline{r}) = E_0 \Psi(\underline{r})$ we suppose that the solution is known

$\updownarrow$

$E_{n\underline{k}}$: solution without external fields (doping)

$$\Psi_{n\underline{k}}(\underline{r}) = e^{i\underline{k}\underline{r}} u_{n\underline{k}}(\underline{r})$$

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

$\uparrow$ spacially slowly varying part

to separate the two parts we go to the momentum space

$\hookrightarrow$ linear combination

$$V(\underline{k}) = \int e^{i\underline{k}\underline{r}} V(\underline{r})\, d^3r \underset{\text{approximation}}{\approx} \delta_{\underline{k}} \cdot V_0$$

$H \Phi = E \Phi$ Ansatz : $\boxed{\Phi(\underline{r}) = \sum_{n,\underline{k}} F_n(\underline{k}) \Psi_{n\underline{k}}(\underline{r})}$ $F_n(\underline{k})$: envelop fn

lin comb. of the solutions

$\hookrightarrow$ substitution to Schrö.

$$\boxed{\sum_{n,\underline{k}} \Psi_{n\underline{k}} \left[E_{n\underline{k}}(\underline{r}) - E + V(\underline{r}) \right] F_n(\underline{k}) = \emptyset}$$

a set of linear equations (no diff. eq. any more)

project with $\Psi_{n'\underline{k}'} \rightarrow \langle \Psi_{n\underline{k}} | \Psi_{n'\underline{k}'} \rangle = \delta_{nn'\underline{k}\underline{k}'}$

$$(*) \quad \sum_{n,\underline{k}} \Big[(E_{n\underline{k}}(\underline{r}) - E)\, \delta_{nn'\underline{k}\underline{k}'} + \overbrace{\langle \Psi_{n'\underline{k}'} | V(\underline{r}) | \Psi_{n\underline{k}} \rangle}^{\text{matrix component}} \Big] F_n(\underline{k}) = \emptyset$$

$$V_{n'\underline{k}'n\underline{k}} = \int u^*_{n'\underline{k}'}(\underline{r})\, u_{n\underline{k}}(\underline{r}) \cdot \underbrace{e^{i(\underline{k}-\underline{k}')\underline{r}} \cdot V(\underline{r})\, d^3r}_{\text{would be the Fourier transf of } V}$$

approximation : the integral can be separated

$u_{n'\underline{k}'} \rightarrow$ localized, $V(\underline{r})$ extended (slowly varying)

$$V_{n'\underline{k}'n\underline{k}} \approx \underbrace{\int u^*_{n'\underline{k}'}(\underline{r})\, u_{n\underline{k}}(\underline{r})\, d^3r}_{\delta_{nn'\underline{k}'\underline{k}}} \; \underbrace{\int e^{i(\underline{k}-\underline{k}')\underline{r}} V(\underline{r})\, d^3r}_{V(\underline{k}-\underline{k}') \text{ Fourier transf.}}$$

$\hookrightarrow$ substitution back to (*)

$$n = n' \Rightarrow \sum_{\underline{k}} \Big[\underbrace{(E_{n\underline{k}}(\underline{r}) - E)}_{\text{shift of the energy level}}\, \delta_{\underline{k}\underline{k}'} + \overbrace{V(\underline{k}-\underline{k}')}^{\text{pot. applied}} \Big] F_{n'}(\underline{k}) = \emptyset$$

multiplication of the wave fn

$\delta_{nn'\underline{k}\underline{k}'}$

it is a Schrö. for $F_n(\underline{k})$

original pb: (known solution)

$$E_n(\underline{q}) = E_c + \frac{\hbar^2 q^2}{2 m_c^*} \quad \text{here } n' \equiv c$$, conduction band

plan wave approx.
=> free e^- gas with an effective mass
↑ everything in (?)

with this EFA equation becomes:

$$(***) \quad \frac{\hbar^2 q^2}{2 m_c^*} F_c(\underline{q}') + \sum_{\underline{q}} V(\underline{q}-\underline{q}')\, F_c(\underline{q}) = (E - E_c) F_c(\underline{q})$$

set of linear equations
↳ we want to show that it is a Schrö. eq.
↓ explanation

Statement: $\underline{q} \rightarrow -i\nabla$
↖ cheating: we said that it wasn't like that

$$(**) \quad \left[-\frac{\hbar^2 \Delta}{2 m_c^*} + E_c + V(\underline{r}) \right] F_c(\underline{r}) = E\, F_c(\underline{r})$$ Schrö. eq.

- FT (Fourier tr.) $F_c(\underline{r}) \rightarrow F_c(\underline{q})$

$$FT(f'(r)) = i q f(q)$$

- $\int f'(r)\, e^{i q r}\, d^3r = i q \int f(\underline{r})\, e^{i \underline{q}\underline{r}}\, d^3r$

$u' \quad v$

$\int u'v = \underbrace{uv}_{\text{vanishes}} - \int u v'$

$$FT(V(\underline{r}) F_c(\underline{r})) = \overbrace{\int V(\underline{q}-\underline{q}')\, F_c(\underline{q})\, d^3r}^{\text{convolution}}$$

FT of (**) becomes (***)

Semi empirical: it needs E_c and m_c^*
it gives intuitively, correctly the effect of external fields

e.g. charge density

- $n(r) = \sum_i |\Psi(r)|^2 f(E_i) = n_{c\phi}(r) \sum_i |F_i(r)|^2 f(E_i)$

↑ Fermi-fn ↑ original charge density i: band index

↳ P:Si [P doped Si]

P has $+1p^+$ & $+1e^-$ ($\rightarrow a_B^* \gg d$)

↳ localized $F(\underline{r})$ => EFA is self consistent

⚠ everything leads back to Schrö. with a perturbation

Transport phenomena

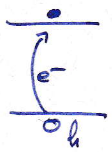
5

- current ($\underline{j}$), thermal current ($\underline{j}_Q$), Seebeck, Peltier

Length-scales $\quad \ell < \delta_\phi < \delta_s < \delta_c$

- charge diffusion length

e



non-equilibrium charge /nemegyensúlyi/

creation $\xrightarrow{\tau_c}$ recombination

$\tau_c \approx 1\mu s - 1ms$ → diffusion $\quad \xleftrightarrow{\tau_c \gg \tau}$

τ_c recombination time

any kind of inhomogeneity

τ momentum relaxation time $\approx 10^{-12} - 10^{-14}$ s

$\boxed{\underline{j} = -D\nabla n}$ $\quad$ D: diffusion constant $\approx \bar{v}\bar{\ell} \approx v_F^2\tau$

j: particle current density $\quad$ v_F Fermi velocity

=> δ_c charge diffusion length

$t=0$ $\xrightarrow{t}$ $\langle \Delta x^2 \rangle = Dt$

=> $\boxed{\delta_c = \sqrt{D\tau_c} \approx v_F\sqrt{\tau\tau_c}}$ $\approx 10\mu m - 1cm$

(solar-cells!)

- spin-diffusion length

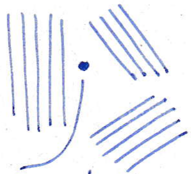
τ_s: spin-lifetime

$\delta_s = v_F\sqrt{\tau\tau_s} \approx 1 - 100\mu m$

- phase-coherence length /fázis koherencia hossz/

$\delta_\phi \approx 100nm - 1\mu m$

$e^{i\underline{k}\cdot\underline{r}}$

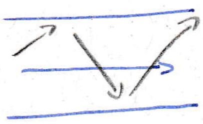


scattering centre → random phase → phase coherence is lost

eg. for weak localization /gyenge lokalizáció/

constructive/destructive interference

ballistic transport



analogy: optical fiber

even if not supraconductor → no scattering

coherent or not?

eszköz mérete < 100nm

- mean free path /szabad úthossz/ 1nm – 100nm

$\ell = v_F \tau$ τ: momentum relaxation time

size ↑

Ohm's law
↳ diffusion, drift

} local equilibrium due to rapid collisions

——— 100nm – 1μm

Landauer - Büttiker formalism – mesoscopic physics

<u>Description</u> (Ohm's law)

<u>Free - electrons (Sommerfeld)</u>		<u>Bloch electrons</u>
quantum number $\underline{k} \in$ periodic b.c.	quantum number	$\underline{k} \in$ per. b.c. + band index
$\varepsilon(\underline{k}) = \frac{\hbar^2 k^2}{2m}$	energy disp	$\varepsilon_n(\underline{k}) = \varepsilon_n(\underline{k}+\underline{G})$ $\quad G \in$ rec. lattice vectors
$\underline{v} = \frac{\hbar \underline{k}}{m} = \frac{1}{\hbar}\frac{\partial \varepsilon}{\partial \underline{k}}$	velocity	$\underline{v}_n(\underline{k}) = \frac{1}{\hbar}\frac{\partial \varepsilon_n(\underline{k})}{\partial \underline{k}}$
$\psi_{\underline{k}}(r) = \frac{1}{\sqrt{V}} e^{i\underline{k}\underline{r}}$	wave functions	$\psi_{n\underline{k}}(\underline{r}) = e^{i\underline{k}\underline{r}} u_{n\underline{k}}(r)$ $u_{n\underline{k}}(\underline{r}+\underline{R}) = u_{n\underline{k}}(\underline{r})$ $R \in$ lattice vector
? no force from the structure (no pot.)		
$m^* = m$	band effective mass	$(\underline{m}^*)^{-1} = \frac{1}{\hbar^2}\frac{\partial^2 \varepsilon}{\partial \underline{k}^2}$ ↳ $m^*_{\text{graphene}} = \infty$?

<u>Notes</u>

· Drude-model: collision with ions → resistivity
Bloch-picture: perfect lattice with ions → $\rho = 0$, $\sigma = \infty$
$\underline{v}_{\underline{k}} = \text{const.}$

· crystal momentum
$\hbar \dot{\underline{k}} = F_{ext}$ → eg. $-e\underline{E}$; Lorentz-force etc

· canonical impulse operator $\underline{p} = \frac{\hbar}{i}\nabla$; $\psi_{n\underline{k}}(r) = e^{i\underline{k}\underline{r}} u_{n\underline{k}}(\underline{r})$

↳ $\underline{p}\,\psi_{n\underline{k}}(\underline{r}) = \hbar \underline{k}\, \psi_{n\underline{k}}(r) + \frac{\hbar}{i} e^{i\underline{k}\underline{r}} \nabla u_{n\underline{k}}(r)$

$p \neq \hbar k$ for Bloch functions ⇒ Bloch functions are no eigenstates of the canonical impulse

↑
only for free e^-

Closed bands and transport

$$\underline{j} = -e \int \underbrace{\frac{d^3 k}{4\pi^3}}_{\text{closed band}} \overbrace{\frac{1}{\hbar}\frac{\partial \varepsilon}{\partial \underline{k}}}^{v} \overset{f(k)=1}{\downarrow} = \emptyset$$

not trivial

$D(k)$ — Anschroft - Mermin

⌐ ~~handwaving proof~~ : . volume is symmetric / even fn
. $\frac{\partial \varepsilon}{\partial \underline{k}}$ -> odd fn (velocity has a well defined direction)
↳ integration of an odd fn over an even fn gives $\emptyset$ ⌐

$$\emptyset = \underbrace{\int \frac{d^3 k}{4\pi^3} \underline{v}(\underline{k})}_{\text{closed band}} = \underbrace{\int \frac{d^3 k}{4\pi^3} \underline{v}(\underline{k})}_{\text{occupied until } \varepsilon} + \underbrace{\int \frac{d^3 k}{4\pi^3} \underline{v}(\underline{k})}_{\text{occupied above } \varepsilon}$$

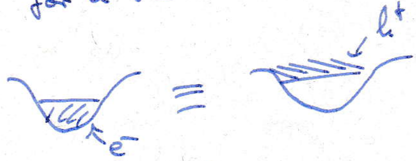
separation — different kinds of charge carriers

$$\boxed{-e \underbrace{\int_{\text{lower states}} \frac{d^3 k}{4\pi^3} \underline{v}(\underline{k})}_{\text{current of } e^-} = e \underbrace{\int_{\text{upper states}} \frac{d^3 k}{4\pi^3} \underline{v}(\underline{k})}_{\text{current due to } h^+}}$$

motivation for h^+ as charge carriers

in Drude: $j = -nev$

for a band:



effective mass is different bcs of band curve (band effective mass)

