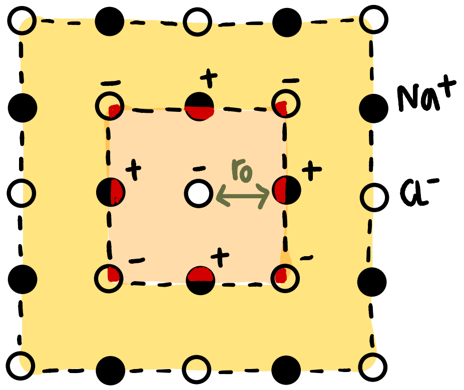
Kristali: → 10^{22-23} gradnikov / cm^3
- ionski
- molekulski
- kovalentni

(1) Kristal Na^+Cl^- (ionski)



Ionizacijska en. = da $Na \to Na^+ + e^-$ (dodana)
$W_i = 1.5\,eV$

Ionizacijska afiniteta = $Cl + e^- \to Cl^-$ (sproščena)
$W_a = 1.1\,eV$

Vezavna en: $2N \cdot W_0 = 2N \cdot 5\,eV$

$$V_{ci} = \frac{e_0 \cdot d_{Mi}}{4\pi\varepsilon_0 \cdot r_0}, \quad d_M = \sum_{j \neq i} \frac{z_j}{r_j / r_0}$$

z-ti naboj

$$W_C = z_i \cdot \frac{e_0^2}{4\pi\varepsilon_0 \cdot r_0}$$

$$W_C = -\frac{e_0^2}{4\pi\varepsilon_0 r_0} \cdot \Big[\underbrace{\Big(\frac{4\cdot\frac{1}{2}}{1} - \frac{4\cdot\frac{1}{4}}{\sqrt{2}}\Big)}_{\text{1.kvadrant}} + \underbrace{\Big(\frac{4\cdot\frac{1}{2}}{1} - \frac{4\cdot 3/4}{\sqrt{2}} - \frac{4\cdot\frac{1}{2}}{2} + \frac{8\cdot\frac{1}{2}}{\sqrt{5}} - \frac{4\cdot\frac{1}{4}}{2\sqrt{2}}\Big)}_{\text{2.kvadrant}} + \dots \Big] =$$

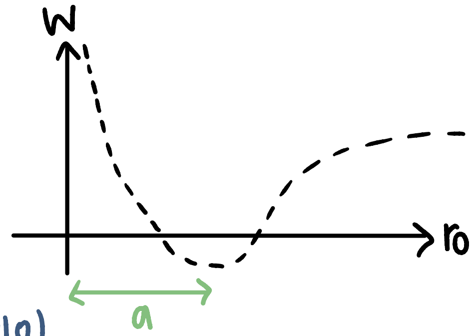
$$= -\frac{e_0^2}{4\pi\varepsilon_0 r_0} \cdot [1.293 + 0.314 + \dots] = -\frac{e_0^2}{4\pi\varepsilon_0 r_0} \cdot 1.61$$

Madelungova konst.

$$\boxed{-2N \cdot \underbrace{W_0(r_0)}_{\text{vezavna en. na neki razdalji } r} = N \cdot W_i - N \cdot W_a - \underbrace{\frac{1}{2} \cdot 2N}_{\text{št. parov}} \cdot \Big(\frac{e_0^2 \cdot d_{Mi}}{4\pi\varepsilon_0 r_0}\Big) + \underbrace{\frac{A}{r_0^{12}}}_{\text{odbojni potencial}}}$$

odbojni potencial (Paulijevo izklj. načelo)

Energijska bilanca



Iščemo ravnovesno razdaljo – to bo razdalja, pri kateri bo minimum en.

$$\Rightarrow \frac{\partial W_0(r_0)}{\partial r_0} = 0 = N \cdot \frac{e_0^2 d_{Mi}}{4\pi\varepsilon_0 r_0^2} - 12 \cdot \frac{A}{r_0^{13}} \Big|_{r=a}$$

$$A = \frac{N}{12} \cdot \frac{e_0^2 \cdot d_{Mi}}{4\pi\varepsilon_0} \cdot a^{11}$$

tovstavimo nazaj v energijsko bilanco

$$-2N \cdot W_0 = NW_i - NW_a - N \cdot \frac{e_0^2 \cdot d_{Mi}}{4\pi\varepsilon_0 a} + N \cdot \frac{e_0^2 d_{Mi}}{4\pi\varepsilon_0} \cdot \frac{1}{12a}$$

