Simetrije v kristalih

Kristalne strukture

Bravaisova rešetka: $\vec{R}_n = n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3$ lokacija osnovne celice n

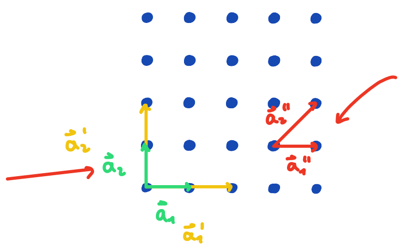
$\vec{a}_i$ ... primitivni osnovni vektorji

$n_i \in \mathbb{Z}$

$\vec{r}_{n,p} = \vec{R}_n + \vec{d}_p$ lokacija delca p v celici n.

↳ vektor baze

primitivna,
saj sta najmanjša
vektorja, ki opišeta
rešetko



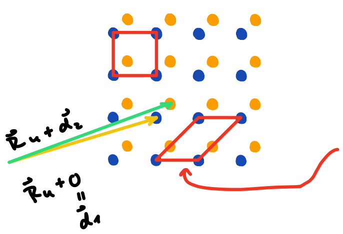
tudi primitivna

Simetrije:

- translacija $T_n = n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3$ operator, ki deluje na rešetko
- točkovne operacije
  - rotacijska os C_n $\alpha = \frac{2\pi}{n}$ najmanjši kot rotacije, da dobimo enako sliko

    edini možni $n = 2, 3, 4, 6$
  - zrcalne ravnine

Baza

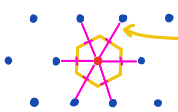


primer osnovnih celic

Osnovne celice niso enolično definirane,

nji hov volumen je vedno enak, $V = (\vec{a}_1, \vec{a}_2, \vec{a}_3)$ mešan produkt

Wigner - Seitzova osnovna celica

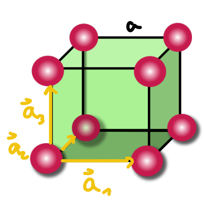


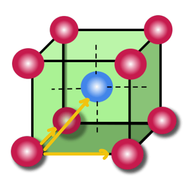
poiščemo najkrajše razdalje do sosednih delcev
in jih razpolovimo, da dobimo enolično defi celico.

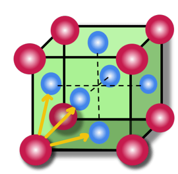
Bravaisove rešetke

Koordinacijsko število N_c = število sosedov

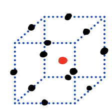
- Preprosta kubična SC
  $N_c = 6$
- Telesno centrirana BCC
  $N_c = 8$
- Ploskovno centrirana FCC
  $N_c = 12$







Če zamaknemo
za a/2



SC:

$\vec{a}_1 = (a, 0, 0)$

$\vec{a}_2 = (0, a, 0)$

$\vec{a}_3 = (0, 0, a)$

BCC:

$\vec{a}_1 = (a, 0, 0)$ $\vec{a}_1' = \frac{1}{2}(a, a, -a)$

$\vec{a}_2 = (0, a, 0)$ $\vec{a}_2' = \frac{1}{2}(a, -a, a)$

$\vec{a}_3 = \frac{1}{2}(a, a, a)$ $\vec{a}_3' = \frac{1}{2}(-a, a, a)$

možni rešetki

FCC:

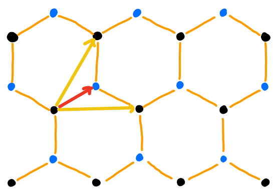
$\vec{a}_1 = \frac{1}{2}(a, a, 0)$

$\vec{a}_2 = \frac{1}{2}(0, a, a)$

$\vec{a}_3 = \frac{1}{2}(a, 0, a)$

Primer B. R. z bazo

- Satje



Osnovno celico sestavljata dve trikotni celici pri $\vec{d}_1$ in $\vec{d}_2$.

$\vec{R}_n = n_i \vec{a}_i$

$\vec{a}_1 = (a, 0)$

$\vec{a}_2 = \left(\frac{a}{2}, \frac{\sqrt{3}}{2} a\right)$

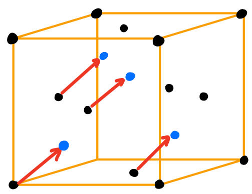
Baza

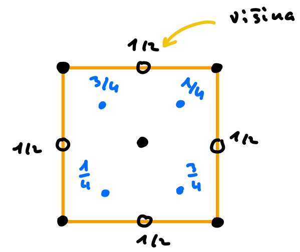
$\vec{d}_1 = 0$

$\vec{d}_2 = \left(\frac{a}{2}, \frac{\sqrt{3}}{6} a\right) = \frac{1}{3}(\vec{a}_1 + \vec{a}_2)$

• zamaknemo za ↗ da dobimo •

- Diamant $N_c = 4$





Tloris

$\vec{d}_1 = 0$

$\vec{d}_2 = \frac{1}{4}(a, a, a)$

Osnovno celico sestavljata dve FCC celici pri $\vec{d}_1$ in $\vec{d}_2$

Recipročna rešetka

Ravni val $e^{i\vec{k}\cdot(\vec{r}+\vec{R}_n)} = e^{i\vec{k}\vec{r}}$ $\quad \forall \vec{R}_n$, $\vec{R}_n = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$

$\Rightarrow \quad e^{i\vec{k}\cdot\vec{R}_n} = 1$ $\quad \vec{k}$ ki izpolnjuje to zvezo tvorijo recipročno rešetko

$$\vec{k} = k_1\vec{A}_1 + k_2\vec{A}_2 + k_3\vec{A}_3 \qquad k_i \in \mathbb{Z}$$

$$\vec{A}_1 = 2\pi \frac{\vec{a}_2 \times \vec{a}_3}{|(\vec{a}_1, \vec{a}_2, \vec{a}_3)|} \qquad \vec{A}_2 = 2\pi \frac{\vec{a}_3 \times \vec{a}_1}{|(\vec{a}_1, \vec{a}_2, \vec{a}_3)|} \qquad \vec{A}_3 = 2\pi \frac{\vec{a}_1 \times \vec{a}_2}{|(\vec{a}_1, \vec{a}_2, \vec{a}_3)|}$$

Velja $\quad \vec{a}_i \cdot \vec{A}_j = 2\pi \delta_{ij}$

$$\vec{k}\cdot\vec{R}_n = 2\pi(k_1 n_1 + k_2 n_2 + k_3 n_3)$$

Primer SC

$\vec{a}_1 = (a, 0, 0) \qquad \vec{A}_1 = \frac{2\pi}{a}(1, 0, 0)$

$\vec{a}_2 = (0, a, 0) \qquad \vec{A}_2 = \frac{2\pi}{a}(0, 1, 0)$

$\vec{a}_3 = (0, 0, a) \qquad \vec{A}_3 = \frac{2\pi}{a}(0, 0, 1)$

Primer FCC

$\vec{a}_1 = \frac{1}{2}(a, a, 0) \qquad \vec{A}_1 = \frac{2\pi}{a}(1, 1, -1)$

$\vec{a}_2 = \frac{1}{2}(a, 0, a) \qquad \vec{A}_2 = \frac{2\pi}{a}(1, -1, 1)$

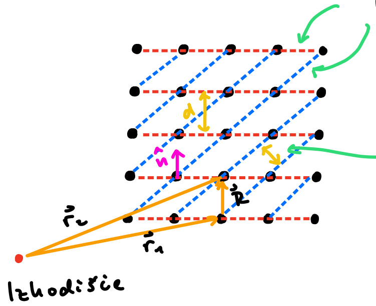
$\vec{a}_3 = \frac{1}{2}(0, a, a) \qquad \vec{A}_3 = \frac{2\pi}{a}(-1, 1, 1)$

$\vec{R}_n \longrightarrow \vec{k}$

Wigner Seitz $\longrightarrow$ 1. Brillouinove cone

Mrežne ravnine

primera družin mrežnih ravnin



Vsaka družina mrež vsebuje vse točke.

konstantna razdalja med mrežami v družini

$\vec{k} = \hat{n}\frac{2\pi}{d}$ $\quad$ vektor recipročne mreže

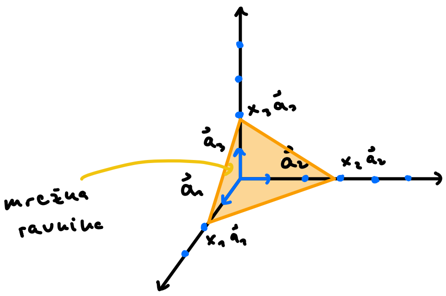
$$\vec{r}_2 - \vec{r}_1 = \vec{R}_n$$

$$\hat{n}\,\vec{R}_n = d \qquad / \, \frac{2\pi}{d}$$

$$\underbrace{\frac{2\pi}{d}\hat{n}}_{\vec{k}} \cdot \vec{R}_n = 2\pi$$

Najmanjši $\vec{k}$ definira razdaljo med mrežami

Millerjevi indeksi



Enačba ravnin $\quad \vec{r}\cdot\hat{n} = c \quad$ velja za $\forall$ vektor na ravnini

$$x_1\vec{a}_1\cdot\vec{k} = c$$
$$x_2\vec{a}_2\cdot\vec{k} = c \qquad \ldots$$
$$x_3\vec{a}_3\cdot\vec{k} = c$$

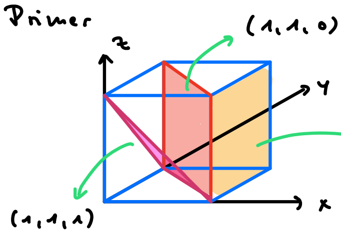
Millerjevi indeksi (h, k, ℓ) so si tuja števila

$$\vec{k} = h\vec{A}_1 + k\vec{A}_2 + \ell\vec{A}_3$$

$$\ldots \quad x_1\, 2\pi\, h = c$$
$$x_2\, 2\pi\, k = c$$
$$x_3\, 2\pi\, \ell = c$$

$$h : k : \ell = \frac{1}{x_1} : \frac{1}{x_2} : \frac{1}{x_3}$$

Primer



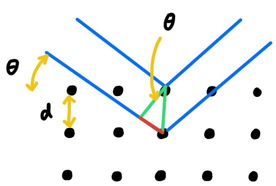
mrežne ravnine $h\ k\ \ell$ $(1,0,0)$

Sipanje na kristalih

X žarki : $\quad hc = 1240\ \text{eVnm}$

$a \sim 0{,}1\ \text{nm}$ razdalje med mrežami

$$E = \frac{hc}{\lambda} = h\nu = 12{,}4\ \text{keV} \qquad \text{pri } \lambda \sim a$$



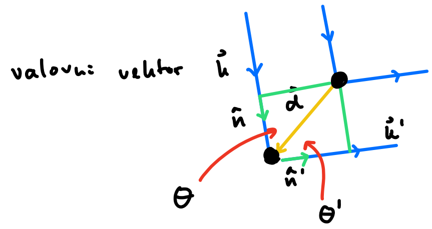
Bragg

- $2d\sin\theta = n\lambda$ $\qquad$ Pogoj za ojačitev

Težave:

- več maksimumov
- x-žarki niso monokromatski
- neskončno mrežnih ravnin

Von Laue



$$\vec k = \frac{2\pi}{\lambda}\hat n$$
$$\vec k' = \frac{2\pi}{\lambda}\hat n'$$

$$\Delta r = (d\cos\theta + d\cos\theta') = n\lambda$$
$$\vec d\cdot\hat n - \vec d\cdot\hat n' = n\lambda \qquad / \frac{2\pi}{\lambda}$$
$$\vec d\left(\frac{2\pi}{\lambda}\hat n - \frac{2\pi}{\lambda}\hat n'\right) = 2\pi n$$
$$\vec d\cdot(\underbrace{\vec k - \vec k'}) = 2\pi n$$
$$\vec d\cdot\vec K = 2\pi n$$

za poljubna dva sipalca v razdalji $\vec d$

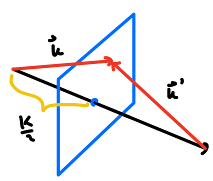
$$\vec R_n\cdot\vec K = 2\pi n \qquad \Rightarrow e^{i\vec R_n\cdot\vec K} = 1$$

vektor recipročne mreže

$$\vec k - \vec k' = \vec K$$
$$\vec k' = \vec k - \vec K$$
$$|\vec k'|^2 = k^2 = k^2 - 2\vec k\cdot\vec K + K^2$$

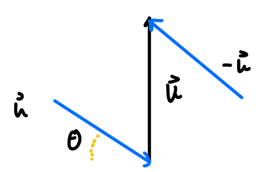
$$\Rightarrow \vec k\cdot\vec K = \frac{K^2}{2} \qquad \Rightarrow \vec k\cdot\hat K = \frac{K}{2}$$ enačba ravnine

$$\hat K = \frac{\vec K}{K}$$



Braggove ravnine

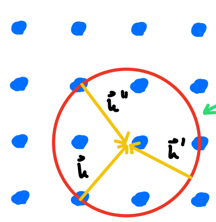
Pokazati moramo, da je Braggov pogoj za interferenco ($2d\sin\theta = n\lambda$) enak von Laue-ovem ($\vec k - \vec k' = \vec K$)



$$\vec k' - \vec k = \vec K$$
$$k\sin\theta = \frac{K}{2}$$
$$\frac{2\pi}{\lambda}\sin\theta = \frac{1}{2}\, n\frac{2\pi}{d}$$
$$2d\sin\theta = n\lambda \quad ✓$$

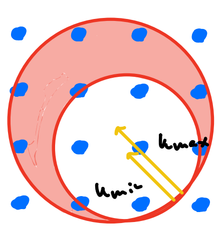
K je najmanjši mrežni vektor

Ewaldova konstrukcija



Ewaldova krogla

Tam kjer ta krog oz. krogla v 3D seka točko na mreži, dobimo ojačitev. Ni pa vedno nujno, da ta krog seka točk.



von Laueva metoda

Svetloba ponavadi ni monokromatska, torej $\lambda \in [\lambda_{min}, \lambda_{max}] \Rightarrow k = [\frac{2\pi}{\lambda_{max}}, \frac{2\pi}{\lambda_{min}}]$.

Metoda rotirajočega kristala

Geometrijski strukturni faktor

Vzemimo poljubno Bravaisovo rešetko $\vec{R}_n$ in to pomnožimo z $(\vec{k}-\vec{k}')$.

$$\vec{R}_n \cdot (\vec{k}-\vec{k}') = 2\pi n$$

Če pa nimamo BR to ni več, ker imamo zraven še bazo.

$$S_{\vec{k}} = \sum_{i=1}^{\overset{\text{število baznih vektorjev}}{p}} e^{i\vec{k}\cdot \underset{\text{vektor baze}}{\vec{d}_i}}$$

Intenziteta je odvisna od $I \propto |S_{\vec{k}}|^2$ in nam pove, kje dobimo ojačitve.

Primer: BCC

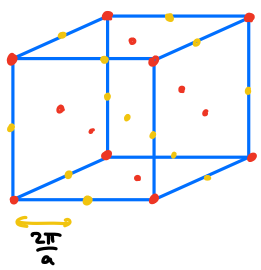
SC: $\vec{a}_1 = (a,0,0)$ $\quad \vec{A}_1 = \frac{2\pi}{a}(1,0,0)$ $\quad \vec{k} = \frac{2\pi}{a}(m_1, m_2, m_3)$

$\vec{a}_2 = (0,a,0)$ $\quad \vec{A}_2 = \frac{2\pi}{a}(0,1,0)$

$\vec{a}_3 = (0,0,a)$ $\quad \vec{A}_3 = \frac{2\pi}{a}(0,0,1)$

SC + baza = BCC $\quad \vec{d}_1 = (0,0,0)$ $\quad \vec{d}_2 = \frac{a}{2}(1,1,1)$

$$S_{\vec{k}} = 1 + e^{i\frac{2\pi}{a}\frac{a}{2}(m_1+m_2+m_3)}$$



● $S_{\vec{k}} = 2$

● $S_{\vec{k}} = 0$

$$S_{\vec{k}} = \sum_{i=1}^{p} f_i(\vec{k})\, e^{i\vec{k}\vec{d}_i}$$

Za kristale z različnimi delci

↳ atomski strukturni faktor

$$f_i(\vec{k}) = \frac{1}{e_0}\int \rho_i(\vec{r})\, e^{i\vec{k}\vec{r}}\, d\vec{r} \approx Z$$

Klasifikacija kristalov

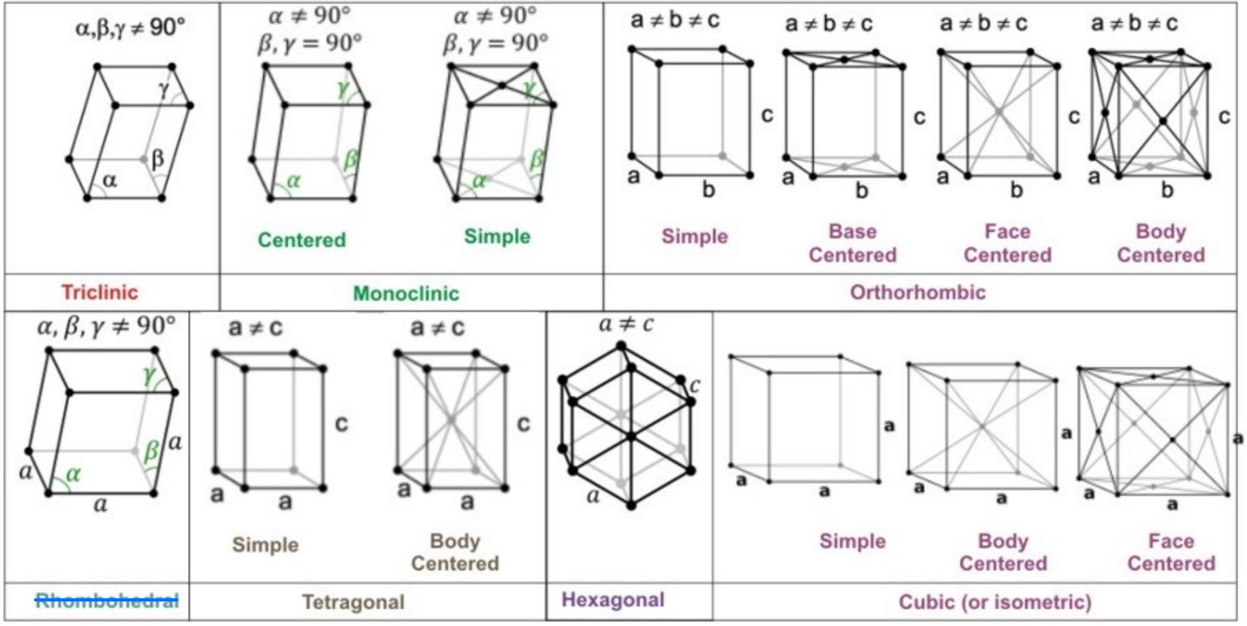
(1) Točkovne simetrije
– tvorijo 32 grup

(2) Translacijske simetrije

$\Big\}$ tvorijo 230 grup

	Bravaisove rešetke sferično sim.	Struktura osnovnih celic
točkovna simetrija	7 kristalnih sistemov	32 točkovnih grup
translacijska simetrija	14 BR	230 prostorskih grup

7 kristalnih sistemov, 14 Bravaisovih rešetk



Trigonalni kristalni sistem

Model prostih elektronov v kristalu

- e^- se nahajajo v konstantnem potencialu

$$-\frac{\hbar^2}{2m}\nabla^2\psi = \varepsilon_k \psi$$

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)\psi = \varepsilon_k \psi$$

$$\psi_{\vec{k}} = A e^{i\vec{k}\cdot\vec{r}} \qquad \varepsilon_k = \frac{\hbar^2 k^2}{2m}$$

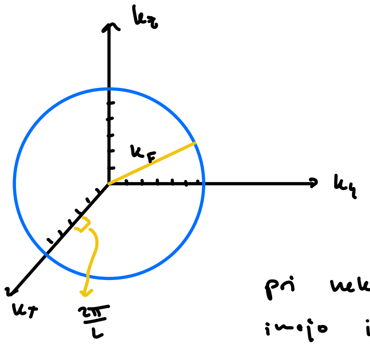
- kristal je končen
  $V = L^3$

$$\psi(x+L,y,z) = \psi(x,y,z) \quad \text{periodični robni pogoji}$$

$$\Rightarrow \quad k_x = n_x \frac{2\pi}{L}$$

$$\varepsilon_{\vec{k}} = \frac{\hbar^2}{2m}\left(\frac{2\pi}{L}\right)^2 (n_x^2 + n_y^2 + n_z^2)$$

n_x n_y n_z	ε_k	deg po spinu	deg
0 0 0	0	2	2
±1 0 0 0 ±1 0 0 0 ±1	1	2	12
⋮			



število elektronov v fermijevi krogli

$$N_{el} = 2\frac{V_F}{\Delta V} = 2\frac{\frac{4}{3}\pi k_F^3}{\left(\frac{2\pi}{L}\right)^3}$$

od spina

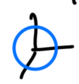
$$\Delta V = \left(\frac{2\pi}{L}\right)^3$$

pri neki $\vec{k}_F$ imajo isto energijo

$$\Rightarrow \boxed{k_F^3 = 3\pi^2 \frac{N_{el}}{V}} \qquad V = L^3$$

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

pri poljubnem k, je znotraj krogle z radijem k N stanj do neke energije / k



Pri $T=0$ elektroni postopoma zapolnijo najnižje stanja.

$$\varepsilon = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2}{2m}\left(3\pi^2 \frac{N}{V}\right)^{\frac{2}{3}}$$

$$\Rightarrow N(\varepsilon) = \left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}} \frac{V}{3\pi^2}\, \varepsilon^{3/2}$$

gostota stanj $D(\varepsilon) = \frac{dN}{d\varepsilon} = \frac{3}{2}\left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}} \frac{V}{3\pi^2}\sqrt{\varepsilon}$

gostota stanj na volumen $g(\varepsilon) = \frac{1}{V}\frac{dN}{d\varepsilon} = \frac{1}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\sqrt{\varepsilon}$

volumska gostota elektronov

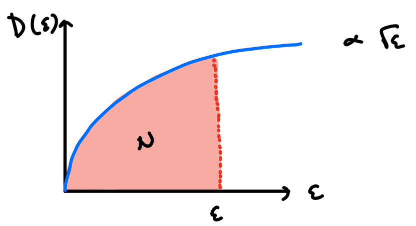
$$\frac{N_{el}}{V} = n = \frac{1}{3\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} \varepsilon_F^{3/2}$$