Boltzmann equation

- statistic physics
- treatment to transport phenomena

distribution function: $f(t, \underline{r}, \underline{k})$
↳ contains all information

$$f^0(\underline{k}) = \frac{1}{1 + e^{\frac{\varepsilon(\underline{k}) - \mu}{k_B T}}}$$ stationary solution — Fermi - Dirac distribution
↳ no time or spatial dependence

measurable physical quantities

$$j = -e \int \underline{v}(\underline{k}) \underbrace{D(\underline{k})}_{\frac{1}{4\pi^3}} f(\underline{k}) \, d^3 k$$

introduction of the T

↖ external forces affect the distribution fn

Boltzmann equation /félklasszikus közelítés/

$$\frac{df}{dt} = \underset{\uparrow}{\frac{\partial f}{\partial t}} + \underset{\frac{\partial f}{\partial \underline{r}}}{\nabla_r f} \cdot \dot{\underline{r}} + \underset{\frac{\partial f}{\partial \underline{k}}}{\nabla_k f} \cdot \dot{\underline{k}} - \frac{\partial f}{\partial t}\Big|_{collision} = 0$$

$f = f(t, \underline{r}, \underline{k})$

collision term introduced heuristically

- $\dot{k}\, \nabla_k f$: force-term (external forces)
  $\hbar \dot{k} = F_{ext}$
- $\dot{\underline{r}}\, \nabla_r f$: diffusion-term ← we neglect yet

Linearisation of the solution

↳ homogeneous solution $f(\underline{k}, t) = f^0(\underline{k}) + g(\underline{k}, t)$

egyensúlyi eloszlás (f^0)

↑ non-equilibrium contribution (g)

relaxation time approximation (no external field)

τ idővel egyensúlyi $f^0(k)$-ba tér vissza

$$\frac{\partial f}{\partial t}\Big|_{coll} = \frac{g}{\tau} \quad \rightarrow \text{Boltzman-eq.}: \frac{\partial g}{\partial t} = -\frac{g}{\tau} \quad \rightarrow g(t) = g_0(t=0)\,\underbrace{e^{-\frac{t}{\tau}}}_{\text{relaxes to } 0}$$

τ: relaxation time = momentum scattering time

$\frac{1}{\tau}$: adott k állapotból időegység alatti másik állapotba való kiszóródás valószínűsége

Stationary solution

without diffusion Boltz. eq. reads

$$\boxed{\dot{\underline{k}}\, \nabla_k f = -\frac{g}{\tau}} \qquad \dot{\underline{k}} = \frac{1}{\hbar} F_{ext} = -\frac{e}{\hbar} \underline{E}$$

↑ DC electric field

$$\nabla_k f = \frac{\partial f}{\partial \underline{k}} = \frac{\partial f}{\partial \varepsilon} \frac{\partial \varepsilon}{\partial \underline{k}} = \frac{\partial f}{\partial \varepsilon} \cdot \hbar\, \underline{v}(\underline{k}) \qquad f^0 = \frac{1}{1 + e^{\frac{\varepsilon(\underline{k}) - \mu}{k_B T}}}$$

$$\dot{\underline{k}}\, \nabla_k f = -e\,\underline{E}\,\underline{v}(\underline{k}) \frac{\partial f}{\partial \varepsilon} = -\frac{g}{\tau} \implies g(\underline{k}) = e\,\underline{E}\,\underline{v}(\underline{k}) \cdot \frac{\partial f}{\partial \varepsilon}\, \tau$$

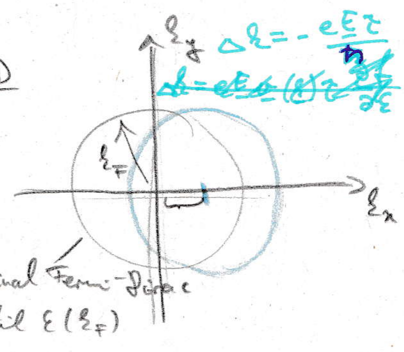
it gives $f(\underline{k}) = f^0(\underline{k}) + g(\underline{k}) = f^0 + e\underline{E}\,\underline{v}(\underline{k}) \frac{\partial f}{\partial \varepsilon} \tau$ ✓

$$\hookrightarrow f(\underline{k}) \approx f^0\left(\underline{k} + \frac{e\underline{E}\tau}{\hbar}\right) \underset{\substack{\uparrow \\ 1^{st} \text{ order} \\ \text{Taylor s.}}}{\approx} f^0(\underline{k}) + \frac{e\underline{E}\tau}{\hbar} \underbrace{\frac{\partial f}{\partial \underline{k}}}_{\frac{\partial f}{\partial \varepsilon} \hbar\, \underline{v}(\underline{k})} = f^0(\underline{k}) + e\underline{E}\,\underline{v}(\underline{k}) \frac{\partial f}{\partial \varepsilon} \tau \ ✓$$

$\implies$ /shift/ translation in $\underline{k}$-space by $\frac{e\underline{E}\tau}{\hbar}$ in 2D

$$\underline{k}_d = -\frac{e\underline{E}\tau}{\hbar}$$

↑ displacement



6

in the Drude model:

$v_D = \frac{eE\tau}{m^*} \rightarrow \hbar k_d \overset{\text{correspondence}}{=} m^* v_D$

↑ drift velocity ↳ these are the same! (Drude – B.eq)

Comments

conceptional difference

Drude model

all e^- move with $v = \underset{\text{small}}{v_D}$

$j = -nev$
↳ all e^- participate

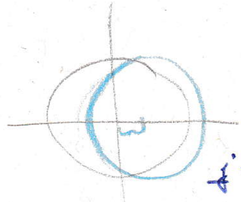
gives back the same result

Bloch (Boltzmann)

moving fast: v_F

only a few e^- near the Fermi surface

$j = -e v_F \underbrace{\frac{n v_D}{v_F}}_{\text{nb of } e^-}$



$j = -e \int D(k) f^0(k)\, v(k)\, d^3k = \phi$

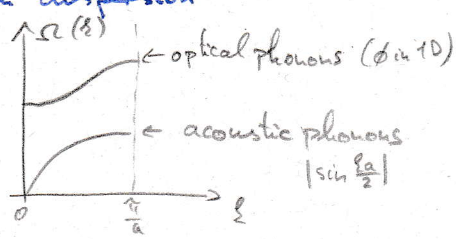
extra charge contribution to current $\sim \frac{v_D}{v_F} = \frac{k_d}{k_F}$

2018. X. 30. 8. hét 8. ea

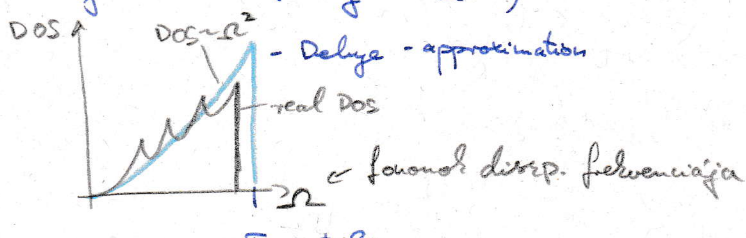
- τ is the central quantity
- origins of τ:
  - phonons
  - impurities ⟷ doping $\begin{cases} \text{low } T: \text{ neutral dopants} \\ \text{high } T: \text{ ionized/charged dopants} \end{cases}$
  - defects
- Matthiesen's rule: $\frac{1}{\tau} = \frac{1}{\tau_{phonon}} + \underbrace{\frac{1}{\tau_{imp}}}_{\text{const.}} + \frac{1}{\tau_{defects}} + \frac{1}{\tau_{e-e}} + \dots$

  $\frac{1}{\tau_{e-e}} \sim T^2$; $\frac{1}{\tau_{e-phonon}} = \begin{cases} \sim T & \text{if } T \gtrsim T_D \\ \sim T^5 & \text{if } T \ll T_D \end{cases}$ ← Debye temperature ($k_B T_D = \hbar \omega_D$) ↳ quantum effects

- phonon dispersion

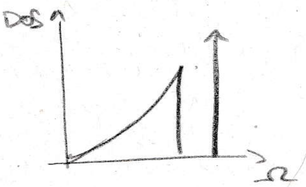


Debye-model (only acoustic)



$T_D \approx \frac{\hbar \Omega_D}{k_B}$

Debye - Einstein model (acoustic + 1 optic mode)



Elias(h)berg - formalism (phonons only)

$\boxed{T \gg 0}$

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

scattering rate

$\tau = 10^{-15} - 10^{-13}\,s$

λ: e-phonon coupling const. $\approx 0.1 - 1$

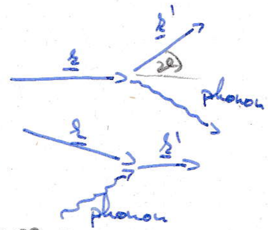
$$\lambda = 2 \int \frac{d\Omega}{\Omega} \underbrace{\alpha^{2} F(\Omega)}$$

notation, not a square

$F(\Omega)$: phonon DOS

$\alpha^2 F(\Omega)$: contains scattering

like $\sim$ $F(\Omega) \times (1 - \cos\vartheta)$



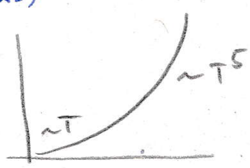
if $\vartheta = 0 \Rightarrow$ forward scattering does not effect τ ($\rightarrow 1-\cos\vartheta = 0$)

$\vartheta = \pi \Rightarrow 1 - \cos\vartheta = 2$, backward scattering gives large contribution to $\frac{1}{\tau}$

Bloch - Grüneisen fn (acoustic, isotropic phonons)

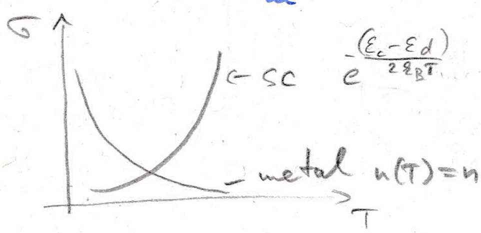
$$\frac{\hbar}{\tau} = 2\pi \lambda k_B T \times \underbrace{\int_0^{\Omega_D} \frac{d\Omega}{\Omega} \left(\frac{\Omega}{\Omega_D}\right)^4 \underbrace{\left[\frac{\frac{\hbar\Omega}{k_B T}}{\sinh\left(\frac{\hbar\Omega}{2k_B T}\right)}\right]^2}_{\sim\left(\frac{\hbar\Omega}{k_B T}\right)^4}}$$

high T limit



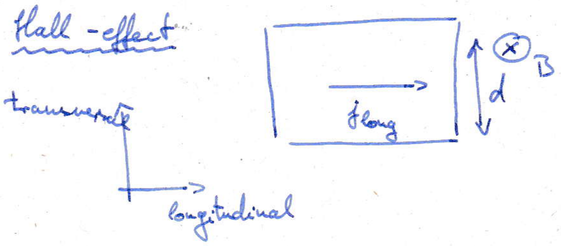
- 1 if $T \to \infty$
- universal fn (with $x = \frac{\hbar\Omega}{k_B T}$) if $T \to 0$

- $\sigma = \frac{n e^2 \tau}{m^*} = \frac{n(T)\, e^2\, \tau(T)}{m^*}$ can be explicitely evaluated (see notes from last year)



Magneto transport

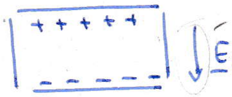
Hall-effect



$F = q\, v \times B$

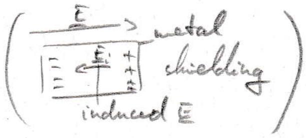
$\uparrow E_{transversal}$

In stationary condition



– irány?