$\vdots$

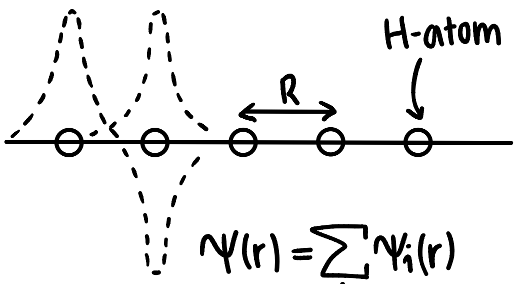
$$-W_0(a) = \frac{W_i - W_a}{2} - \frac{e_0^2 d_{Mi}}{8\pi\varepsilon_0 a} \cdot \frac{11}{12}$$

$$\boxed{a = \frac{11}{12} \cdot \frac{e_0^2}{4\pi\varepsilon_0} \cdot \frac{d_{Mi}}{W_i - W_a + 2W_0}} = \dots = 2 \cdot 10^{-4}\,\mu m = 0.2\,nm$$

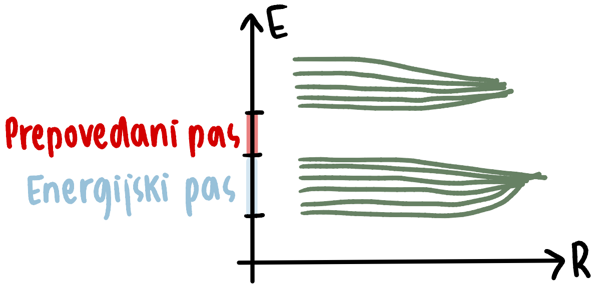
Konstanta fine strukture

$$\boxed{\begin{aligned} \alpha &= \frac{e_0^2}{4\pi\varepsilon_0 \hbar c} \approx \frac{1}{137} \\ \hbar c &= 0.197\,eV\,\mu m \end{aligned}}$$

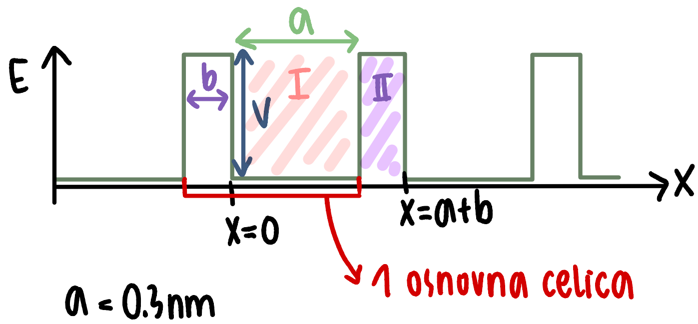
(2) Elektroni v kristalu (Kronig-Penneyjev model)



$$\psi(r) = \sum_i \psi_i(r)$$



Najpreprostejši model kristala : Kronig-Penneyev model



$$V(x) = V\cdot b \sum_{i=-\infty}^{\infty} \delta(x+a\cdot i)$$

$V \to \infty$
$b \to 0$

$a = 0.3\,\mathrm{nm}$
$Vb = 2.5\,\mathrm{meV\cdot nm}$

Blochov izrek: $\hat{H}(\vec{r}) = \hat{H}(\vec{r}+\vec{r}_0) \Rightarrow \psi_{k_L}(\vec{r}) = \underbrace{e^{i\vec{k}_L\cdot\vec{r}}}_{\text{Prosti val}} \cdot u_{\vec{k}_L}(\vec{r})\ ;\ u_{\vec{k}_L}(\vec{r}) = u_{\vec{k}_L}(\vec{r}+\vec{r}_0)$ Periodična funkcija

ali $\Downarrow$

$$\psi_{\vec{k}_L}(\vec{r}+\vec{r}_0) = e^{i\vec{k}_L\cdot\vec{r}_0}\cdot\psi_{\vec{k}_L}(\vec{r})$$