↳ Fermijeva energija

$$\left(\frac{2m}{\hbar^2}\right)^{3/2} = 3\pi^2 n\, \varepsilon_F^{-3/2}$$

$$\Rightarrow D(\varepsilon) = V\,\frac{3}{2}\,\frac{n}{\varepsilon_F}\sqrt{\frac{\varepsilon}{\varepsilon_F}}$$

$$g(\varepsilon) = \frac{3}{2}\,\frac{n}{\varepsilon_F}\sqrt{\frac{\varepsilon}{\varepsilon_F}} \qquad g(\varepsilon_F) = \frac{3}{2}\,\frac{n}{\varepsilon_F}$$



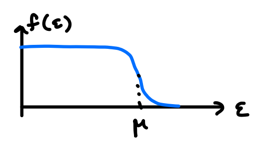
$$N = \int_0^{\varepsilon} D(\varepsilon)\, d\varepsilon$$

Pri končni temperaturi

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

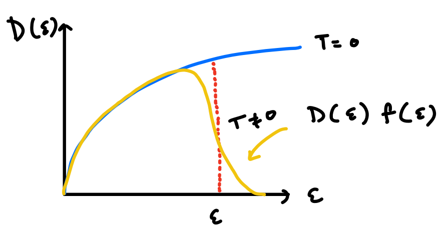
Fermi – Diracova porazdelitev

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



$\varepsilon_F \rightarrow \mu(T)$ kemijski potencial

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



Notranja energija

$$u = \frac{2}{V} \sum_{\vec{k}=0}^{\infty} \varepsilon(\vec{k})\, f(\varepsilon(\vec{k})) = \frac{2}{V} \int_0^{\infty} \frac{d^3k}{\frac{8\pi^3}{V}}\, \varepsilon(\vec{k})\, f(\varepsilon(\vec{k})) =$$

$$= \frac{1}{4\pi^3} \int_0^{\infty} d^3k\, \varepsilon(\vec{k})\, f(\varepsilon(\vec{k})) \underset{\varepsilon = \frac{\hbar^2 k^2}{2m}}{=} \int_0^{\infty} d\varepsilon\, \varepsilon f(\varepsilon)\, g(\varepsilon)$$

Pri $T=0$ $\quad \bar{\varepsilon}_0 = \int_0^{\varepsilon_F} d\varepsilon\, \varepsilon\, g(\varepsilon) = \int_0^{\varepsilon_F} d\varepsilon\, \varepsilon\, \frac{3}{2} \frac{n}{\varepsilon_F^{3/2}} \varepsilon^{1/2} = \frac{3}{5} n\, \varepsilon_F$

Pri končni temperaturi $T>0$

$$u = \int_0^{\infty} d\varepsilon\, \varepsilon\, g(\varepsilon)\, f(\varepsilon) \qquad n = \int_0^{\infty} d\varepsilon\, g(\varepsilon)\, f(\varepsilon)$$

Sommerfeldov razvoj za majhne temperature $(T \ll T_F)$ $\qquad \varepsilon_F = k_B T_F$

$$\int_0^{\infty} H(\varepsilon)\, f(\varepsilon)\, d\varepsilon = \int_0^{\mu(T)} H(\varepsilon)\, d\varepsilon + \frac{\pi^2}{6} (k_B T)^2 H'(\varepsilon = \mu) + \mathcal{O}(T^4)$$

$$n = \int_0^{\mu} g(\varepsilon)\, d\varepsilon + \frac{\pi^2}{6} (k_B T)^2 g'(\mu) =$$

$$n = \underbrace{\int_0^{\varepsilon_F} g(\varepsilon)\, d\varepsilon}_{n} + \int_{\varepsilon_F}^{\mu} g(\varepsilon)\, d\varepsilon + \frac{\pi^2}{6} (k_B T)^2 g'(\mu)$$

ε_F je skoraj enak μ

$$n \doteq n + (\mu - \varepsilon_F)\, g(\varepsilon_F) + \frac{\pi^2}{6} (k_B T)^2 g'(\varepsilon_F)$$

$$\mu = \varepsilon_F - \frac{\pi^2}{6} (k_B T)^2 \underbrace{\frac{g'(\varepsilon_F)}{g(\varepsilon_F)}}_{\frac{1}{2\varepsilon_F}} \qquad g(\varepsilon) \propto \varepsilon^{1/2}$$

$$\mu = \varepsilon_F \left(1 - \frac{\pi^2}{12} \left(\frac{k_B T}{\varepsilon_F}\right)^2\right) = \varepsilon_F \left(1 - \frac{\pi^2}{12} \left(\frac{T}{T_F}\right)^2\right)$$

Specifična toplota el. plina

$$c_V = \frac{du}{dT}$$

$$u_T = \underbrace{\int_0^{\varepsilon_F} \varepsilon\, g(\varepsilon)\, d\varepsilon}_{\bar{\varepsilon}_0} + (\mu - \varepsilon_F)\, \varepsilon_F\, g(\varepsilon_F) + \frac{\pi^2}{6} (k_B T)^2 \left(g(\varepsilon_F) + \varepsilon_F\, g'(\varepsilon_F) \right)$$

$$\varepsilon_F\, (\underbrace{\dots}_{=0})$$

$$u_T = \bar{\varepsilon}_0 + \frac{\pi^2}{6} (k_B T)^2 g(\varepsilon_F) \quad \Rightarrow \quad c_V = \frac{\partial u}{\partial T} = \frac{\pi^2}{3} k_B^2\, T\, \underbrace{g(\varepsilon_F)}_{\frac{3}{2}\frac{n}{\varepsilon_F}}$$

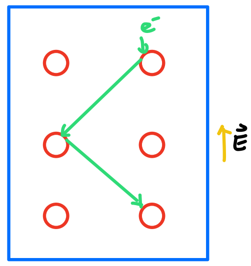
$$\Rightarrow \quad c_V = \frac{\pi^2}{2} k_B\, n\, \frac{k_B T}{\varepsilon_F}$$

št. valenčnih el.

c_V na mol snovi $\qquad C = \frac{z N_A}{n} c_V = \frac{z N_A V}{N_{el}} c_V = \frac{\pi^2}{2} \underbrace{k_B N_A}_{R}\, z \frac{T}{T_F} = \frac{\pi^2}{2} R z \frac{T}{T_F} = \gamma T$

Drudejev model el. upornosti / prevodnosti

- Z elektronov se premo enakomerno gibljejo pod vplivom $\vec{E}$.
- Med trki se e^- gibljejo prosto.
- Trki so trenutni in naključni
- τ ... čas med trki, $P = \frac{1}{\tau}$
- Trki vzpostavijo termično ravnovesje

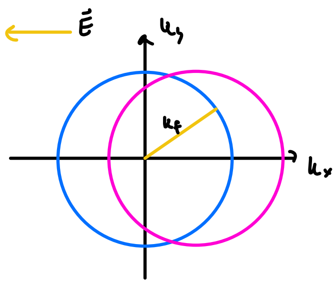


$$m_e \dot{\vec{v}} = -e_0 \vec{E} - \underbrace{\frac{m\vec{v}}{\tau}}_{\text{dušenje}}$$

$$\Rightarrow \quad \vec{v} = -\frac{e_0 \tau}{m} \vec{E}$$

$$\vec{j} = -n e_0 \vec{v} = \underbrace{\frac{n e_0^2 \tau}{m}}_{\sigma} \vec{E}$$ gostota el. toka

$$\vec{j} = \sigma \vec{E}$$



$$\varepsilon_F = \frac{\hbar^2 k_F^2}{2m}$$

Če ni dušenja

- $m \frac{d\vec{u}}{dt} = \hbar \frac{d\vec{k}}{dt} = -e\vec{E} \Rightarrow \vec{k}(t) = \vec{k}(0) - \frac{e\vec{E}}{\hbar} t$

Ocena premika Fermijeve krogle

$$\boxed{\delta k = -\frac{eE}{\hbar}\tau}$$

$k_F,\ \varepsilon_F,\ v_F = \frac{\hbar k_F}{m} \Rightarrow$ Povprečna prosta pot $l = v_F \tau$

Elektronska stanja v periodičnem potencialu

- Šibek periodični potencial $\quad U(\vec{r}) = U(\vec{r} + \vec{R}) \quad \forall \vec{R}$ B.R.
- Enodelčni problem $\quad H\psi = \varepsilon\psi \quad H = -\frac{\hbar^2 \nabla^2}{2m} + U(\vec{r})$
- Zaradi periodičnega potenciala $\Rightarrow$ rešitev $\psi_{n\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} u_{n\vec{k}}(\vec{r})$ $\quad u_{n\vec{k}}(\vec{r}+\vec{R})$ periodično

n: indeks pasu

$$\vec{k} = \frac{n_x}{N_x}\vec{A}_x + \frac{n_y}{N_y}\vec{A}_y + \frac{n_z}{N_z}\vec{A}_z \qquad |\vec{k}| = \frac{2\pi}{a} \text{ minimalni } k$$

$$\psi(\vec{r}) = \sum_{\vec{q}} c_{\vec{q}} e^{i\vec{q}\cdot\vec{r}} \qquad \vec{q}: \text{ periodični RP} \qquad |\vec{q}| = \frac{2\pi}{L}$$

$$U(\vec{r}) = \sum_{\vec{k}} U_{\vec{k}} e^{i\vec{k}\cdot\vec{r}} \qquad \vec{k} = k_1\vec{A}_1 + k_2\vec{A}_2 + k_3\vec{A}_3 \quad k_i \in \mathbb{Z} \qquad \vec{A}_1 = 2\pi \frac{\vec{a}_2 \times \vec{a}_3}{(\vec{a}_1, \vec{a}_2, \vec{a}_3)}$$

$$U(\vec{r}+\vec{R}) = U(\vec{r}) \Rightarrow U(\vec{r}+\vec{R}) = \sum U_{\vec{k}} e^{i\vec{k}(\vec{r}+\vec{R})} = U(\vec{r}) \quad \text{ker } e^{i\vec{k}\vec{R}} = 1$$

$$-\frac{\hbar^2}{2m}\nabla^2 \psi(\vec{r}) = \sum_{\vec{q}} c_{\vec{q}} \underbrace{\frac{\hbar^2 q^2}{2m}}_{\varepsilon^0_{\vec{q}}} e^{i\vec{q}\cdot\vec{r}}$$

$$U(\vec{r})\psi(\vec{r}) = \sum_{\vec{k},\vec{q}'} c_{\vec{q}'} U_{\vec{k}} e^{i(\vec{q}'+\vec{k})\vec{r}} \qquad \vec{q} = \vec{q}' + \vec{k}$$

$$= \sum_{\vec{k},\vec{q}} c_{\vec{q}-\vec{k}} U_{\vec{k}} e^{i\vec{q}\vec{r}}$$

$(H-\varepsilon)\psi = 0$

$$\sum_{\vec g} e^{i\vec g\vec r}\Big(\underbrace{(\varepsilon^0_{\vec g}-\varepsilon)\,c_{\vec g} + \sum_{\vec K} c_{\vec g-\vec K}\, U_{\vec K}}_{=0}\Big) = 0$$

ortogonalnost ravnih valov

$$(\varepsilon^0_{\vec g}-\varepsilon)\,c_{\vec g} + \sum_{\vec K} c_{\vec g-\vec K}\, U_{\vec K} = 0$$