E_{stat} charge accumulation due to the electric field



build up potential

$$E_{stat} = -F_{\substack{trans \\ (Lor)}} = -q\,\nabla\varphi$$

Drude-model

$$\to \quad v_D = \frac{e E_{long}\,\tau}{m^*} = \mu\, E_{long}$$

$\uparrow$ mobility

Hall-voltage : $V_H = d\, v_D B = \frac{d e E_{long}\,\tau}{m^*} B$

m $\quad \left[\frac{F}{q}\right] = \frac{m}{s}\cdot\frac{Vs}{m^2} = \frac{V}{m}$ electric field

Hall-resistivity : $\rho_H = \frac{E_{trans}}{j_{long}} = \frac{v_D B}{n e v_D} = \frac{B}{ne}$ $= R\cdot B$

/Hall-ellenállás/

[Ω·m] !

$$[\rho_H] = \frac{V}{m}\cdot\frac{m^2}{A} = \Omega\cdot m$$

Hall-constant : $R := \frac{\rho_H}{B} = \frac{1}{n\cdot e}$

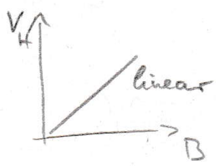
$\uparrow$ large for SCs

n has a sign !

for e^-: $n = -10^{23}\,\frac{1}{cm^3}$

$|n_{SC}| \sim 10^{10} - 10^{16}\,\frac{1}{cm^3}$

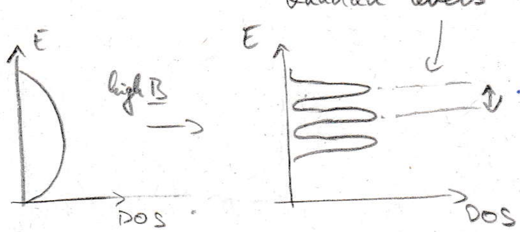
$|n_{metal}| \sim 10^{21}\,\frac{1}{cm^3}$



Quantum Hall-effect

$g\mu_B B \gg \frac{\hbar}{\tau} \Rightarrow$ QHE

Zeeman energy



$\updownarrow \hbar\omega_c$, broadening $\frac{\hbar}{\tau}$

cyclotron eff. : $\omega_c = \frac{eB}{m^*}$; $\hbar\omega_c = \frac{e\hbar B}{m^*} = \underbrace{\frac{1}{\pi}\frac{m^*}{m}}_{\sim g}\underbrace{\frac{e\hbar}{2m}}_{\mu_B\ (\text{Bohr-magneton})} B$

legkisebb körpálya $\to r_c = \sqrt{\frac{\hbar}{m\omega_c}}$

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

Hall-effect more precisely:

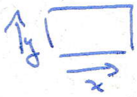
$$\begin{pmatrix} j_x \\ j_y \end{pmatrix} = \begin{pmatrix} \sigma_{xx} & -\sigma_{xy} \\ \sigma_{xy} & \sigma_{yy} \end{pmatrix}\begin{pmatrix} E_x \\ E_y \end{pmatrix}$$

Hall eff

$\xrightarrow{\text{inversion}}$ $\sigma \neq \frac{1}{\rho}$

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

if $\sigma_{xx} \gg \sigma_{xy}$; $\mu = \frac{e\tau}{m^*}$



$j_y = 0 \iff \sigma_{xy} \neq 0$

$\sigma_{xx} = \sigma_{yy}$ if isotropic

$$\rho_{xy} = \frac{\sigma_{xy}}{\sigma_{xy}^2+\sigma_{xx}^2} = \frac{B}{en}$$

$\rho_{xy} = R_H$

$\hookrightarrow$ measurements n, μ (that's why HE is important)

- $n = \dfrac{1}{e\left(\frac{\partial\rho_{xy}}{\partial B}\right)_{B=0}}$ $\leftarrow R_H = \dfrac{E_{trans}}{j_{long}}$

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

mágneses ellenállás

$\boxed{e\text{-}n\mu\tau}$

$B\odot$

$\underline{v} = \mu(\underbrace{\underline{E}}_{E_{stat}} + \underbrace{\underline{v}\times\underline{B}}_{E_{Lorentz}})$ $\Rightarrow R(B) = \dfrac{R(B=0)}{1+(\mu B)^2}$

Thermal effects in SCs

Boltzmann equation

B.E. : $(*)\ \dfrac{df}{dt} = \dfrac{\partial f}{\partial t} + \underbrace{\dot{k}\,\nabla_k f}_{\text{force}} + \underbrace{\dot{r}\,\nabla_r f}_{\text{diffusion}} = -\dfrac{g}{\tau}$

$f(k, r, t)$; $\hbar\dot{k} = F_{ext}$; diffusion (spacial grad of particle distribution × velocity)

- experiment shows $\nabla T \to$ current (Seebeck)

  $j \to j_Q$ (Peltier)

  heat current density

- how to introduce ∇T into $(*)$?

  $\to T(r)$

  $\mu(r)$ (chemical pot.)

  $f^0(k,r,t) = \dfrac{1}{e^{\frac{\varepsilon-\mu}{k_B T}}+1}$ e.g. $\varepsilon = \varepsilon(k)$, $\mu = \mu(r)$, $T(r)$

- we neglect diffusion
- let $x = \beta(\varepsilon-\mu)$; $\beta = \frac{1}{k_B T}$

$$\Rightarrow \frac{df}{dt} = \frac{\partial f}{\partial t} + \dot{k}\, \nabla_k f + \frac{\partial f}{\partial x} \cdot \frac{\partial x}{\partial T} \nabla T \cdot \dot{r} + \frac{\partial f}{\partial x} \cdot \frac{\partial x}{\partial \mu} \nabla \mu \cdot \dot{r}$$

- $\frac{\partial f}{\partial x} = \frac{\partial f}{\partial \varepsilon} \cdot \frac{\partial \varepsilon}{\partial x} = \frac{1}{\beta} \frac{\partial f}{\partial \varepsilon}$
- $\frac{\partial x}{\partial T} = \frac{\partial x}{\partial \beta} \cdot \frac{\partial \beta}{\partial T} = (\varepsilon - \mu) \cdot \beta \cdot \left(-\frac{1}{T}\right)$
- $\frac{\partial x}{\partial \mu} = -\beta$

$$\Rightarrow \frac{df}{dt} = \frac{\partial f}{\partial t} + \frac{\partial f}{\partial \varepsilon} \underset{\dot{r}(k)}{\underset{\uparrow}{v}}(k) \left[F_{ext} - \nabla \mu - (\varepsilon - \mu) \frac{\nabla T}{T} \right] \Rightarrow \nabla T \text{ induces current}$$

$eE + \nabla \mu \rightarrow$ thermal current

- $\nabla_k f = \frac{\partial f}{\partial \varepsilon} \cdot \underset{\hbar v}{\underset{\downarrow}{\frac{\partial \varepsilon}{\partial k}}} \quad \rightarrow \quad \dot{k} \cdot \nabla_k f = \underset{\hbar \dot{k}}{\underset{\uparrow}{F}} \cdot v \cdot \frac{\partial f}{\partial \varepsilon}$

· reminder:

$$\left.\frac{df}{dt}\right|_{stationary} = \frac{\partial f}{\partial \varepsilon} v(k) \, (-eE) = -\frac{g}{\tau} \rightarrow \boxed{f = f^0 + \underbrace{e E \tau v(k) \frac{\partial f}{\partial \varepsilon}}}$$

distribution fn is shifted (in DC voltage)

Particle current

$j_n = \int \underbrace{\frac{d^3k}{4\pi^3}}_{D(k)} v_k f(k)$ – particle current

$\underset{e^- \text{ current}}{j} = -e j_n$ – charge current

$j_E = \int \frac{d^3k}{4\pi^3} \varepsilon_k v_k f(k)$ – energy current

$j_Q \rightarrow T dS = dE - \mu dN$ – heat current

average energy of the system

normalisation for area

$T d j_Q = j_E - \mu j_n$

$$\boxed{j_Q = \int \frac{d^3k}{4\pi^3} v_k f(k) \frac{\varepsilon - \mu}{T}}$$

without derivation (phenomenological)

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

cross coefficients are equal

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

K_0, K_1, K_2 can be obtained from B.E.

Onsager - reciprocity relations
/4th law thermodynamics/

részleges egyensúly: egyensúlyban folyamat és inverze azonos valséggel megy végbe

eg. ~~ele~~ 1. heat cond:

$$\underline{j}_Q = -\kappa \underline{\nabla} T \quad \text{(Fourier-law)}$$

$$\underline{j} = \emptyset \rightarrow K_0 \left(E + \frac{\nabla\mu}{e}\right) = K_1 \frac{\nabla T}{T} \rightarrow \kappa = \frac{K_2}{T} - \frac{K_1^2}{K_0 T}$$

2. electric conductivity:

$$\underline{j}_Q = 0$$

$$\underline{j} \;\hookrightarrow\; -K_1\left(E + \frac{\nabla\mu}{e}\right) = K_2 \frac{\nabla T}{T} \rightarrow \frac{\nabla T}{T} = -\frac{K_1}{K_2}\left(E + \frac{\nabla\mu}{e}\right)$$

$$\hookrightarrow j = \sigma \left(E + \frac{\nabla\mu}{e}\right)$$

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

Wiedemann - Franz law:

$$\frac{\kappa}{\sigma} = L T$$

$\uparrow$ Lorentz - nb $\quad L = \frac{\pi^2}{3}\left(\frac{k_B}{e}\right)^2$

$$\boxed{\kappa = \frac{\sigma}{T} \frac{K_2}{K_0}}$$

3. Seebeck effect:

$$\left.\begin{matrix} E = \emptyset \\ \underline{\nabla} T \neq \emptyset \end{matrix}\right\} \rightarrow \underline{j} \neq \emptyset \qquad \text{short circuit}$$

$$\left.\begin{matrix} \underline{j} = \emptyset \\ \underline{\nabla} T \neq \emptyset \\ \underline{E} \neq \emptyset \end{matrix}\right\} \qquad \text{broken/open circuit}$$

means: definition

$$\left(\underline{E} + \frac{\underline{\nabla}\mu}{e}\right) \triangleq S \underline{\nabla} T \rightarrow S := -\frac{1}{T} \frac{K_1}{K_0}$$

Seebeck

4. Peltier:

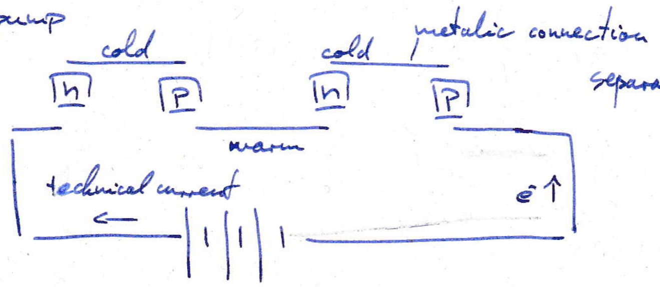
$$\begin{matrix} \underline{j} \neq \emptyset \\ \underline{j}_Q \neq \emptyset \end{matrix} \qquad \underline{j}_Q \triangleq \Pi \underline{j} \rightarrow \Pi := -\frac{K_1}{K_0}$$

Peltier

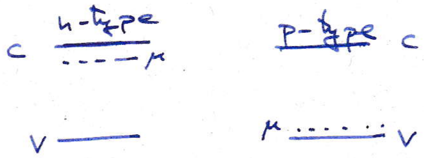
5. Kelvin relation: $\Pi = S \cdot T$ special case of Onsager relations