$k_L = \frac{2\pi}{L}\cdot n,\ n \in \left\{-\frac{N}{2}, \dots, \frac{N}{2}\right\}$ število celic

L: celotna dolžina kristala

Kolikšna je energijska vrzel ΔE med najnižjima energijskima pasovoma?

$$\psi_I = A\cdot e^{ikx} + B\cdot e^{-ikx}, \quad k = \sqrt{\frac{2mE}{\hbar^2}}$$

$$\psi_{II} = C\cdot e^{\kappa x} + D e^{-\kappa x}, \quad \kappa = \sqrt{\frac{2m(V-E)}{\hbar^2}}$$

Robni pogoji: (a) $\psi_I(x=0) = \psi_{II}(x=0)$ (c) $\psi_I'(x=0) = \psi_{II}'(x=0)$

(b) $\psi_I(x=a) = \psi_{II}(x=a)$ (d) $\psi_I'(x=a) = \psi_{II}'(x=a)$

$\Rightarrow$ (a) $A+B = C+D$
(c) $A\cdot ik - B\cdot ik = C\kappa - D\kappa$

(b) $\psi_I(x=a) = \psi_{II}(x=a)$, $\tilde{x} + (a+b) = a$
$\Downarrow$
$\tilde{x} = -b$

Blochov izrek pa pravi: $\psi_I(x=a) = \psi_{II}(x=a) = e^{ik_L(a+b)}\cdot\psi_{II}(-b)$, $k_L = \frac{2\pi}{L}\cdot n = \frac{2\pi}{N\cdot(a+b)}\cdot n$

$$\Rightarrow A\cdot e^{ika} + B\cdot e^{-ika} = e^{ik_L(a+b)}\cdot\left(C e^{-\kappa b} + D e^{\kappa b}\right)$$ → zato ker smo pri $-b$!

(d) $\psi_I'(x=a) = \psi_{II}'(x=a) = e^{ik_L(a+b)}\cdot\psi_{II}'(-b)$

$$\Rightarrow ik\left(Ae^{ika} - Be^{-ika}\right) = e^{ik_L(a+b)}\left[C\kappa\cdot e^{-\kappa b} - D\kappa e^{\kappa b}\right]$$

Iz robnih pogojev smo dobili sistem 4 enačb za 4 neznanke

$\underline{\underline{A}} \cdot \vec{x} = 0 \rightarrow$ Rešitev tega sistema bo netrivialna samo, če je $\det(A) = 0$

2.VAJE 21.2.2022

Determinanta:

$$\det \begin{bmatrix} 1 & 1 & -1 & -1 \\ ik & -ik & -K_V & K_V \\ e^{ika} & e^{-ika} & -e^{-K_V b} e^{ik_L(a+b)} & -e^{K_V b} e^{ik_L(a+b)} \\ ike^{ika} & -ike^{-ika} & -K_V e^{-K_V b} e^{ik_L(a+b)} & K_V e^{K_V b} e^{ik_L(a+b)} \end{bmatrix} = 0$$

Izraz vržemo v Mathematico in dobimo enačbo:

$$\frac{K_V^2 - k^2}{2K_V k} \cdot \mathrm{sh}(K_V b) \cdot \sin(ka) + \mathrm{ch}(K_V b) \cdot \cos(ka) = \cos(k_L(a+b)) \;;\; k = \sqrt{\frac{2mE}{\hbar^2}},\; K_V = \sqrt{\frac{2m(V-E)}{\hbar^2}}$$

Poenostavitev: Smo v limiti $V \to \infty$, $b \to 0$, $V \cdot b = \text{konst.}$

$\Rightarrow K_V \gg k$

$\Rightarrow \mathrm{sh}\, x \approx x,\; \mathrm{ch}\, x \approx 1 + \mathcal{O}(x^2)$

$$\mathrm{sh}(K_V b) = \mathrm{sh}\left(\sqrt{\frac{2m(V-\cancel{E})}{\hbar^2} b^2}\right) = \mathrm{sh}\left(\overbrace{\sqrt{\frac{2mV \cdot b}{\hbar^2}}}^{\text{konst.}} \cdot \underbrace{\sqrt{b}}_{\text{majhno}}\right) \approx \sqrt{\frac{2mV \cdot b^2}{\hbar^2}} = K_V b$$

$$\mathrm{ch}(K_V b) \approx 1$$

$$\Rightarrow \frac{K_V^{\cancel{2}} \cdot a}{2\cancel{K_V} k \cdot a} \cdot K_V b \cdot \sin(ka) + \cos(ka) = \cos(k_L(a+b))$$