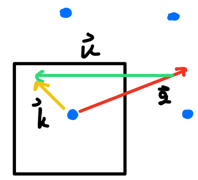
$$u_{\vec K} = \int u(\vec r)\, e^{-i\vec K\vec r}\, d^3r$$

izbira ničle $u(\vec r)$

$$u_{\vec K=0} = 0 = \int u(\vec r)\, d^3r$$

Naj bo $\vec k = \vec g + \vec K$ vektor znotraj prve Brillouinove cone

$\Rightarrow \vec g = \vec k - \vec K$



$$(\varepsilon^0_{\vec k-\vec K}-\varepsilon)\,c_{\vec k-\vec K} + \sum_{\vec K''} c_{\vec k-\vec K-\vec K''}\, U_{\vec K''} = 0$$

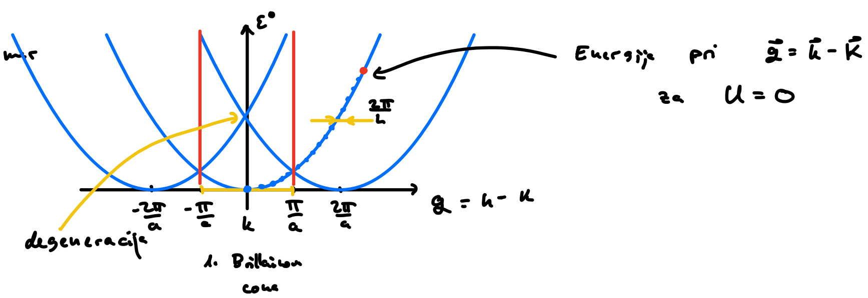
Naj bo $\vec K + \vec K'' = \vec K'$

$$(\varepsilon^0_{\vec k-\vec K}-\varepsilon)\,c_{\vec k-\vec K} + \sum_{\vec K'} c_{\vec k-\vec K'}\, U_{\vec K'-\vec K} = 0$$

(a) Kaj če je $u(\vec r) = u_0 = \text{konst.} = 0 \Rightarrow U_{\vec K} = 0 \quad \forall \vec K$

$\Rightarrow \varepsilon = \varepsilon^0_{\vec k-\vec K}$ $\qquad \varepsilon^0_{\vec k} = \frac{\hbar^2 k^2}{2m}$

1D primer

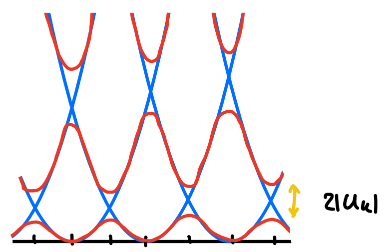


(b) $U_{\vec K}$ majhen

gledamo energijo stran od degeneracije

$$|\varepsilon^0_{\vec k-\vec K_1} - \varepsilon^0_{\vec k-\vec K}| \ll U_{\vec K-\vec K_1}$$

poljuben $\vec K$



$c_{\vec k-\vec K_1} \sim 1 \qquad c_{\vec k-\vec K} \sim 0 \quad \forall \vec K \neq \vec K_1$

$$(\varepsilon^0_{\vec k-\vec K_1}-\varepsilon)\,c_{\vec k-\vec K_1} + \sum_{\vec K\neq\vec K_1} c_{\vec k-\vec K}\, U_{\vec K-\vec K_1} = 0$$

$\vec K \neq \vec K_1$ $\qquad (\varepsilon^0_{\vec k-\vec K}-\varepsilon)\,\underbrace{c_{\vec k-\vec K}}_{} + c_{\vec k-\vec K_1}\, U_{\vec K_1-\vec K} = 0$

izpostavimo in vstavimo zgoraj

$$(\varepsilon^0_{\vec k-\vec K_1}-\varepsilon)\,\cancel{c_{\vec k-\vec K_1}} - \sum_{\vec K} \frac{\cancel{c_{\vec k-\vec K_1}}\, U_{\vec K-\vec K_1}\, U_{\vec K_1-\vec K}}{(\varepsilon^0_{\vec k-\vec K}-\varepsilon)} = 0$$

$$\varepsilon = \varepsilon^0_{\vec k-\vec K_1} - \sum_{\vec K} \frac{|U_{\vec K-\vec K_1}|^2}{\varepsilon^0_{\vec k-\vec K}-\varepsilon} \approx \varepsilon^0_{\vec k-\vec K_1} + \sum_{\vec K} \frac{|U_{\vec K-\vec K_1}|^2}{\varepsilon^0_{\vec k-\vec K_1} - \varepsilon_{\vec k-\vec K}} = \varepsilon^0_{\vec k-\vec K_1} - O(U^2)$$

najnižja energija $\Longrightarrow$ Negativno, energija se zmanjša

(c) $|\varepsilon^0_{\vec k-\vec u_1} - \varepsilon^0_{\vec k-\vec u_2}| \sim U_{\vec u_1-\vec u_2}$ opazujemo kaj se zgodi z energijo pri degeneraciji

$$(\varepsilon_{\vec k-\vec u_1} - \varepsilon)\, c_{\vec k-\vec u_1} + c_{\vec k-\vec u_2}\, U_{\vec u_2-\vec u_1} = 0$$
$$(\varepsilon_{\vec k-\vec u_2} - \varepsilon)\, c_{\vec k-\vec u_2} + c_{\vec k-\vec u_1}\, U_{\vec u_1-\vec u_2} = 0$$

kjer $c_{\vec k-\vec u_1} \sim c_{\vec k-\vec u_2} \sim 1$ ostali pa 0.

$$\vec g = \vec k - \vec u_1 \Rightarrow \vec k = \vec g + \vec u_1 \qquad \vec k - \vec u_2 = \vec g - (\vec u_2 - \vec u_1) = \vec g - \vec u$$

$$(\varepsilon^0_{\vec g} - \varepsilon)\, c_{\vec g} + c_{\vec g-\vec u}\, U_{\vec u} = 0$$
$$(\varepsilon^0_{\vec g-\vec u} - \varepsilon)\, c_{\vec g-\vec u} + c_{\vec g}\, U_{-\vec u} = 0$$

zanima nas ε v bližini $\varepsilon^0_{\vec g} \approx \varepsilon^0_{\vec g-\vec u}$

$\Downarrow$

Točke degeneracije, se zgodijo na Braggovih ravninah.

$$\begin{cases} g^2 = (\vec g - \vec k)^2 = g^2 - 2\vec g \vec k + k^2 \\ \vec g \hat n = \frac{k}{2} \quad \text{Braggova ravnina} \end{cases}$$

$$\det \begin{vmatrix} \varepsilon^0_{\vec g} - \varepsilon & U_{\vec u} \\ U_{-\vec u} & \varepsilon^0_{\vec g-\vec u} - \varepsilon \end{vmatrix} = 0$$

$$\ldots \Rightarrow \varepsilon = \frac{1}{2}\left(\varepsilon^0_{\vec g} + \varepsilon^0_{\vec g-\vec u}\right) \pm \frac{1}{2}\sqrt{(\varepsilon^0_{\vec g} - \varepsilon^0_{\vec g-\vec u})^2 + 4U_{\vec u}^2}$$

ε pri $\varepsilon^0_{\vec g} = \varepsilon^0_{\vec g-\vec u}$

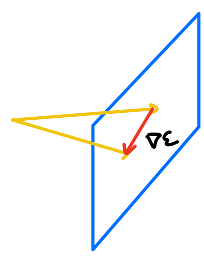
$\varepsilon = \varepsilon^0_{\vec g} \pm |U_{\vec u}|$ Reža je $2|U_{\vec u}|$

Iščemo
$$\nabla_{\vec g}\, \varepsilon = \frac{\hbar^2}{4m} \nabla_{\vec g}\left(g^2 + (\vec g - \vec u)^2\right) + 0 =$$
$$= \frac{\hbar^2}{2m}(\vec g + \vec g - \vec u) =$$
$$= \frac{\hbar^2}{m}\left(\vec g - \frac{\vec k}{2}\right)$$

$g^2 = |\vec g - \vec k|^2$

$g^2 = g^2 + k^2 - 2\vec g \cdot \vec k$

$\vec g \cdot \hat n = \frac{k}{2}$

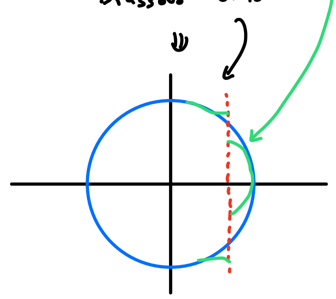


leži na Braggovi ravnini

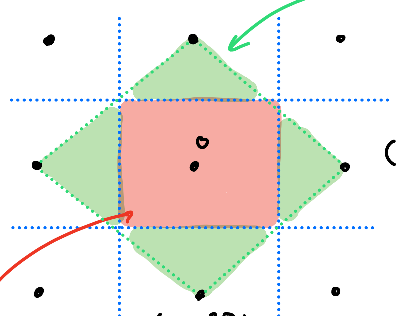
$\Downarrow$

Fermijeva krivulja mora biti $\perp$ na Braggovo črto

$\Downarrow$

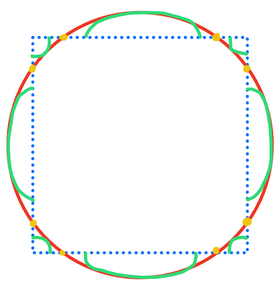


2. Brillouinova cona



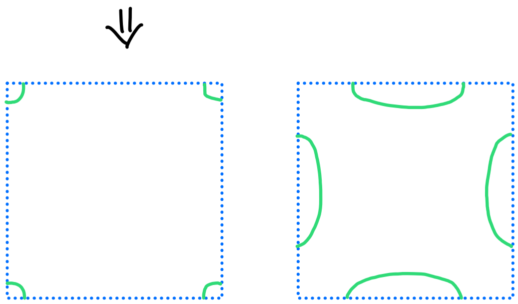
1. Brillouinova cona

1. B.C.



- Brez potenciala
- Točke degeneracije
- 1. B.C., Braggova črta
- s potencialom

Fermijeva površina



Gostota stanj

$H(\varepsilon_n(\vec{k}))$

poljubna funkcija odvisna od $\varepsilon_n(\vec{k})$

$$\frac{1}{V}\sum_k H(\varepsilon_n(\vec{k})) = \frac{1}{4\pi^3}\int d^3k\, H(\varepsilon_n(\vec{k})) =$$