Thermoelectric (Peltier) device

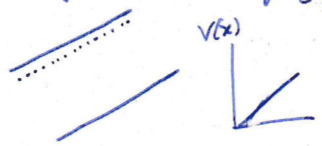
heatpump

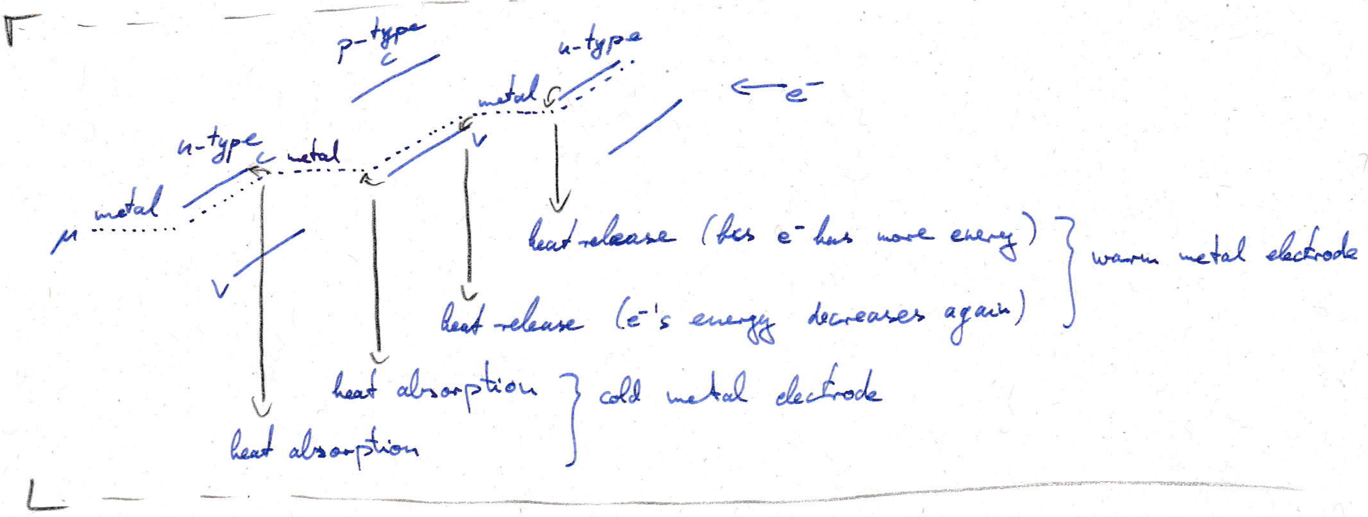


separated series of n and p SCs



with voltage / under voltage:
↳ occures mostly on SCs





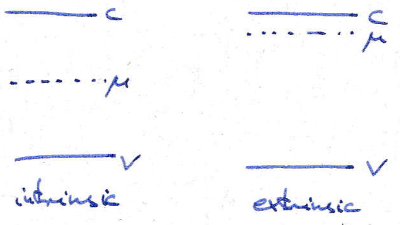
- A single n junction would act as a TE device (thermoelectric)
- Best operation: n p in series and heat conduction in parallel
- an n - n - n ... would not be a thermoelectric device (Σ heat absorption $= \Sigma$ heat release)

Diffusion-effects in SCs

intrinsic SC:

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

mass action law : $\boxed{n \cdot p = n_i^2(T)}$ valid also for extrinsic SCs



=> doped SC : majority | minority | charge carriers

↳ n-type $\quad p \ll n \approx n_d$

↑ high T enough to ionise all the ~~doping~~ dopants ↓

p-type $\quad n \ll p \approx n_a$

Non-equilibrium charge concentrations

- charge carriers can be injected, excited, pumped, etc.
- equilibrium: n_0, p_0 ; $n_0 \cdot p_0 = n_i^2(T)$
- non-equilibrium: n, p (e.g. light excitation, charge pumping, thermal excitation)
- recombination rate: $R \sim p \cdot n$
- thermal/any/excitation rate: $G_{thermal} = C \cdot n_0 p_0 = R^0$ continuous generation and annihilation / recomb.

$\uparrow$ equilibrium recomb. rate

↳ $R = C \cdot n \cdot p$

in non-equilibrium : $\overset{\text{net recombination rate}}{U} = R - G_{therm} = C(n \cdot p - n_0 \cdot p_0)$

↳ recombination rate is defined by the minority charge carriers – bottle-necks the recombination rate

$$U = C\left[\underbrace{(n-n_0)(p-p_0)}_{np + n_0p_0 - n_0 p - n p_0} + n_0(p-p_0) + p_0(n-n_0)\right] = C\left[np + n_0p_0 - n_0p - p_0 n + n_0 p - n_0 p_0 + p_0 n - p_0 n_0\right]$$

$(n-n_0)(p-p_0)$ is neglected (2nd order)

$$\Rightarrow \boxed{U \approx C\left[n_0(p-p_0) + p_0(n-n_0)\right]}$$

n-type $\quad p_0 \ll n_0 \approx n_d \quad \rightarrow \quad U \approx C \cdot n_0 (p - p_0)$

p-type $\quad n_0 \ll p_0 \approx n_a \quad\quad U \approx C \cdot p_0 (n - n_0)$

} => recombination is given by minority charge carriers

· charge carrier life time : $\tau_n, \tau_p \gg \tau$
$\sim 1\mu s - 1ms$ — momentum life time / momentum scattering time $\sim 10^{-15} - 10^{-13}$ s

Equations of continuity

divergence — denotes technical current

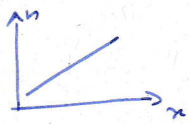
Sólyom

$$\left.\begin{aligned} \frac{\partial n}{\partial t} - \frac{1}{e}\nabla j_n &= -\frac{p-p_0}{\tau_p} \\ \frac{\partial p}{\partial t} + \frac{1}{e}\nabla j_p &= -\frac{p-p_0}{\tau_p} \end{aligned}\right\} n\text{-type}$$

$$\left.\begin{aligned} \frac{\partial p}{\partial t} + \frac{1}{e}\nabla j_p &= -\frac{n-n_0}{\tau_n} \\ \frac{\partial n}{\partial t} - \frac{1}{e}\nabla j_n &= -\frac{n-n_0}{\tau_n} \end{aligned}\right\} p\text{-type}$$

$p > p_0$ -> negative (n) charge decreases
recombination acts to increase n

Spatial inhomogeneity



· $\boxed{j_n = -D\nabla n}$ Diffusion current
particle current; diffusion const.

· $j = nev_D = ne\mu E$ Drift current (eg. external field $\mathcal{E}$)
electric current; mobility

$\hookrightarrow \boxed{j = -ne\mu\nabla V}$ voltage

equilibrium / stationary situation

· $j_{Drift} + j_{Diff} = \emptyset$
! $-e\,j_n$ } electric current

$-ne\mu\nabla V + eD\nabla n = 0$

· $n(r)$ trough the distribution fn : $n \sim f = \frac{1}{e^{\frac{\varepsilon-\mu}{k_BT}}+1}$; $f(V(r)) = \frac{1}{e^{\frac{\varepsilon - eV(r) - \mu}{k_BT}}+1} \approx e^{-\frac{\varepsilon - eV - \mu}{k_BT}}$, $T \gg \emptyset$

$\hookrightarrow \nabla n = n(r)\frac{e}{k_BT}\cdot\nabla V$

$\hookrightarrow ne\mu\nabla V = \frac{e^2D}{k_BT}n\nabla V \Rightarrow \boxed{\mu = \frac{e}{k_BT}D}$ Einstein-relation

mobility, diffusion <- not intuitive that they are related

(special case of fluctuation-dissipation theorem)

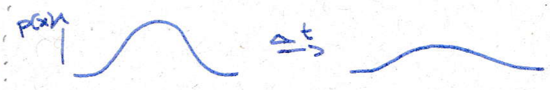
diffúzió -> inhomogén töltéseloszlás

charge inhomogeneity

/ koncentráció csak egy irányban változik

n-type $\frac{1}{e}\nabla j_p = -\frac{p-p_0}{\tau_p}$

$j_p^{diff} = -D_p \nabla p$



↳ $\boxed{1D}$ $x=0$-ban töltéseket injektálunk

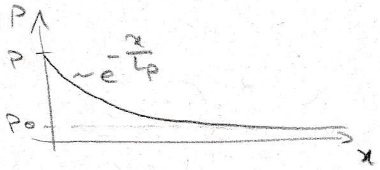
$$\frac{\partial^2 p}{\partial x^2} = \frac{p-p_0}{D\cdot\tau_p}$$

$$\boxed{p(x) = p_0 + \left[p(x=\phi)-p_0\right] e^{-\frac{x}{L_p}}}$$

$\boxed{L_p = \sqrt{D\tau_p}} = v\sqrt{\tau\tau_p}$ (mean free path)

$D = v\,l = v^2\tau$

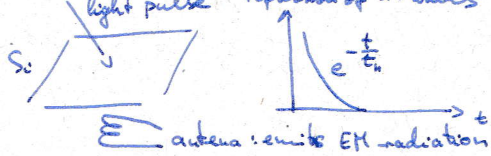
charge diffusion / recombination length /diffúziós hossz/



solar cell: if charges recombine within the material → no net current

measuring τ_n, τ_p

light pulse — reflection of EM waves

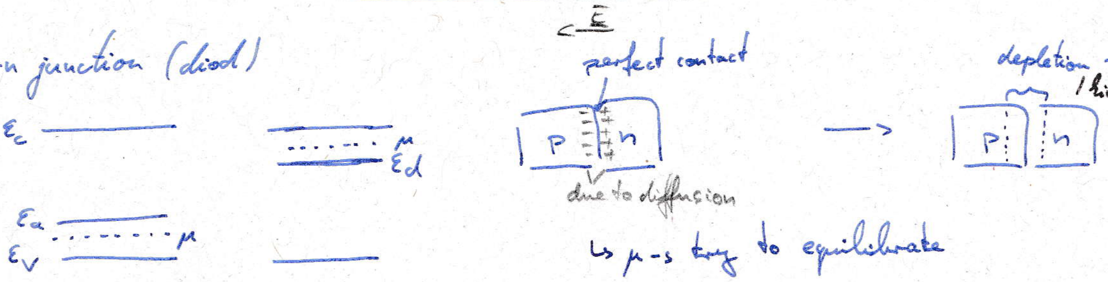


antenna: emits EM radiation

τ_n is limited by · impurities · doping

Semiconductor devices

· p-n junction (diod)



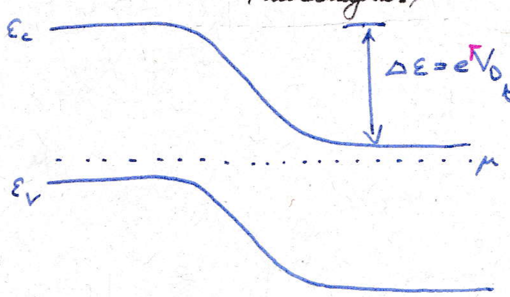
perfect contact

due to diffusion

depletion region: no free charge carrier /kiürített réteg/

↳ μ-s try to equilibrate

↓ band-bending /sávelhajlás/



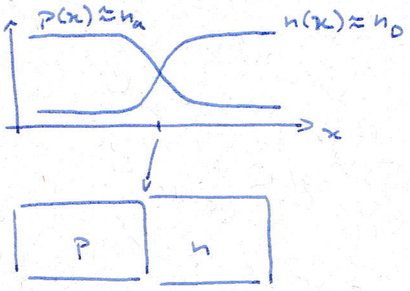
$\Delta\varepsilon = eV_D$ ← diffusion potential / contact pot.