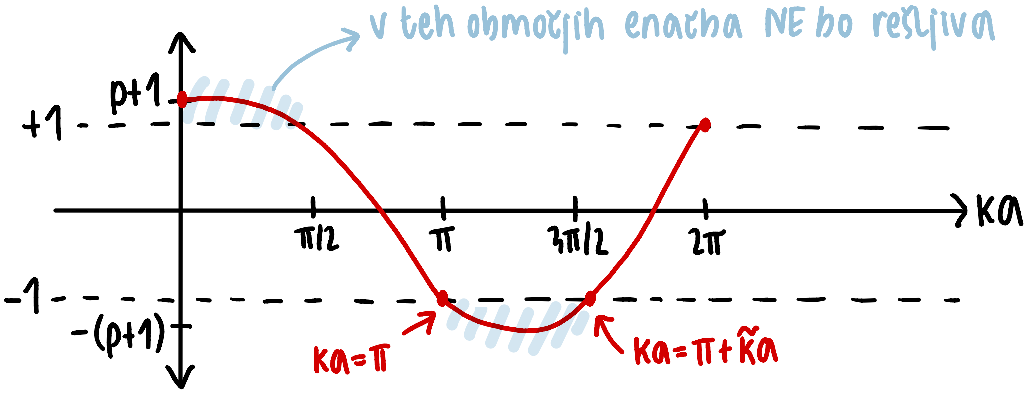
zato, da bo tudi koeficient pred sin brezdimenzijski

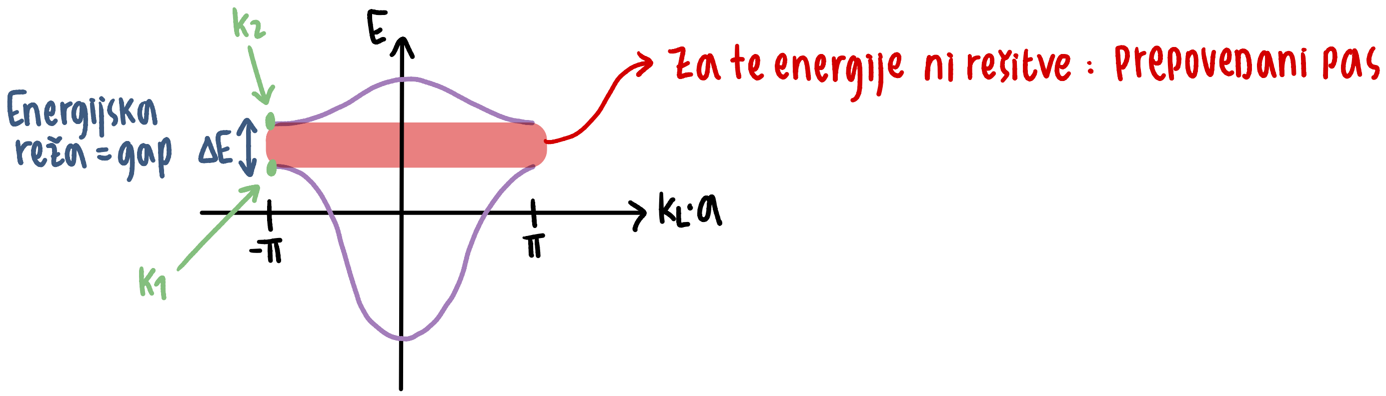
$$\frac{(K_V a) \cdot (K_V b)}{2} \cdot \frac{\sin(ka)}{ka} + \cos(ka) = \cos(k_L(a+b))$$

p

$$p \cdot \frac{\sin(ka)}{ka} + \cos(ka) = \overbrace{\cos(k_L(a+b))}^{\in[-1,1]}$$

Zanima nas disperzija, torej $E(k_L)$. Enačbo rešimo grafično:





Zdaj bomo ocenili širino reže, tako da bomo razvili funkcijo okoli točke, kjer vemo, da nimamo rešitve: $k\cdot a = \pi$

$$p = \frac{(\kappa a)\cdot(\kappa b)}{2} = \frac{2m\,(Vb)\cdot a}{2\cdot\hbar^2} = \frac{2\cdot(mc^2)\cdot Vb\cdot a}{c^2\hbar^2} = \ldots = 0.1 \ll 1$$

1.) $k\cdot a = \pi$
2.) $k\cdot a = \pi + \tilde{k}\cdot a$ $\Rightarrow$ $p\cdot\frac{\sin(\pi+\tilde{k}a)}{\pi+\tilde{k}\cdot a} + \cos(\pi+\tilde{k}a) = -1$

$$+p\cdot\frac{\sin(\tilde{k}a)}{\pi+\tilde{k}\cdot a} + \cos(\tilde{k}a) = +1$$

$$p\cdot\frac{\tilde{k}a}{\pi+\tilde{k}a} + \cancel{1} - \frac{(\tilde{k}a)^2}{2} = \cancel{1}$$

$$2p\tilde{k}a = (\tilde{k}a)^2\cdot(\pi+\tilde{k}a)$$

$$\tilde{k}a\,(2p - \tilde{k}a(\pi+\tilde{k}a)) = 0$$

$\sin(\pi+\tilde{k}a) =$
$= \sin\pi\cdot\cos(\tilde{k}a) + \sin(\tilde{k}a)\cdot\underbrace{\cos\pi}_{-1} =$
$= \emptyset - \sin(\tilde{k}a)$

$\cos(\pi+\tilde{k}a) =$
$= \cos\pi\cdot\cos(\tilde{k}a) - \sin\pi\cdot\sin(\tilde{k}a) =$
$= -\cos(\tilde{k}a) - \emptyset$

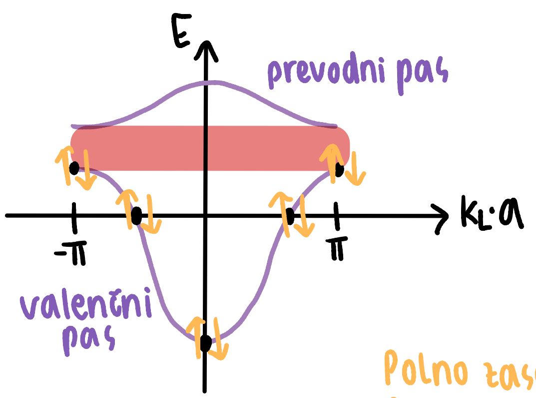
1. rešitev: $\tilde{k}a = 0$
$\rightarrow$ To je ravno točka $ka = \pi$

2. rešitev: $\tilde{k}a = \frac{2p}{\pi+\tilde{k}a} \approx \frac{2p}{\pi}$ $\Rightarrow ka = \pi + \frac{2p}{\pi}$

Vstavimo v izraz za energijo:

$$E = \frac{\hbar^2 k^2}{2m}\,,\quad \Delta E = \frac{\hbar^2}{2m}\cdot(k_2^2 - k_1^2) = \frac{\hbar^2}{2m}\left[\left(\frac{\pi}{a}+\frac{2p}{\pi a}\right)^2 - \left(\frac{\pi}{a}\right)^2\right] \approx \frac{\hbar^2}{2m}\cdot\frac{4p}{a^2} = 0.17\,\text{eV}$$

$k_L = \frac{2\pi}{L}\cdot n\,,\ n\in\left[-\frac{N}{2}, \frac{N}{2}\right]$, N = št. osnovnih celic v kristalu
$L = N\cdot a$
2N elektronov

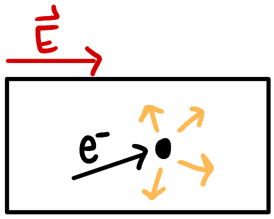


Recimo, da imamo le 5 mest $\rightarrow$ na vsako mesto gresta 2 stanji ($\uparrow$ in $\downarrow$)

Polno zaseden valenčni pas = izolator
Delno zaseden valenčni pas = prevodnik

μ = kemijski potencial = črta, pod katero so vsa zasedena stanja v valenčnem pasu