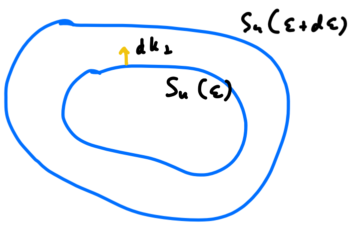
$$= \sum_n \int g_n(\varepsilon)\, H(\varepsilon)\, d\varepsilon = \int g(\varepsilon)\, H(\varepsilon)\, d\varepsilon$$

po pasovih

gostota stanj

$$g_n(\varepsilon) = \int \frac{d^3k}{4\pi^3}\, \delta(\varepsilon - \varepsilon_n(\vec{k}))$$

$$d\varepsilon\, g_n(\varepsilon) = \int \frac{d^3k}{4\pi^3} \begin{cases} 1 ; & \varepsilon < \varepsilon_n(\vec{k}) < \varepsilon + d\varepsilon \\ 0 ; & \text{sicer} \end{cases}$$



$$d\varepsilon\, g_n(\varepsilon) = \int_{S_n(\varepsilon)} \frac{dS\, dk_\perp}{4\pi^3}$$

$$d\varepsilon = \nabla_k \varepsilon_n(\vec{k})\, d\vec{k} = |\nabla_k \varepsilon_n(\vec{k})|\, dk_\perp$$

$$g_n(\varepsilon) = \int_{S_n(\varepsilon)} \frac{dS}{4\pi^3} \frac{1}{|\nabla_k \varepsilon_n(\vec{k})|}$$

$$g(\varepsilon) = \sum_n g_n(\varepsilon)$$

Preverimo za proste elektrone

$$\varepsilon = \frac{\hbar^2 k^2}{2m} \qquad |\nabla \varepsilon| = \frac{\hbar^2 k}{m}$$

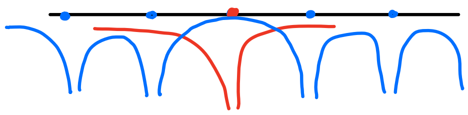
$$g(\varepsilon) = \underbrace{\frac{4\pi k^2}{4\pi^3}}_{\text{krogla}} \frac{m}{\hbar^2 k} = \frac{1}{\pi^2}\frac{m}{\hbar^2} k \quad \propto \sqrt{E} \quad ✓$$

Metoda tesne vezi

$$(\varepsilon^0_{\vec k-\vec K} - \varepsilon)\, c_{\vec k-\vec K} + \sum_{\vec K'} c_{\vec k-\vec K'}\, U_{\vec K'-\vec K} = 0$$

$$\psi_{n,\vec k} = e^{i\vec k\cdot\vec r}\, u_{n,\vec k}(\vec r) \quad ; \quad \psi_{nk}(\vec r+\vec R) = e^{i\vec k\vec R}\, \psi_{nk}(\vec r)$$

$$\underset{\substack{\uparrow \\ \text{H enega samega atoma}}}{H = H_{at}} + \Delta U(\vec r)$$



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

$\psi_n(\vec r)$ so lokalizirane.

Kako konstruirati Blochovo ψ

nastavek
$$\psi_{n\vec k}(\vec r) = \sum_{\vec R} e^{i\vec k\vec R}\, \varphi(\vec r-\vec R) \qquad \varphi = \sum_n b_n \psi_n(\vec r)$$
$$= \sum_{n\vec R} e^{i\vec k\cdot\vec R}\, b_n \psi_n(\vec r-\vec R)$$

$$(H_{at} + \Delta U)\,\psi(\vec r) = \varepsilon(\vec k)\,\psi(\vec r) \qquad / \int \psi_m^*\, d\vec r$$

$$\int \psi_m^*(\vec r)\, H_{at}\, \psi(\vec r)\, d\vec r = E_m \int \psi_m^*(\vec r)\, \psi(\vec r)\, d\vec r$$

$$\int \psi_m^* \psi_n\, d\vec r = \sum_{n\vec R} b_n e^{i\vec k\cdot\vec R} \int \psi_m^*(\vec r)\, \psi_n(\vec r-\vec R)\, d\vec r =$$
$$= \underset{\text{pri } \vec R=0}{b_m} + \sum_{n\vec R\neq 0} b_n e^{i\vec k\vec R} \underbrace{\int \psi_m^*\, \psi_n(\vec r-\vec R)\, d\vec r}_{\ll \text{ za } \vec R\text{, ki niso sosedje}}$$

$$(\varepsilon(\vec k) - E_m) \int \psi_m^*(\vec r)\, \psi(\vec r)\, d\vec r = \int \psi_m^*(\vec r)\, \Delta U(\vec r)\, \psi(\vec r)\, d\vec r$$

$$(\varepsilon(\vec k) - E_m)\, b_m + (\varepsilon(\vec k) - E_m) \sum_{n\vec R\neq 0} \int \psi_m^*(\vec r)\, \psi_n(\vec r-\vec R)\, d\vec r\; b_n e^{i\vec k\vec R} =$$
$$= \underbrace{\sum_n b_n \int \psi_m^*(\vec r)\, \Delta U(\vec r)\, \psi_n(\vec r)\, d\vec r}_{\text{pri } \vec R=0} + \sum_{n\vec R\neq 0} b_n e^{i\vec k\vec R} \int \psi_m^*\, \Delta U(\vec r)\, \psi_n(\vec r-\vec R)\, d\vec r$$

Poseben primer stanje - s , $b_n = 0$ razen za $n=0$ $\Rightarrow \sum_n b_n = b_0$

Rešujemo prejšnji sistem

$$\varepsilon(\vec k) = \overset{E_m}{E_s} - \frac{\beta + \sum_{\vec R} \gamma(\vec R)\, e^{i\vec k\vec R}}{1 + \sum_{\vec R} \alpha(\vec R)\, e^{i\vec k\vec R}}$$

$$\varphi(\vec r) = b_0 \psi_0$$
$$\alpha(\vec R) = \int \varphi^*(\vec r)\, \varphi(\vec r-\vec R)\, d\vec r$$

$$\beta(\vec R) = -\int \varphi^*(\vec r)\, \Delta U(\vec r)\, \varphi(\vec r)\, d\vec r$$
$$\gamma(\vec R) = -\int \varphi^*(\vec r)\, \Delta U(\vec r)\, \varphi(\vec r-\vec R)\, d\vec r$$

Lahko zamenimo α

$$\Rightarrow \quad \mathcal{E}(\vec{k}) = E_s - \beta - \sum_{\uparrow} \gamma(\vec{R}) \cos \vec{k}\vec{R}$$

najbližji sosedi

Primer FCC $\quad \vec{R}_i = \left\{ \frac{a}{2}(\pm 1, \pm 1, 0), \frac{a}{2}(\pm 1, 0, \pm 1), \frac{a}{2}(0, \pm 1, \pm 1) \right\}$

najbližji sosedi

Zaradi simetrije $\gamma(R_i) = \gamma$

$$\mathcal{E}(\vec{k}) = -\beta - 4\gamma \Big(\cos\left(a \frac{k_x + k_y}{2}\right) + \cos\left(a \frac{k_x - k_y}{2}\right) + \cos\left(a \frac{k_x + k_z}{2}\right) +$$

$$+ \cos\left(a \frac{k_x - k_z}{2}\right) + \cos\left(a \frac{k_y + k_z}{2}\right) + \cos\left(a \frac{k_y - k_z}{2}\right) \Big)$$

Primer 1D $\quad R_1 = a \quad R_2 = -a$

$$\mathcal{E}(k) = E_s - \beta - 2\gamma \cos ka$$

Gibanje e^- v periodičnem potencialu

$\psi_{n\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}}\, u_{n\vec{k}}(\vec{r})$ $\quad$ ni lastno stanje operatorja $\hat{p}$

periodična funkcija

$$\hat{p}\, \psi_{n\vec{k}}(\vec{r}) = \hbar \vec{k}\, \psi_{n\vec{k}}(\vec{r}) + e^{i\vec{k}\cdot\vec{r}}\, \hat{p}\, u_{n\vec{k}}(\vec{r})$$

	Prost e^-	Blochov e^-
opis stanj	$\vec{q}$	$n,\ \vec{k} \in 1BC$
energija	$\mathcal{E}^0 = \frac{\hbar^2 q^2}{2m}$	$\mathcal{E}_n(\vec{k})$
hitrost	$\frac{\hbar \vec{k}}{m}$	$v_n(\vec{k}) = \frac{1}{\hbar}\frac{\partial \mathcal{E}_n(\vec{k})}{\partial \vec{k}}$
val. funkcija	$\frac{1}{\sqrt{V}} e^{i\vec{q}\cdot\vec{r}}$	$\psi_{n\vec{k}}(\vec{r})$

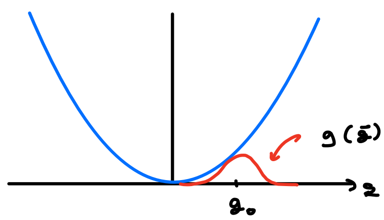
periodična $\mathcal{E}_n(\vec{k}+\vec{K})$

grupna hitrost

Gibanje prostega e^-

$$\vec{v} = \frac{\hbar \vec{k}}{m}$$

$$\hbar \dot{\vec{k}} = -e(\vec{E} + \vec{v} \times \vec{B})$$



$$\psi(\vec{r}, t) = \sum_{\vec{q}} g(\vec{q})\, e^{i\vec{q}\cdot\vec{r}}\, e^{-\frac{\mathcal{E}^0(\vec{q})}{\hbar} t}$$

časovni razvoj

Valovni paket

Razvoj energije $\quad \mathcal{E}^0(q) = \mathcal{E}^0(q^0) + (\vec{q} - \vec{q}_0) \left.\frac{\partial \mathcal{E}(q)}{\partial q}\right|_{q_0}$

$\Rightarrow$ grupna hitrost

Blochove enačbe

Smo v periodičnem potencialu

$\mathcal{E}_n(\vec{k})$ vhodni podatek

1. Indeks pasu se ohranja, n
2. $\vec{v}_n(\vec{k}) = \frac{1}{\hbar}\frac{\partial \mathcal{E}_n(\vec{k})}{\partial \vec{k}} = \frac{1}{\hbar}\nabla_{\vec{k}}\,\mathcal{E}_n(\vec{k})$
3. $\hbar\dot{\vec{k}} = -e\left(\vec{E}(\vec{r},t) + \vec{v}_n(\vec{k})\times\vec{B}(\vec{r},t)\right)$

Blochove enačbe

$\vec{k}$ ... kristalni valovni vektor

uporabimo za izračun $\vec{k}$

Izpeljava ?