Driving force of diffusion

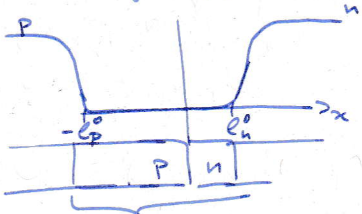
$j_{drift} + j_{diff} = \phi$

$env_D E + eD\nabla n = \phi$

built-in E field



Schottky - approximation



depletion layer

$l \sim$ few 10nm
(unrelated to L_n, L_p)

$E \sim 10^4 - 10^6 \frac{V}{cm}$ < gate voltag (→ $\sim 10^8 \frac{V}{cm}$)

charge neutrality
$p \cdot l_p^0 = n l_n^0$

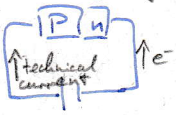
$p \approx n_a, n \approx n_d$
⇒ $n_d \cdot l_n^0 = n_a l_p^0$

heavily doped material → small depletion layer
lightly doped → large depletion layer

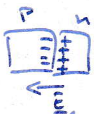
pn junction + bias

majority charge carr. (+) →
← majority charge carr. (-)
} ⇒ recombination / annihilation → light emission

forward bias
/nyitó irány

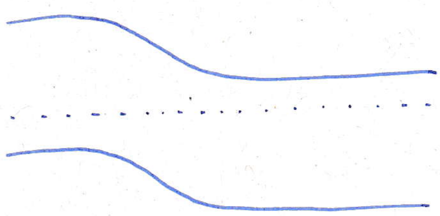


reversed bias
/záró irány

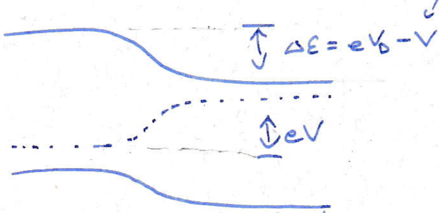


depletion layer grows : $E_{built\,in} \uparrow\uparrow E_{ext}$

we can tune the device by changing the bias voltage



$V > \phi$
forward



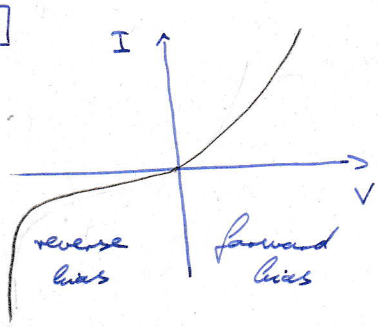
schottky equation / diode equation:

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

↑ reverse current

9

p n

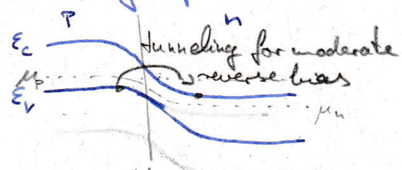


/lavina letörés/
avalanche breakdown

- destroys
- weakly doped
- minority charg. carr. accelerated
→ additional charg. carr.

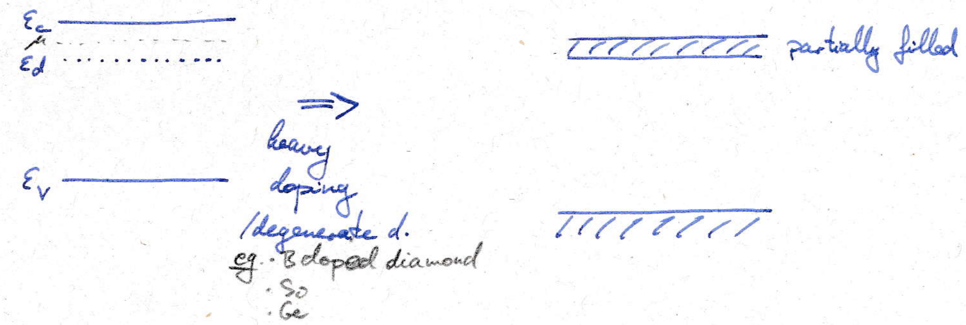
Zener - effect

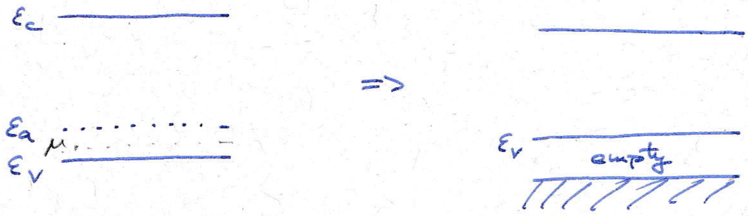
- doesn't destroy
- heavily doped



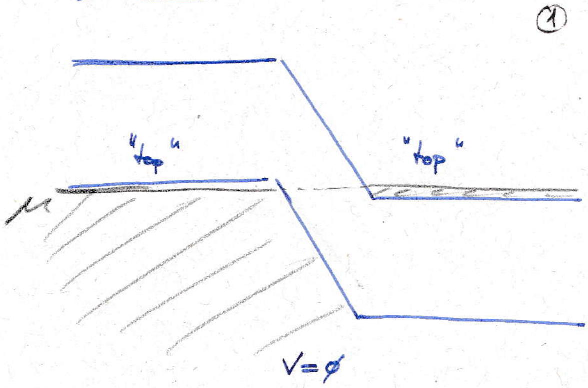
thin depletion layer

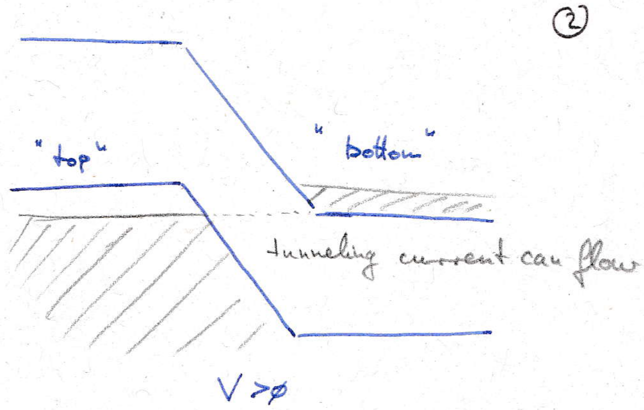
Tunnel-diode / Esaki diode

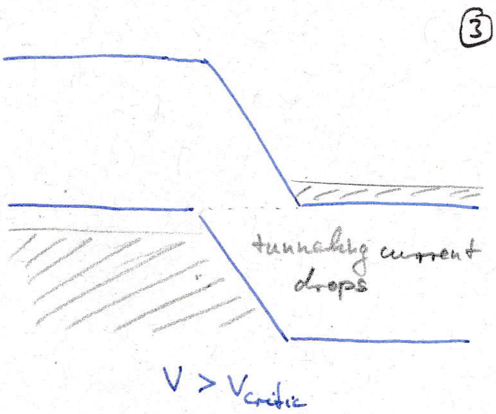


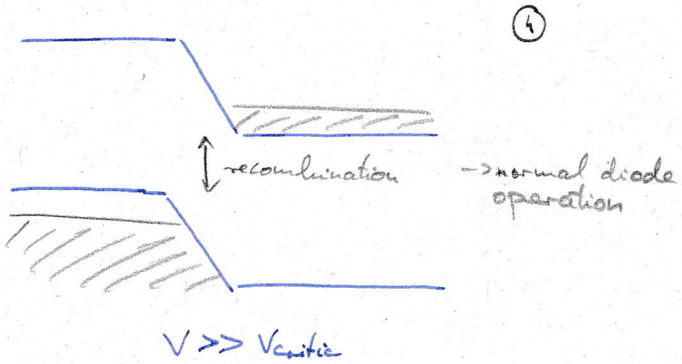


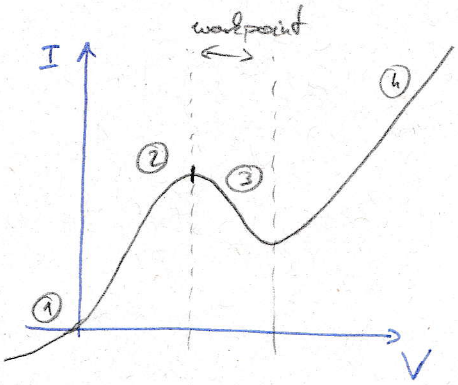
$\boxed{p^{++}}\boxed{n^{++}}$



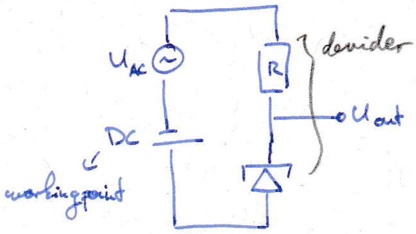






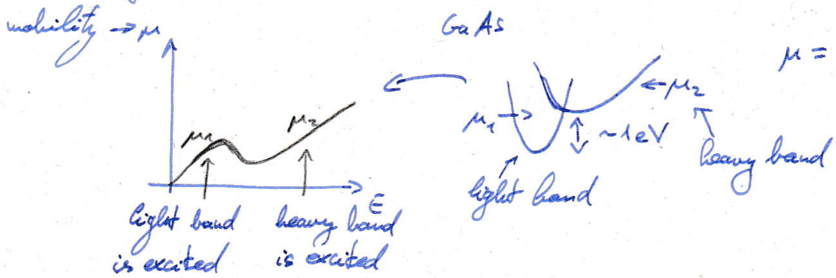


negative differential resistance : $\left.\frac{dI}{dV}\right|_{\text{workpoint}} = -\frac{1}{r}$



$U_{out} = U_{AC} \cdot \frac{-r}{R-r} = U_{AC} \frac{r}{r-R} > U_{AC}$ if $R < r$ analogue amplifier (or oscillator)

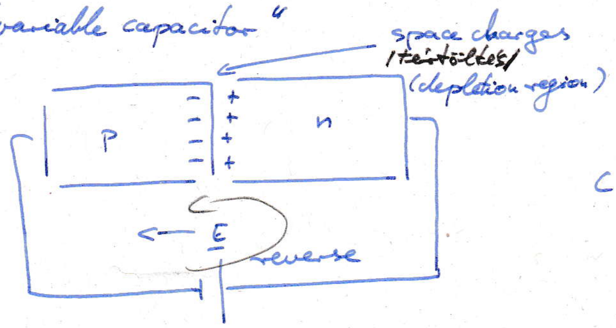
<u>Gunn diode</u> or ; $-\boxed{n^{++}}\boxed{n}\boxed{n^{+}}-$



$\mu = \frac{e\tau}{m^*}$ → different m^* : $m_1^* < m_2^*$

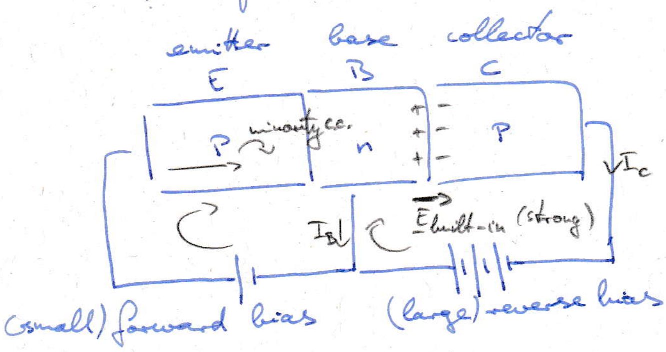
<u>Varactor-diode</u>

"variable capacitor"



$C \sim \frac{1}{\sqrt{V_{reverse}}}$

<u>Bipolar junction transistor</u> (BJT) $\neq \boxed{pn} + \boxed{np}$



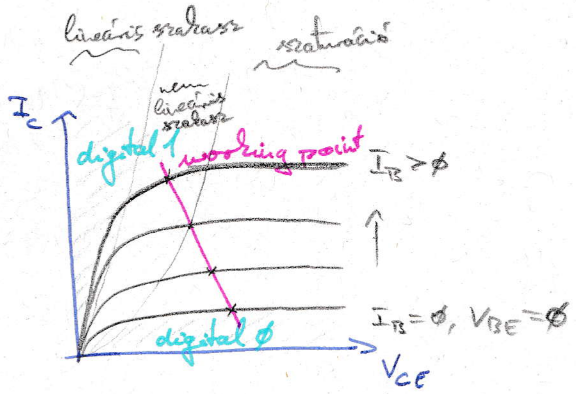
$\boxed{n}$
Base < L
charge diffusion length

V_{BC} → sweeps through minority cc. from base to coll

I_c depends on the charge injected on the left-hand side : $V_{BE} \sim I_B$ ⇒ I_c is controlled by I_B

$\frac{I_c}{I_B} = \beta \approx 10 \ldots 100$ <u>current amplification factor</u>

$I_c = I_E - I_B$ - recombined

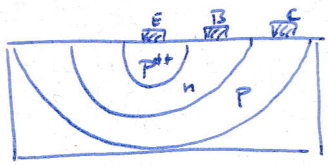


$V_{BC} \nearrow$ charge carriers depend on V_{BE}
=> saturation

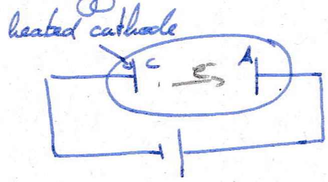
- transistor logic TTL
- analog amplifier : $I_C \sim I_B$

. BJT: minority carrier device

. technical realisation:

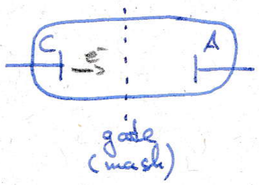


. analogy: electron tube (1904.)