Čopič V/24 – Drudejev model



Elektroni se sipajo

τ = relaksacijski čas (čas, v katerem se v povprečju sipa e^-)

Newtonova en.: $\boxed{\frac{d\langle\vec{p}\rangle}{dt} = -\frac{\langle\vec{p}\rangle}{\tau} + q\cdot\vec{E}}$ Drudejeva en.

q: $-e_0$ za e^-, e_0 za vrzel

$$\langle\vec{j}\rangle = n\cdot q\cdot\langle\vec{v}\rangle = n\cdot q\cdot\frac{\langle\vec{p}\rangle}{m}$$

$$\langle\vec{j}\rangle = \sigma\cdot\vec{E}$$

σ ↳ specifična prevodnost

$$\boxed{\langle\vec{j}\rangle = \frac{n\cdot q^2\tau}{m}\cdot\vec{E}}$$

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

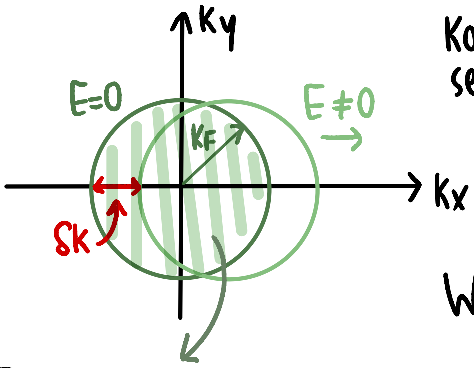
Stacionarno stanje: $\frac{d\langle\vec{p}\rangle}{dt} = 0$, $\langle\vec{p}\rangle = q\vec{E}\tau$

Zanima nas povprečna hitrost potovanja elektronov v bakru v zunanjem el. polju in razmerje te hitrosti proti hitrosti elektronov s Fermijevo energijo. Obravnavamo torej približek $k \ll \pi/a$

$\beta_{Cu} = 0.0032\ m^2/Vs$ = gibljivost
$W_F = 0.7\,eV$ = Fermijeva en.
$E = 1\,V/m$

a) $\beta = \frac{\langle\vec{v}\rangle}{E} \Rightarrow \langle v\rangle = \beta\cdot E = 0.0032\,\frac{m^{\cancel{2}}}{\cancel{V}s}\cdot 1\,\frac{\cancel{V}}{\cancel{m}} = 3.2\,mm/s$

b) Fermijeva energija



Zasedena so vsa stanja znotraj te krogle

Ko vklopimo zunanje el. polje, se krogla zamakne

Radij te krogle je k_F, njen volumen pa $V = \frac{4\pi k_F^3}{3}$

$$W_F = \frac{\hbar^2 k_F^2}{2m} = \frac{m\cdot v_F^2}{2} \Rightarrow v_F = \sqrt{\frac{2\cdot W_F}{m}} = c\cdot\sqrt{\frac{2\cdot W_F}{mc^2}} = \ldots = 1.6\cdot 10^6\,\frac{m}{s}$$

$$\Rightarrow \frac{\langle v\rangle}{v_F} = 2\cdot 10^{-9}$$

Čopič V/23

Izračunati želimo povprečno prosto pot prevodniških e^- v Na in Cu.

$\sigma_{Cu} = 5.9\cdot 10^{-7}\ 1/\Omega m$
$\sigma_{Na} = 2.2\cdot 10^{-7}\ 1/\Omega m$
$\rho_{Cu} = 8.9\ g/cm^3$
$\rho_{Na} = 0.97\ g/cm$

Gibljejo se e^- na robu Fermijeve krogle $\Rightarrow \langle l\rangle = v_F\cdot\tau$

a) $\tau = ?$ $\quad \sigma = \frac{q^2\cdot n\cdot\tau}{m} \Rightarrow \tau = \frac{m\cdot\sigma}{q^2 n}$

$\rho = \frac{m}{V} = \frac{M}{V}\cdot\frac{N}{N_A} = \frac{M}{N_A}\cdot n$

$\Rightarrow \tau = \frac{m\cdot\sigma}{q^2}\cdot\frac{M}{N_A\rho}$