$$\mathcal{E}_n(\vec{k}) - e\phi(\vec{r},t) = \text{konst} \quad \text{za } \forall t \quad \Big/ \frac{d}{dt}$$

$$\underbrace{\frac{1}{\hbar}\frac{\partial \mathcal{E}_n(\vec{k})}{\partial \vec{k}}}_{\vec{v}_n(\vec{k})}\dot{\vec{k}}\hbar - e\frac{\partial\phi}{\partial\vec{r}}\underset{\vec{v}_n(\vec{k})}{\underset{\parallel}{\dot{\vec{r}}}} = 0$$

$$\vec{v}_n(\vec{k})\left(\dot{\vec{k}}\hbar - e\vec{E}(\vec{r},t) + \underbrace{e\vec{v}\times\vec{B}}\right) = 0$$

lahko prištejemo karkoli
kar je $\perp$ na $\vec{B}$

Primer: $\vec{E} = \text{konst}$, 1D

pokrivalni integral

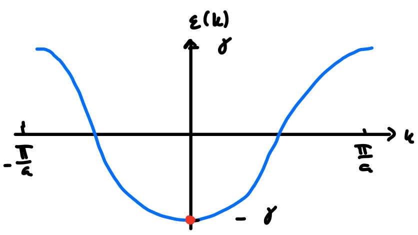
$$\mathcal{E}(\vec{k}) = -\gamma\cos ka$$

$$\hbar\dot{k} = -eE \Rightarrow k(t) = k(0) - \frac{eE}{\hbar}t$$

$$\mathcal{E}(k,t) = \mathcal{E}\left(k_0 - \frac{eE}{\hbar}t\right)$$

$$v(k(t)) = v\left(k_0 - \frac{eE}{\hbar}t\right)$$

$$\mathcal{E}(k) = -\gamma\cos\frac{eE}{\hbar}ta \qquad k(0) = 0$$



Blochove oscilacije $\quad \frac{eE}{\hbar}a\,t_B = 2\pi \qquad t_B = \frac{h}{eEa}$

$$v = \frac{1}{\hbar}\frac{\partial\mathcal{E}(k)}{\partial k} = -\frac{\gamma a}{\hbar}\sin ka = -\frac{\gamma a}{\hbar}\sin\frac{eEa}{\hbar}t$$

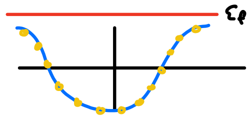
$$x = \int v\,dt = x_0 + \frac{\gamma a\hbar}{\hbar\, eEa}\cos\frac{eEa}{\hbar}t$$

Amplituda Bloch oscilacij $\quad x_B = \frac{\gamma}{eE}$

Zapolnjen pas, j_{el} in j_a

$$\vec{j} = -ne\vec{v}$$

$$j_{n,el} = -e \int_{BC} \frac{d^3k}{4\pi^3} \frac{1}{\hbar} \frac{\partial \varepsilon_n(\vec{k})}{\partial \vec{k}} = 0$$



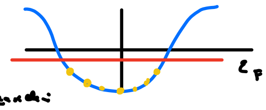
Polno zapolnjen pas ne prispeva k el. ali energijskem toku

$$j_{n,a} = \int_{BC} \frac{d^3k}{4\pi^3} \underbrace{\varepsilon_n(\vec{k}) \frac{1}{\hbar} \nabla_k \varepsilon_n(\vec{k})}_{\frac{1}{2\hbar}\nabla_k \varepsilon_n^2(\vec{k})} = 0$$

V 1BC je 2N stanj, N el. stanj, zaradi spina

Pojem vrzeli

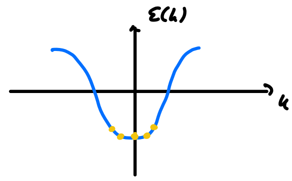
Kaj pa ne polno zapolnjen pas?



$$0 = -e \int_{\text{zasedeni}} \frac{d^3k}{4\pi^3} \vec{v}_n(\vec{k}) - e \int_{\text{nezasedeni}} \frac{d^3k}{4\pi^3} \vec{v}_n(\vec{k}) = \vec{j}_{\text{zasedeni}} + \vec{j}_{\text{nezasedeni}}$$

Efektivna masa

$$\varepsilon_n(\vec{k}_0 + \delta\vec{k}) = \varepsilon_n(\vec{k}_0) + \sum_{i=x,y,z} \underbrace{\frac{\partial \varepsilon_n(\vec{k})}{\partial k_i}}_{=0} \delta k_i + \frac{1}{2} \sum_{ij} \frac{\partial^2 \varepsilon_n}{\partial k_i \partial k_j} \delta k_i \delta k_j$$



$$\varepsilon^0(k) = \frac{\hbar^2 k^2}{2m} \qquad \frac{1}{m} = \frac{1}{\hbar^2} \frac{\partial^2 \varepsilon}{\partial k^2} \text{ v minimumu}$$

$$[M_n^{-1}(\vec{k})]_{ij} = \pm \frac{1}{\hbar^2} \frac{\partial^2 \varepsilon_n}{\partial k_i \partial k_j}$$

($+$: e^-, $-$: vrzeli) Tenzor efektivne mase

Blochov e^- v statičnem mag. polju

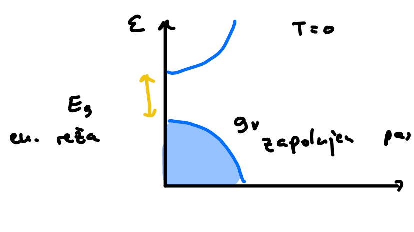
$$\vec{v}(\vec{k}) = \frac{1}{\hbar} \frac{\partial \varepsilon(\vec{k})}{\partial \vec{k}} \qquad \hbar\dot{\vec{k}} = -e\vec{v}(\vec{k}) \times \vec{B} \qquad \vec{B} = (0,0,B)$$

$$\Rightarrow \dot{k}_z = 0 \qquad k_z \text{ ... konst. gibanja}$$

$$\dot{\varepsilon}(\vec{k}) = \nabla_k \varepsilon(\vec{k}) \dot{\vec{k}} \hbar = \vec{v}(\vec{k}) (-e) (\vec{v}(\vec{k}) \times \vec{B}) = 0$$

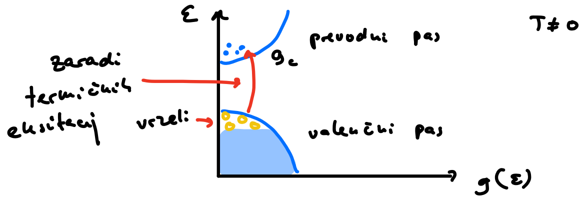
$\varepsilon(\vec{k})$ ... konst. gibanja

Homogeni polprevodniki



Polprevodnik $E_g \sim 1eV$

Izolator $E_g \sim 5eV$



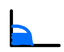
n_c ... gostota elektronov v prevodnem pasu
p_v ... gostota vrzeli v prevodnem pasu

$$n_c \propto e^{-E_g/2k_BT}$$

Primer $E_g = 4\,eV$ $\quad n_c \sim 10^{-35}$ $\quad$ pri $k_BT \sim 0{,}025\,eV$

$E_g = 0{,}25\,eV$ $\quad n_c \sim 10^{-2}$ $\quad$ sobna T

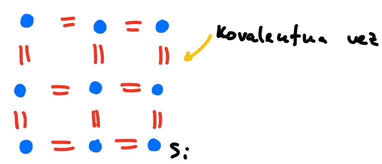
	Specifična upornost [Ω cm]
kovina	10^{-6}
polprevodnik	$10^{-3} - 10^{9}$
izolator	10^{22}



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

- Kovine: σ pada s T ker τ pada s T.
- Polprevodnik: σ močno naraste s T, ker $n \propto e^{-E_g/2k_BT}$

Polprevodniki kristali zrejo v strukturo diamanta

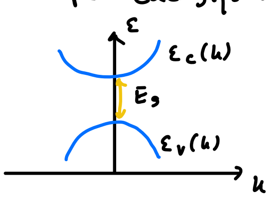


- Jih tvorijo: Si, Ge, (C) IV skupina

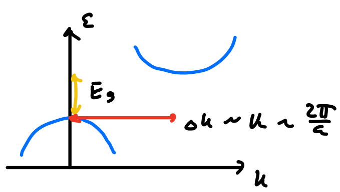
Tipične energijske reže

Si	1,12	1,17
Ge	0,67	0,75
InAs	0,35	0,43
	pri 300 K	0K

Tipe energijskih rež



Direktna reža



Indirektna reža

ⓐ Merimo direktno režo

$\hbar\omega_f = E_g$ se močno poveča absorpcija

ⓑ Merimo indirektno režo

Ni mogoč zgornji proces

$\hbar\omega_f = E_g \pm \hbar\omega(\vec{q})$

emisija fononov
absorpcija

Naj bo $E_g \sim 1\,eV$, k_f val. vektor fotona, primerjam z $k = \frac{2\pi}{a}$

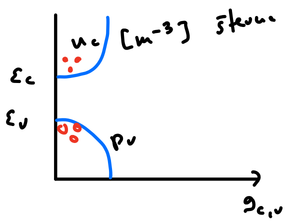
$$E_f = E_g = h\nu = h\frac{c}{\lambda} \Rightarrow \lambda = \frac{hc}{E_g} \doteq 10^3\,nm$$

$$\Rightarrow k_f \sim \frac{2\pi}{\lambda} \sim 10^{-2}\,nm^{-1} \ll k$$

Zanima nas dogajanje okoli min in max

$$\varepsilon_c(k) = \varepsilon_c + \underbrace{\frac{\hbar^2}{2}\sum_{\mu\nu} k_\mu (M_c^{-1})_{\mu\nu} k_\nu}_{\frac{\hbar^2 k^2}{2m}} \overset{\text{v lastnem sist}}{=} \varepsilon_c + \frac{\hbar^2}{2}\left(\frac{k_1^2}{m_{1c}} + \frac{k_2^2}{m_{2c}} + \frac{k_3^2}{m_{3c}}\right)$$

$$\varepsilon_v(k) = \varepsilon_v - \frac{\hbar^2}{2}\sum_{\mu\nu} k_\mu (M_v^{-1})_{\mu\nu} k_\nu = \varepsilon_v - \frac{\hbar^2}{2}\left(\frac{k_1^2}{m_{1v}} + \frac{k_2^2}{m_{2v}} + \frac{k_3^2}{m_{3v}}\right)$$



$$n_c = \int_{\varepsilon_v}^{\infty} d\varepsilon\, g_c(\varepsilon)\,\frac{1}{e^{\varepsilon-\mu/kT}+1}$$

$$p_v = \int_{-\infty}^{\varepsilon_v} d\varepsilon\, g_v(\varepsilon)\,\Big(\underbrace{1 - \frac{1}{e^{\varepsilon-\mu/kT}+1}}_{\frac{1}{e^{\mu-\varepsilon/kT}+1}}\Big)$$