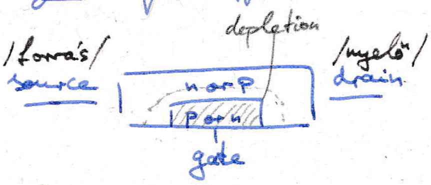
first diode: in reverse bias there is no current

. triode (1906.)



anode current is controlled by V_{CG} (chatode-gate voltage)
high impedance controll device, $I_G = \phi$

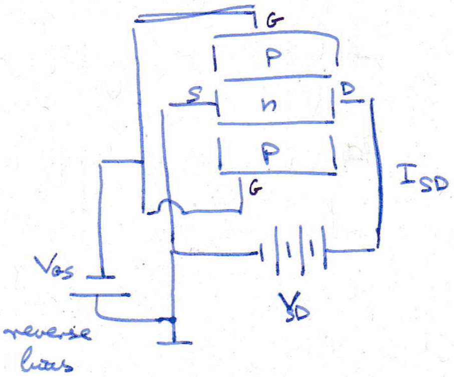
10 Junction field effect transistor



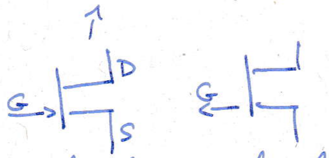
gate-source : forward -> I_{SD} large
reverse -> I_{SD} small

I_{SD} controlled by V_{GS}

$I_G = \phi$ -> large impedance control (eg. input to oscilloscope)



JFET	BJT
- large control imp. $I_G = \phi$	- finit control imp. I_B finite
- good for digital switching	- better for analoge application

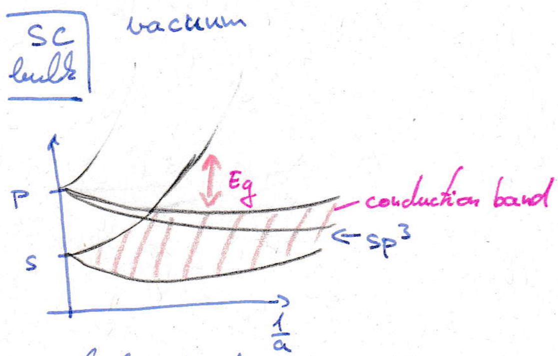


n-channel p-channel

Schottky - barrier, surface states

$\boxed{10}$

„lógó kötés"

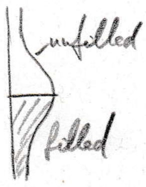


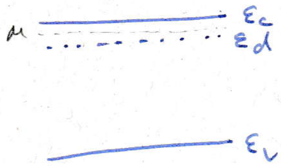
s-p hybridisation

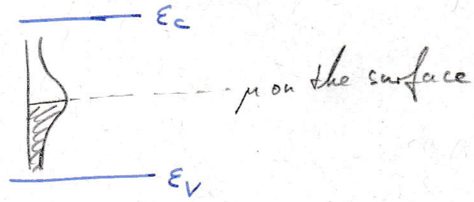
surface sp³ states with dangling bonds

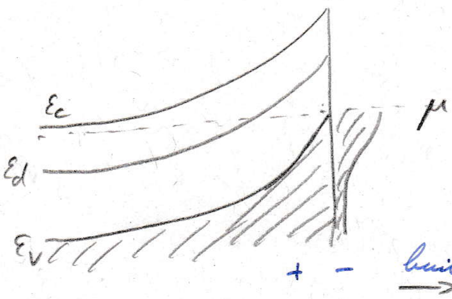
↳ midgap states

atom szerű állapot









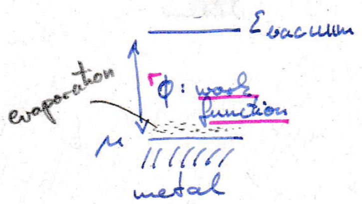
band-bending (sávelhajlás)

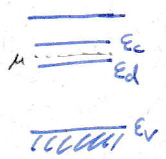
ionized donors near the surface

↳ surface charge

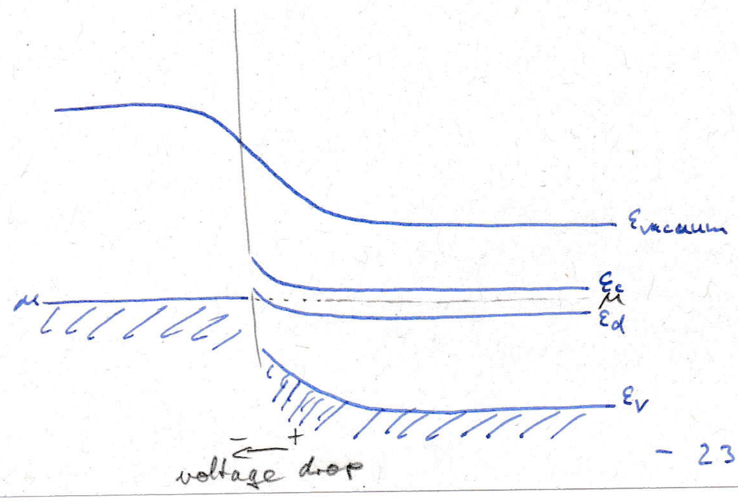
built-in electric field

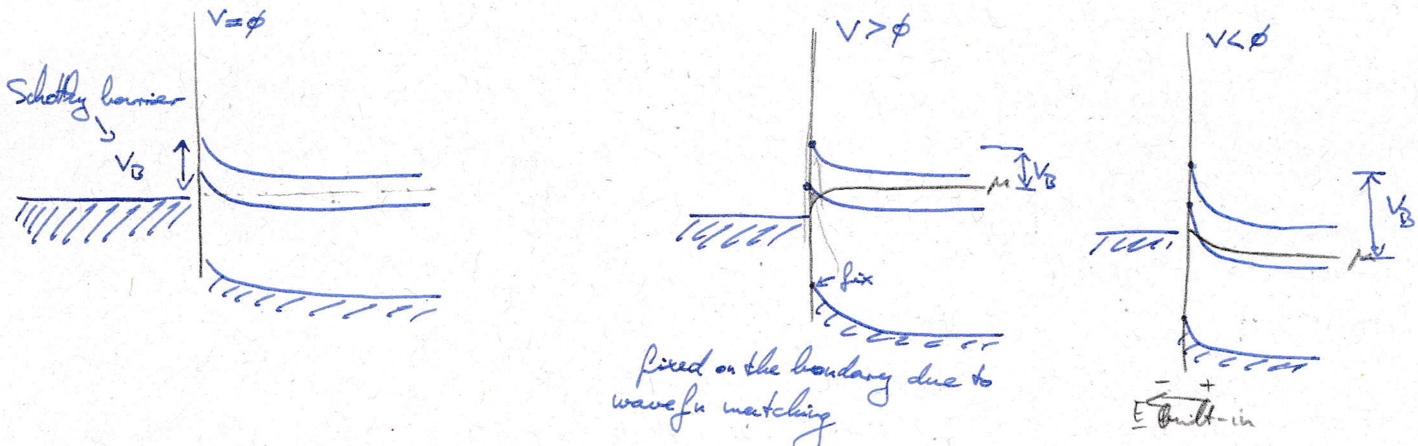
Metal - SC junction





junction





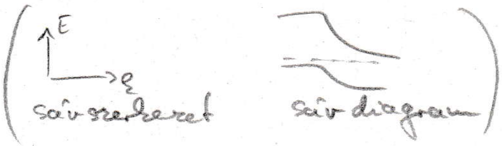
V_B is smaller

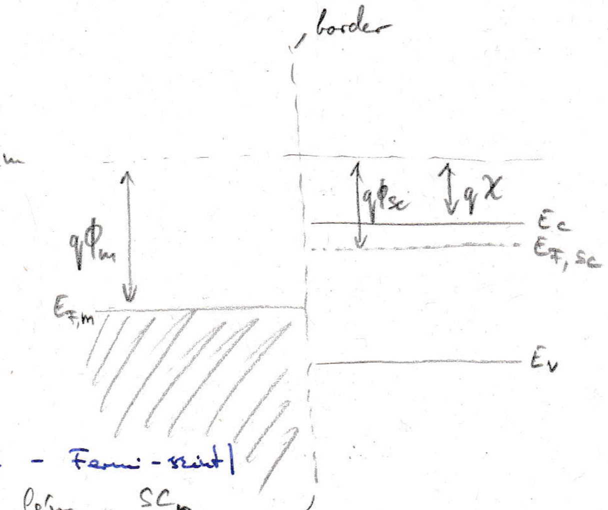
V_B is larger

Devices - part 2

Volk János
volk@mfa.kfki.hu

Metal - SC contacts





Metal - n-type SC $\boxed{\phi_M > \phi_{sc}}$

$q\phi_M$ ← pozitív irány

ϕ_m : potenciál -> $q\phi_m$ kilépési munka : |vákuum-szint - Fermi-szint|

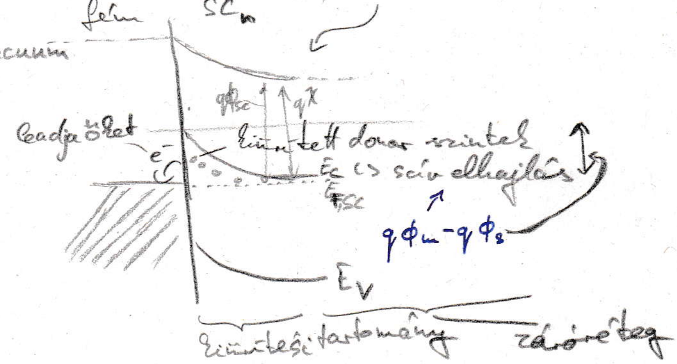
χ : elektron affinitás : |vákuum-szint - E_c|

$q\phi_{sc}$: sc kilépési munkája

kontakt potenciál: $\phi_M - \phi_{sc}$

schottky-gát: $q\phi_m - q\chi$

idealizált : aminél kevesebb nem lehet



Metal - p-type SC $\boxed{\phi_M < \phi_{sc}}$

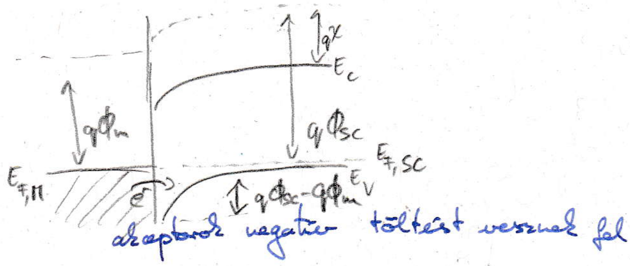
$q\phi_{sc} > q\phi_m$

χ : anyagra jellemző

Fermi-szint függ az adalékolás mértékétől

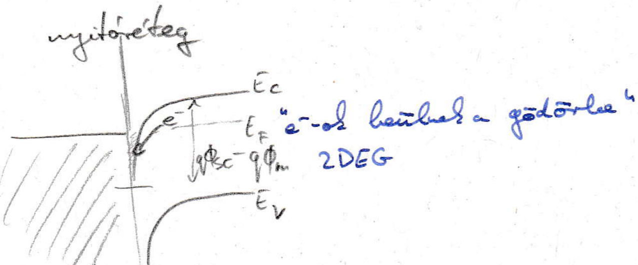
Schottky gát:

$q\phi_{Bp0} = E_G - q(\phi_M - \chi)$



Metal - n-type SC $\boxed{\phi_M < \phi_{sc}}$

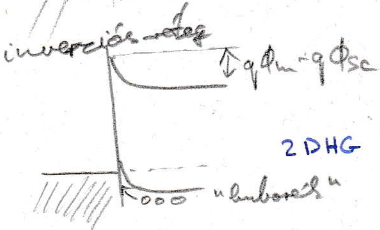
ohmikus kontaktus



Metal - p-type SC $\boxed{\phi_M > \phi_{sc}}$

valóságban ritka : nehéz megfelelően nagy kilépési munkával rendelkező fémet találni (max. ~5.7 eV, Pt)

ohmikus kontaktus



Realisztikus Schottky

- felületi csapda helyek (D_{it}) -> töltéseket megfogják => sáv nem tud hajlani => Fermi level pinning
  - -> kovalens félvezetőknél (GaAs, Si)
  - -> van fém induced változata is
  - -> Schottky - Mott limit

$D_{it} \to \infty$; $\phi_{barr} = E_G - \phi_0$

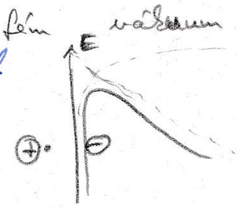
$D_{it} \to 0$; $\phi_{barr} = \phi_m - \chi$

in between

Metal - n-type + bias

záró irány ↓ ↑ nyitó irány   p-type-nál fordítva

Schottky gát csökkenés
- magyarázat tükörtöltéssel a fém oldalon

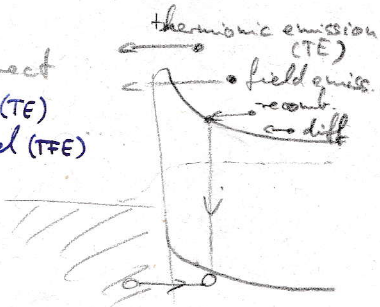


Current transport on Schottky contact   numbering on the slide isn't correct

$N_d < 10^{17}\frac{1}{cm^3}$ -> széles kiürítési tart. (TE)

$10^{17}\frac{1}{cm^3} N_d < 10^{18}\frac{1}{cm^3}$ -> alagutazás gerjesztéssel (TFE)

$10^{18}\frac{1}{cm^3} N_d$ -> alagutazás (FE)



Thermionic emission regime
- start from Poisson Δ equation

$\hookrightarrow$ $J_{te} = J_{te0}\left(e^{\frac{qV}{\eta kT}} - 1\right)$

ideality factor, good if ≈ 1 ← tisztán thermionic

$\eta > 1$: TFE

telítési áram

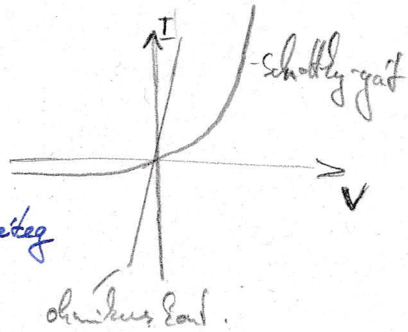
Ohmic contact : fém-SC kontaktus kis ellenállással

source, drain

↑ small resistence

new device : start with the optimisation of the ohmic contact

megvalósítás : Schottky-gát minimalizálása / erősen adagolt átmeneti réteg



Transmission Line Method (TLM)

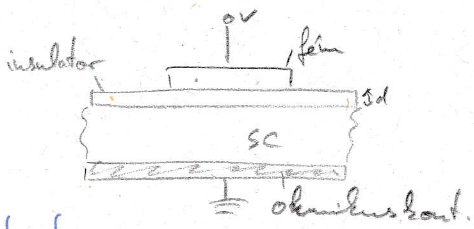
lower layer thickness -> lower slope

Metal - Insulator - SC (MIS) capacitor

insulator may contain charge

inversion : minority charge carriers' accumulation in the contact

Ψ_p determines the bending

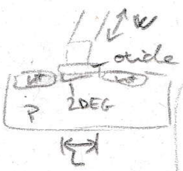


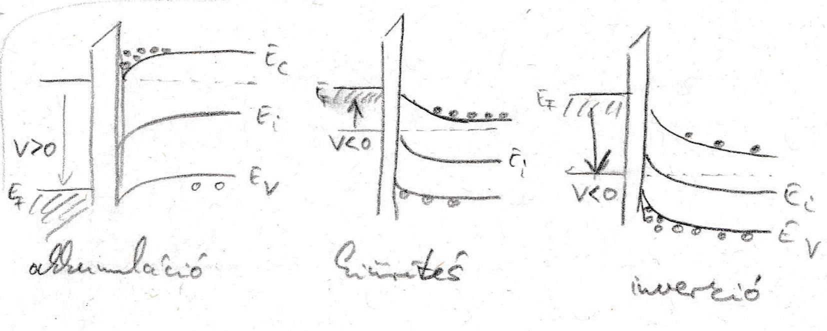
- fém - SC : azonos nagyságú töltés (ellentétes előjel)
- szigetelőn keresztül nem folyik áram

charges have to be equal in the two sides of the contact

L: channel length

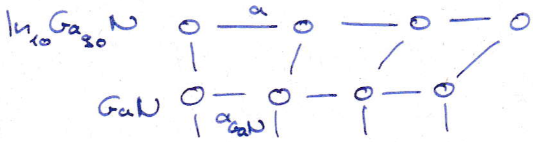
W: width of the device





FIN-FET

absorption limit: $\lambda[nm] = \frac{1240}{E_g[eV]}$ -> below this energy transparent
$> \lambda$
-> $< \lambda$ absorbing



lattice missmatch <- should not be light

2018. XI. 27. 13. hét

polar SCs -> piezo

MBE: molecular beam epitaxy

crystal polarity: images show the ideal case but the surface isn't always like that => that's why it's better to describe it by the polarity

stress: F $\xrightarrow{\text{induces}}$ ΔP_0
polarization

strain / deformáció

pulling -> $+\Delta P_0$
pushing -> $-\Delta P_0$

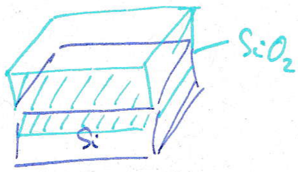
- closed pack crystal structure
  $u_c = u_{hcp}$

- on top of GaN layer we want to grow an $Al_x Ga_{1-x} N$ layer
  ↳ strain bcs of lattice mismatch -> ΔP_{pz} (piezo effect)
  in addition to P_{sp}
  spontaneous pol.

$In_y Ga_{1-y} N$
↓
$\boxed{GaN}$ -> compression

- P_{sp} and P_E can be adjusted / changed by changing the alloy rate
- field is built-in the material
  -> tilt of the CB
- QW is in the GaN's side
  ↑ higher charge
  higher density
- sheet resistance: $R_{SH} = \frac{\Omega}{\square}$ <- with 4 point ~~resistivity~~ measurement

- on the surface of Si native oxide -> annealing
- oxide growing on Si
  - wet : thicker
  - dry : purer



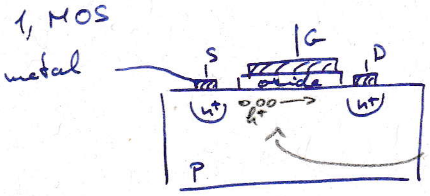
- ALD (deposition technique) : follows the shape of the surface
- usually physical & chemical etching at the same time

2018.
XII. 4.
14. hét

CMOS

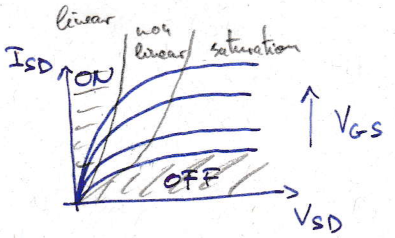
complementary MOS
 ↳ metal-oxide-SC

1, MOS



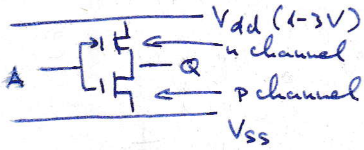
n-channel MOS

- $V_{GS} > \emptyset$ -> conductivity in the channel $I_{SD} > \emptyset$
- $V_{GS} < \emptyset$ -> $I_{SD} = \emptyset$



finite current flows
typically: I_{SD} = few mA
small MOS: few μA -> if we have millions of it on a device it gets important ($10^6 \dots 10^9$)

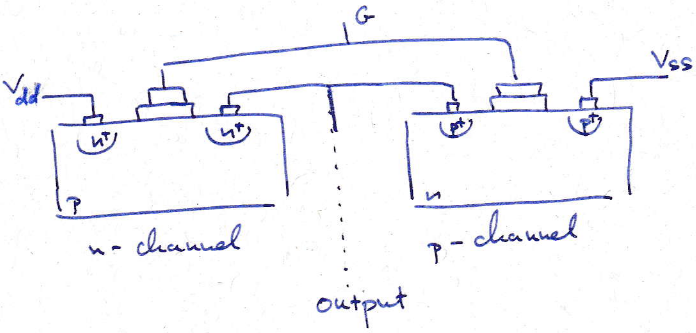
if MOSs are in serie → ON-OFF-ON-OFF-... current never flows



(typically $\emptyset$, GND)

} NOT gate

2, CMOS



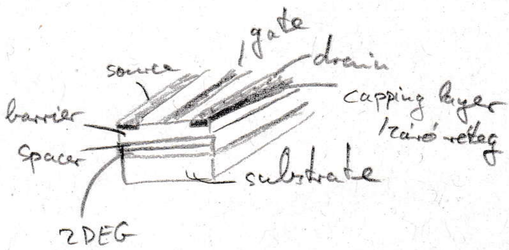
↳ always made in pairs

- $V_G > \emptyset$ => n-channel MOS conducts
  p-channel MOS is closed
  output = V_{dd}
- V_G small => n-channel is closed
  ($V_G < \emptyset$) here p-channel is open
  (there is a type of MOS that conducts at $V_G \approx 0$ too.)
  output = V_{ss}

No net current flows between V_{dd} and V_{ss}
↳ except for a small switching current.

HEMT: high-electron-mobility-transistor

- high frequency → cell phone, radar
- high gain -> amplifier
- high switching speed
- low noise
- SC heterojunction (wide bandgap element doped with donors -> injection to narrow band elem



Optical properties of SCs

Drude-modell

direct current

DC: $m^*\dot{v} = -eE - \frac{m v}{\tau} \longrightarrow \sigma_{DC} = \frac{n e^2 \tau}{m^*}$ — $\varepsilon_0 \cdot \omega^2_{plasma}$ (see below)

alternating current

AC: $m\dot{v} = -eE(t) - \frac{m v(t)}{\tau} \rightarrow \sigma(\omega) = \sigma_1(\omega) + i\sigma_2(\omega)$ with $\sigma_1(\omega) = \frac{\sigma_{DC}}{1+\omega^2\tau^2}$

$\sigma_2(\omega) = \frac{\sigma_{DC} \cdot \omega\tau}{1+\omega^2\tau^2}$

dispersive Lorentzian fn

$E = E_0 e^{i\omega t}$

Ansatz: $v(t) = v_0 e^{i\omega t}$

$-i\omega m^* v(t) = -eE(t) - \frac{m^* v(t)}{\tau}$

$j(t) = ne\,v(t) = \sigma E(t)$

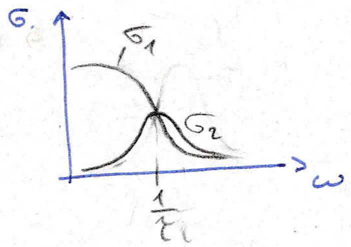
$$\sigma(\omega) = \frac{ne^2\tau}{m} \underbrace{\frac{1}{1-i\omega\tau}}_{\frac{1}{1+\omega^2\tau^2} + \frac{i\omega\tau}{1+\omega^2\tau^2}}$$

Hilbert transformation

$\sigma_1 \Leftrightarrow \mathcal{H}(\sigma_2)$

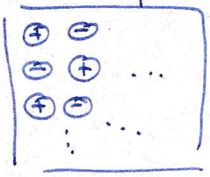
$\sigma_1(\omega) = -\frac{1}{\pi} \mathbb{P} \int \frac{\sigma_2(\omega)}{\omega - \omega'} d\omega'$ Kramers-Kronig relation