Pri $T=0$ $\quad n_c = p_v = 0 \Rightarrow \varepsilon_v < \mu < \varepsilon_c$

$k_B T \sim 0{,}025\,eV$

Približek nedegeneriranega polprevodnika: $\mu - \varepsilon_c \gg k_B T$, $\varepsilon_v - \mu \gg k_B T$ dober približek

$$\frac{1}{e^{\varepsilon-\mu/kT}+1} \sim e^{-\varepsilon-\mu/kT} \qquad \frac{1}{e^{\mu-\varepsilon/kT}+1} \sim e^{-\frac{\mu-\varepsilon}{kT}}$$

$$n_c = \int_{\varepsilon_c}^{\infty} d\varepsilon\, g_c(\varepsilon)\, e^{-\frac{\varepsilon-\varepsilon_c}{kT}}\, e^{-\frac{\varepsilon_c-\mu}{kT}} \equiv N_c(T)\, e^{-\varepsilon_c-\mu/kT}$$

exp odvisnost od T

potenčna odv. od T

$$p_v = \int_{-\infty}^{\varepsilon_v} d\varepsilon\, g_v(\varepsilon)\, e^{-\varepsilon_v-\varepsilon/kT}\, e^{-\mu-\varepsilon_v/kT} \equiv P_v(T)\, e^{-\mu-\varepsilon_v/kT}$$

$$N_c = \int_{\varepsilon_c}^{\infty} d\varepsilon\, g_c(\varepsilon)\, e^{-\varepsilon-\varepsilon_c/kT} \qquad g_c(\varepsilon) = \sqrt{2|\varepsilon-\varepsilon_c|}\,\frac{m_c^{3/2}}{\pi^2\hbar^3}$$

$$x = \frac{\varepsilon-\varepsilon_c}{k_B T} \qquad dx = \frac{d\varepsilon}{kT}$$

$$N_c = \frac{\sqrt{2}\, m_c^{3/2} (kT)^{3/2}}{\pi^2\hbar^3}\underbrace{\int_0^\infty dx\, x^{1/2} e^{-x}}_{\sqrt{\pi}/2} = \frac{1}{4}\left(\frac{2 m_c k_B T}{\pi\hbar^2}\right)^{3/2}$$

$$\boxed{\begin{array}{ll} N_c = \frac{1}{4}\left(\frac{2 m_c k_B T}{\pi\hbar^2}\right)^{3/2} & P_v = \frac{1}{4}\left(\frac{2 m_v k_B T}{\pi\hbar^2}\right)^{3/2} \\ n_c = N_c\, e^{-\varepsilon_c-\mu/kT} & p_v = P_v\, e^{-\mu-\varepsilon_v/kT} \end{array}}$$

Primer čistega prevodnika $n_c = p_v$

$n_i \equiv n_c = p_v$ $\qquad n_i^2 = n_c p_v = N_c P_v\, e^{-\varepsilon_c - \varepsilon_v / kT}$ (ni več μ)

intrinsic

$$n_i = \sqrt{N_c P_v}\; e^{-E_g/2k_0T} \qquad E = \varepsilon_c - \varepsilon_v$$

Iščemo μ: $n_c = p_v$ (ohranitev naboja)

$$N_c\, e^{-\varepsilon_c - \mu / kT} = P_v\, e^{-\mu - \varepsilon_v/kT} \qquad / \ln$$

$$-\frac{\varepsilon_c - \mu}{kT} = \ln \frac{P_v}{N_c} - \frac{\mu - \varepsilon_v}{kT}$$

$$\mu = \frac{1}{2}(\varepsilon_c + \varepsilon_v) + \frac{1}{2} k_0 T \ln \frac{P_v}{N_c}$$

$$\mu = \varepsilon_v + \frac{1}{2} E_g + \frac{3}{4} k_0 T \ln \frac{m_v}{m_c}$$

Pri $T=0$ je μ na sredini reže

Čisti polprevodnik

$n_i = n_c = p_v \qquad n_c = N_c(T)\, e^{-\varepsilon_c - \mu_i / k_0T} \qquad n_v = N_v(T)\, e^{-\mu_i - \varepsilon_v / k_0 T}$

Dopirani polprevodniki

$n_c - p_v = \Delta n \neq 0 \qquad n_c = N_c(T)\, e^{-\varepsilon_c - \mu / k_0T}$

$n_c p_v = n_i^2 \qquad n_v = N_v(T)\, e^{-\mu - \varepsilon_v / k_0T}$

spremeni se le μ

$n_c - p_v = \Delta n \qquad / \cdot n_c$

$n_c^2 - n_i^2 = n_c \Delta n$

$$\Rightarrow n_c = \frac{1}{2}\left(\Delta n \pm \sqrt{\Delta n^2 + 4 n_i^2}\right) \qquad \Rightarrow \begin{Bmatrix} n_c \\ p_v \end{Bmatrix} = \frac{1}{2}\left(\sqrt{\Delta n^2 + 4n_i^2} \pm \Delta n\right)$$

$\frac{\Delta n}{n_i}$ ... merilo za vpliv nečistoč

$\frac{\Delta n}{n_i} \gg 1$ za močno dopiran polprev.

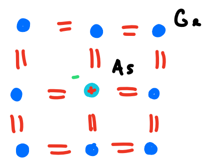
$$n_c = N_c\, e^{-\beta(\varepsilon_c - \mu)}$$
$$n_i = N_c\, e^{-\beta(\varepsilon_c - \mu_i)}$$
$$n_c = n_i\, e^{-\beta(\mu - \mu_i)} \qquad \Rightarrow \qquad \Delta n = 2 n_i \sinh \beta(\mu - \mu_i)$$
$$p_v = n_i\, e^{-\beta(\mu - \mu_i)}$$

Nivoji nečistoč

1. Donorske nečistoče: prispevajo dodatne e^-
2. Akceptorske nečistoče: prispevajo dodatne vrzeli

$3s^2 3p^1$	$3s^2 3p^2$	$3s^2 3p^3$
Al	Si	P
$4s^2 4p^1$	$4s^2 4p^2$	$4s^2 4p^3$
Ga	Ge	As
Akceptorske		Donorske

Donorske



$\Rightarrow$ Predstavljamo si lahko kot H atom v dielektriku

$m_e = m^*$

$\frac{m^*}{m_e} = 0{,}1$

H atom

Bohrov radij

$a_0 = \frac{4\pi\varepsilon_0 \hbar^2}{m e^2} = 0{,}53 \cdot 10^{-10}\,m$

$R_y = \frac{\hbar^2}{2 m a_0^2} \doteq 13{,}6\,eV$

$\varepsilon_{Ge} = 16 > \varepsilon_{Si}$

Dielektrična konst.

Za nas $r_0 = \frac{m}{m_0}\varepsilon a_0$

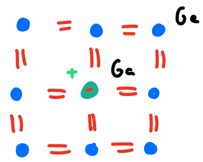
$\varepsilon_B = \frac{m^*}{m}\frac{1}{\varepsilon^2} R_y \sim 0{,}0127\,eV$

Binding energy

As v Ge

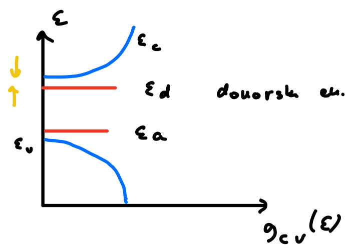
šibko vezan e^- As

Akceptorske



$\varepsilon_c - \varepsilon_d = \varepsilon_b^d$

$\varepsilon_a - \varepsilon_v = \varepsilon_b^a$



Donorske $\varepsilon_b = \varepsilon_c - \varepsilon_d$ [eV]

	P	As	Sb
Si	0,044	0,049	0,039
Ge	0,012	0,013	0,0096

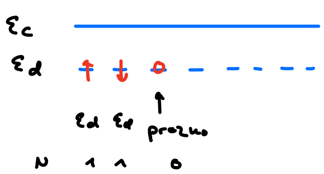
Zasedenost nivojev nečistoč

$n_c = N_c\, e^{-\beta(\varepsilon_c - \mu)} \qquad p_v = P_v\, e^{-\beta(\mu - \varepsilon_v)}$

Donorski nivoji

$$\langle n \rangle = \frac{\sum_j N_j e^{-\beta(\varepsilon_j - N_j \mu)}}{\sum_j e^{-\beta(\varepsilon_j - N_j\mu)}}$$

Primer



$$\langle n \rangle = \frac{2 e^{-\beta(\varepsilon_d - \mu)} + 0}{2 e^{-\beta(\varepsilon_d - \mu)} + 1} = \frac{1}{1 + \frac{1}{2} e^{\beta(\varepsilon_d - \mu)}}$$

Gostota el. v donorskih nečistočah

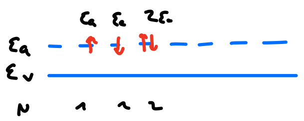
št. donorjev pri T=0

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

ker $\varepsilon_d - \mu \gg k_B T$

⇒ $n_d \ll N_d$ ⇒ Pri sobni T so nivoji nečistoč ionizirani, večina jih gre v prevodni pas

Akceptorski nivoji



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

$$\langle p\rangle = 2-\langle n\rangle = \frac{1}{1+\frac{1}{2}e^{\beta(\mu-\varepsilon_a)}}$$

gostota vrzeli v akcep. pasu

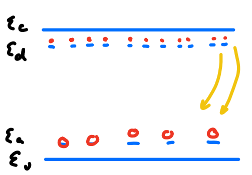
$$p_a = N_a\langle p\rangle = \frac{N_a}{1+\frac{1}{2}e^{\beta(\mu-\varepsilon_a)}}$$

koncentracija akceptorskih nečistoč

Za čist polprevodnik $n_c = p_v$ (ohranitev naboja)

Vzemimo N in P dopiran

N_d in N_a, $N_d > N_a$



⇒ Pri $T=0$ gredo e^- v najnižje stanje

$$n_c + n_d = N_d - N_a + p_v + p_a \qquad \text{splošno}$$

Pri sobni T, $n_d \ll N_d$, $p_a \ll N_a$

⇒ $n_c - p_v = N_d$ za donorske

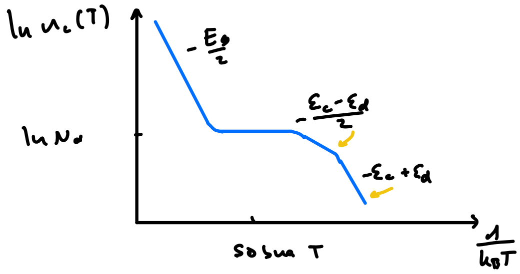
$n_c - p_v = -N_a$ za akceptorske

Močno dopiran polprevodnik $\Delta n \gg n_i$ $\qquad \Delta n = n_c - p_v$

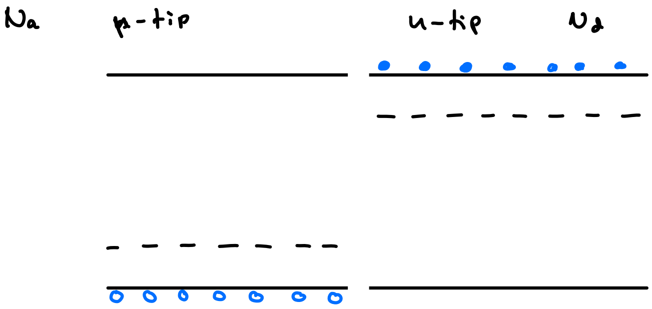
$\Delta n = N_d \gg n_i$: $\quad n_c = N_d$, $\quad p_v = n_i^2/N_d \ll n_c$

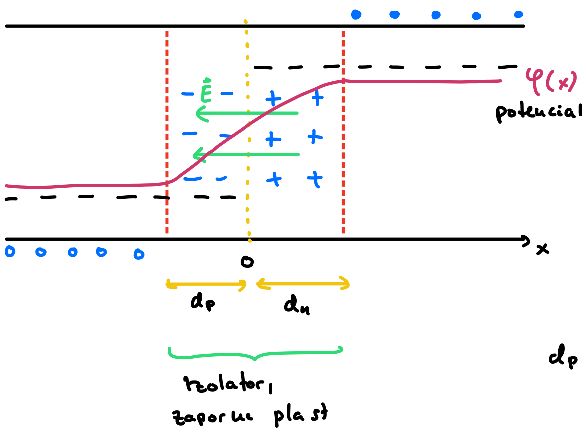
$$\left\{ \begin{matrix} n_c \\ p_v \end{matrix} \right\} = \frac{1}{2}\left(\sqrt{\Delta n^2 + 4n_i^2} \pm \Delta n\right)$$