$\sigma_2(\omega) = \frac{1}{\pi} \mathbb{P} \int \frac{\sigma_1(\omega)}{\omega - \omega'} d\omega'$



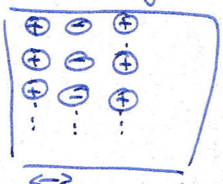
Plasma oscillation

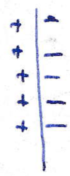
neutral plasma



assume → non-equilibr. situation

double layers





Gaussian theorem

$\oint E\,dA = \frac{Q}{\varepsilon_0}$

$E = \frac{Q}{A\varepsilon_0}$ volume density of particles

$Q = \rho V = e n_e A x$

volume charge density

$\Downarrow$

restoring forces

$F = -eE = -\frac{e^2 n_e x}{\varepsilon_0}$

$\Rightarrow E = \frac{e n_e x}{\varepsilon_0}$

$m\ddot{x} = -\frac{e^2 n_e x}{\varepsilon_0}$ harmonic oscillator

eigen oscillation $\rightarrow$ $\boxed{\omega^2_{plasma} = \frac{n_e e^2}{m\varepsilon_0}}$ $\frac{1}{\cancel{s^2}} \cdot \frac{A^2 s^2}{VAs} \cdot \frac{\cancel{s^2}}{s^2} \cdot \frac{Vs}{As} = \frac{1}{s^2}$ ✓

(angular-) plasma frequency

↳ tends back to the equilibrium with this oscillation

$\hookrightarrow \sigma_{DC} = \varepsilon_0 \omega_{plasma}^2 \tau$

$\sigma_{AC} = \sigma_{DC} \dots \qquad \sigma_{AC} = \frac{\varepsilon_0 \omega_p^2 \tau}{1+\omega^2\tau^2} + i \frac{\varepsilon_0 \omega_p^2 \omega \tau^2}{1+\omega^2\tau^2}$

typical energies: $\tau = 10^{-13} \dots 10^{-15}\,s$

$\frac{1}{\tau} = 10 - 1000\,THz$

visible light: $100\,THz$

$\omega_{plasma} \sim m \Rightarrow \omega_{plasma} \simeq 10\,eV$ for a good metal (eg. Au)

$\hookrightarrow$ UV range

$\omega_{plasma}^{SC} < 1\,eV$

$\hookrightarrow$ IR range

Optical reflectivity

Fresnel-formula

n_1 | n_2 - refraction index

normal incidence

/merőleges beesés/

$$R = \left|\frac{n_1 - n_2}{n_1 + n_2}\right|^2 = r^2, \quad \Gamma = \frac{z_e - z_0}{z_e + z_0}$$

R: reflected energy/power; z_e: load impedance; z_0: wave impedance

impedence matching

$N(\omega) = n(\omega) + i\kappa(\omega)$

complex index of refraction; extiction coeff. /extinkciós koefficiens/

$$\hookrightarrow R = \frac{(n-1)^2 + \kappa^2}{(n+1)^2 + \kappa^2} \quad \text{with } \begin{array}{l} n_1 = 1 \\ n_2 = N(\omega) \end{array} \text{ from vacuum into material}$$

Maxwell-equation

$$\nabla \times H = j + \frac{\partial D}{\partial t} = \sigma E + \varepsilon_0 \frac{\partial E}{\partial t} \Rightarrow \nabla \times H = \sigma E - i\omega \varepsilon_0 E_0$$

j: free current; $\frac{\partial D}{\partial t}$: displacement current /eltolási áram/

with $E = E_0 e^{i\omega t}$ convention

we want to plug the free current term into the displacement term

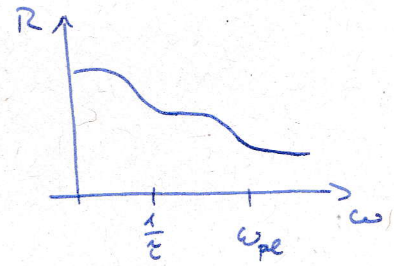
$$\hookrightarrow \nabla \times H = \varepsilon_0 \frac{\partial E}{\partial t}\Big(1 + \underbrace{\frac{\sigma}{-\varepsilon_0 i\omega}}_{\text{free current term}}\Big) = \varepsilon_0 \frac{\partial E}{\partial t}\underbrace{\Big(1 + \frac{i\sigma}{\varepsilon_0\omega}\Big)}_{\frac{A}{V\cdot m}\cdot\frac{Vs}{A s}\cdot s = 1}$$

ε_0: permittivity of vacuum /dielectric const.

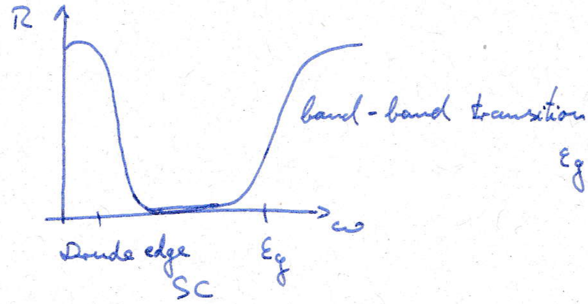
$$\Rightarrow \varepsilon_r(\omega) = 1 + \frac{i\sigma}{\varepsilon_0\omega} \text{ rel. permittivity}$$

back to the Fresnel formula:

$$r = 1 - \frac{\omega_{pl}^2}{\omega^2 + \frac{i\omega}{\tau}}$$ depends on both ω_{pl} and $\frac{1}{\tau}$ independent of each other



metal

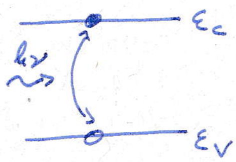


SC

$\varepsilon_g = 0.8 - 3\,eV$

$\omega_{pl}^{SC} \ll \omega_{pl}^{metal}$ bcs n is small

Photoconductivity



$\Delta n = \Delta p \sim I_{light}$

change in the nb of e^-

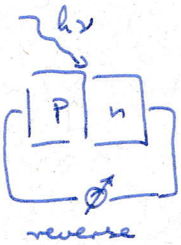
$\sigma = n e \mu_e + p e \mu_h$

$\Delta\sigma = \sigma_0 \left(\frac{1 + \frac{\mu_e}{\mu_h}}{n_0 \frac{\mu_e}{\mu_h} + p_0} \right)$ large for intrinsic SC (bcs less charge carriers)

↳ n_0, p_0 exponentially dependent on T

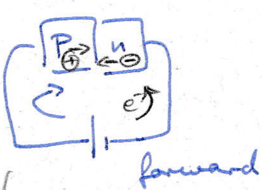
⇒ keep it at const. T

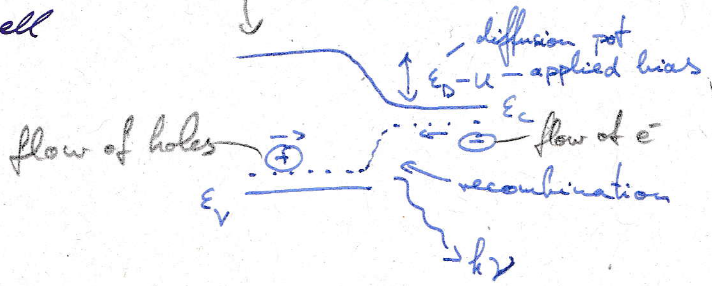
Solar cells and diodes (LEDs)



solar cell

LED

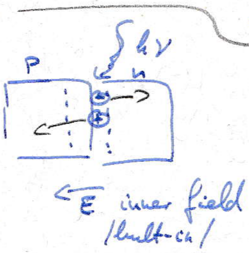




↳ μ shifted up

other representation:
e^- flow → energy drops (right to left)
↳ plus energy have to be somewhere

radiative recombination



the built-in field separates ⊕ and ⊖ charges

↳ ⊕ is protected in p
⊖ is protected in n
bcs majority charge carrier

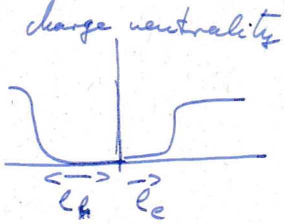
with of depletion layer : l

diffusion length : L ← $L \approx v_F \sqrt{\tau \tau_c}$ ≈ 1 mm – 1 cm

scattering time ≈ $10^{-15} - 10^{-13}$ s

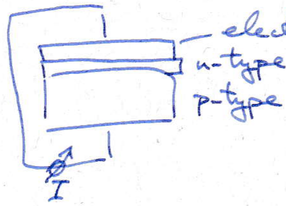
charge carrier lifetime μs – 1 ms

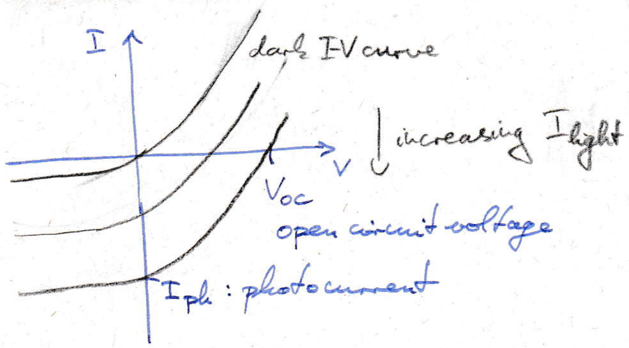
for ℓ: Schottky approximation
↳ small if N_A, N_D large (high doping)



solar cell	LED
$\ell \ll L$	$\ell \gg L$
↳ charge carriers can leave the depletion layer	↳ chance for recombination
↳ heavy doping	↳ low doping

Solar cell



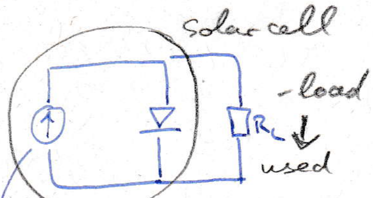


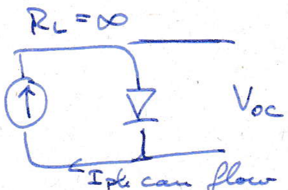
$$I = I_s\left[e^{\frac{eV_{oc}}{k_BT}} - 1\right] - I_{ph} = \emptyset \quad \text{for short circuit}$$

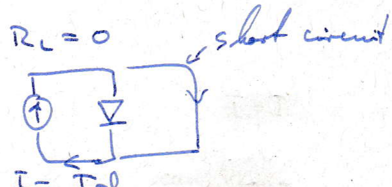
infinite load = open circuit

$$V = V_{oc} \to V_{oc} = \frac{k_BT}{e}\ln\left[\frac{I_{ph}}{I_s}+1\right] \approx \frac{k_BT}{e}\ln\frac{I_{ph}}{I_s}$$

↳ equivalent circuit modell

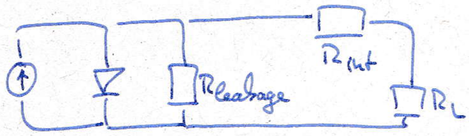






ideal current generator
(if $\cancel{I} \Rightarrow I_{ph}$ couldn't flow)
↳ always generate the same current, only depends on light intensity

Realistic equivalent circuit



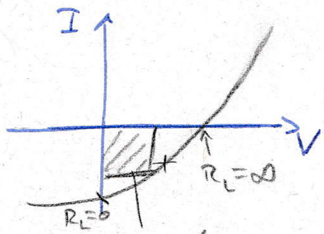
leakage :  current on the surface

Optimal working point <- maximális teljesítmény
(reality: complicated electronics)

inverter

I_{ph} depends on light
V_{oc} ~const.
} $\xrightarrow{\text{DC + inverter}}$ AC

Voltage ~230V <- should appear even with low light intensity
I_{AC}



$R_L = \frac{U}{I}$

optimal function: $U \cdot I = P$ (power) $= P_{max}$

largest area -> gives R_L
teljesítmény