$\Delta n = -N_a$: $\quad p_v = N_a$, $\quad n_c = n_i^2/N_a$



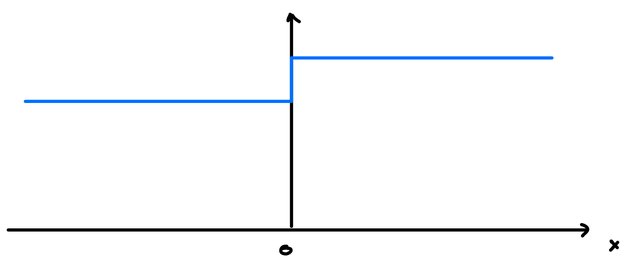
Nehomogeni polprevodniki, p-n stik





e^- in vrzeli se rekombinirajo, ostanejo ioni

$d_p, d_n \sim 10 - 1000\ nm$



$$N_a(x) = \begin{cases} N_a & x<0 \\ 0 & x>0 \end{cases} \qquad N_d(x) = \begin{cases} 0 & x<0 \\ N_d & x>0 \end{cases}$$

$$H_{c,v} = \varepsilon_{c,v}(x) - e\varphi(x)$$

$$\varepsilon_c(x) = \varepsilon_c - e\varphi(x)$$

$$\varepsilon_v(x) = \varepsilon_v - e\varphi(x)$$

$$n_c(x) = N_c(T)\, e^{-\beta(\varepsilon_c - e\varphi(x) - \mu)}$$

$$p_v(x) = P_v(T)\, e^{-\beta(\mu - \varepsilon_v + e\varphi(x))}$$

$$n_c(x \to \infty) = N_d = N_c(T)\, e^{-\beta(\varepsilon_c - e\varphi(\infty) - \mu)}$$

$$p_v(x \to -\infty) = N_a = P_v(T)\, e^{-\beta(\mu - \varepsilon_v + e\varphi(-\infty))}$$

$$\frac{N_d N_a}{N_c(T) P_v(T)} = e^{-\beta(\varepsilon_c - \varepsilon_v + e(\underbrace{\varphi(-\infty) - \varphi(\infty)}_{-\Delta\varphi}))}$$

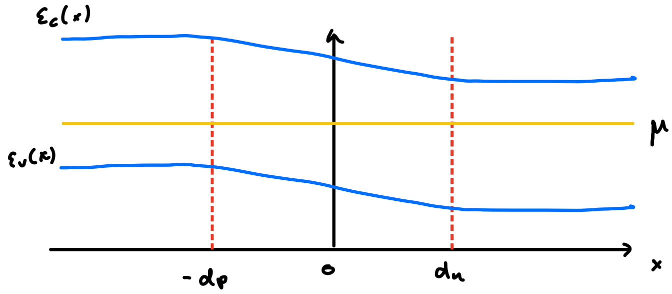
$$e\Delta\varphi = \underbrace{\varepsilon_c - \varepsilon_v}_{E_g} + k_B T \ln \frac{N_d N_a}{N_c(T) P_v(T)}$$

$$\frac{n_c(x)}{N_d} = e^{-\beta e(\varphi(\infty) - \varphi(x))}$$

$$n_c(x) = N_d\, e^{-\beta e(\varphi(\infty) - \varphi(x))}$$

$$p_v(x) = N_a\, e^{-\beta e(\varphi(-\infty) - \varphi(x))}$$

$$\varepsilon_c(x) = \varepsilon_c - e\varphi(x)$$

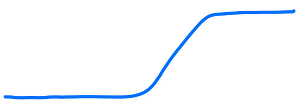


v term. din. ravnovesju je μ povsod enak

$$\nabla^2\varphi = \frac{\rho(x)}{\varepsilon\varepsilon_0}$$
$$\Downarrow$$
$$\frac{d^2\varphi}{dx^2} = \frac{\rho(x)}{\varepsilon\varepsilon_0}$$

$$\varphi(x) = \begin{cases} \varphi(\infty) & x > d_n \\ \varphi(\infty) - \frac{e^2 N_d}{2\varepsilon\varepsilon_0}(x-d_n)^2 & 0 < x < d_n \\ \varphi(-\infty) + \frac{eN_a}{2\varepsilon\varepsilon_0}(x+d_p)^2 & -d_p < x < 0 \\ \varphi(-\infty) & x < -d_p \end{cases} \Leftarrow$$

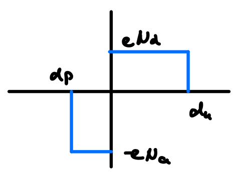
$$\rho(x) = e\left(N_d(x) - N_a(x) - n_c(x) + p_v(x)\right) = \begin{cases} 0 & x > d_n \\ eN_d & 0 < x < d_n \\ -eN_a & -d_p < x < 0 \\ 0 & x < -d_p \end{cases}$$



Iščemo d_n, d_p. Zveznost in odvedljivost pri $x=0$

Robni pogoji pri $x = 0^+, 0^-$

1. $\varphi(0^+) = \varphi(0^-)$
2. $\varphi'(0^+) = \varphi'(0^-)$



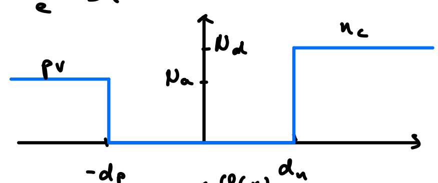
2. $\frac{eN_d}{\varepsilon\varepsilon_0} d_n = \frac{eN_a}{\varepsilon\varepsilon_0} d_p \Rightarrow N_d d_n = N_a d_p$ (kondenzator naboja)

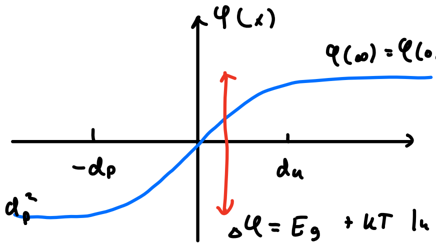
1. $\varphi(\infty) - \frac{eN_d d_n^2}{2\varepsilon\varepsilon_0} = \varphi(-\infty) + \frac{eN_a d_p^2}{2\varepsilon\varepsilon_0}$

$$N_d d_n^2 + N_a d_p^2 = \frac{2\varepsilon\varepsilon_0}{e}\Delta\varphi \qquad \Delta\varphi = \varphi(\infty) - \varphi(-\infty)$$

$$d_n^2\left(N_d + \frac{N_d^2}{N_a}\right) = d_n^2 \frac{N_d}{N_a}(N_a + N_d) = \frac{2\varepsilon\varepsilon_0}{e}\Delta\varphi$$

$$\boxed{\begin{matrix} d_n \\ d_p \end{matrix} = \sqrt{\frac{(N_a/N_d)^{\pm 1}}{(N_a+N_d)} \frac{2\varepsilon\varepsilon_0\Delta\varphi}{e}}}$$

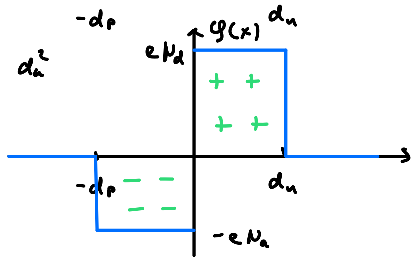




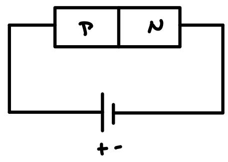
$\varphi(\infty) = \varphi(0) + \frac{eN_d}{2\varepsilon\varepsilon_0} d_n^2$

$\varphi(-\infty) = \varphi(0) - \frac{eN_a}{2\varepsilon\varepsilon_0} d_p^2$

$\Delta\varphi = E_g + kT \ln \frac{N_a N_d}{N_c P_v}$



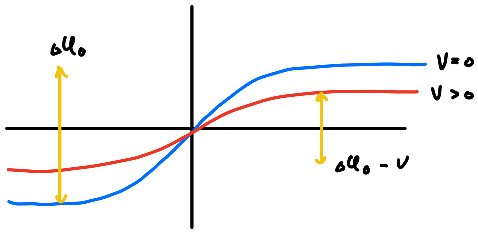
P-N stik priključen na napetost



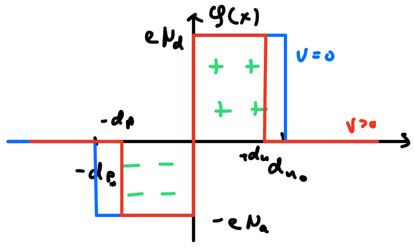
$V > 0$ v prevodni smeri

$$\Delta\varphi = \Delta\varphi_0 - V$$

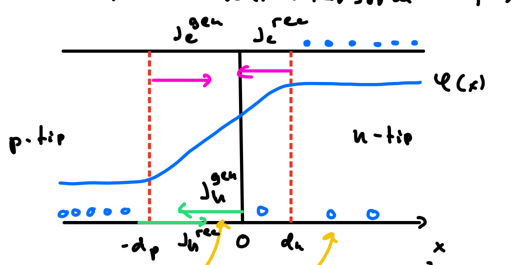
$$d_n = \sqrt{c\,\Delta\varphi}$$
$$d_n(V=0) = \sqrt{c\,\Delta\varphi_0}$$
$$d_n(V>0) = \sqrt{c(\Delta\varphi_0 - V)} = d_n(V=0)\sqrt{1 - \frac{V}{\Delta\varphi_0}}$$



$\Delta\varphi$ se zmanjša in d_n se zmanjša



I-V karakteristika P-N stika



$p_0 = \frac{n_i^2}{N_d} \ll n_e$

pade po potencialu

Imamo tudi nekaj vrzeli

Nosilci toka so e^- in vrzeli

$$j_e = -e\,J_e$$
$$j_h = +e\,J_h$$

gostota el. toka — Sretok toka

Pri $V=0$ $J_e = J_h = 0$

Pri $V \neq 0$ $J_h = J_h^{gen} + J_h^{rec}$

generacijski tok — rekombinacijski tok

$$J_h^{gen} \neq J_h^{gen}(T)$$
$$J_h^{rec} = J_h^{rec}(T) \propto e^{-\beta e(\Delta\varphi_0 - V)}$$

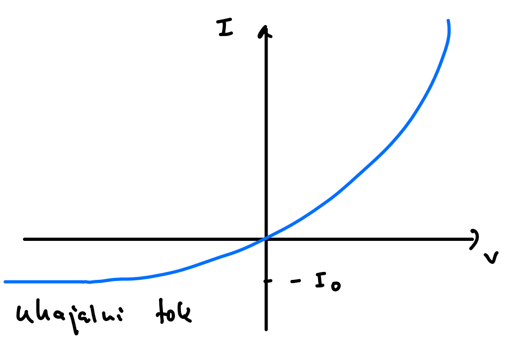
Pri $V=0$ $J_h = 0 \Rightarrow J_h^{gen} = J_h^{rec} \Rightarrow J_h^{rec} = J_h^{gen} e^{\beta e V}$

$$J_h(V) = J_h^{rec}(V) - J_h^{gen} = \underline{J_h^{gen}(e^{\beta e V} - 1)}$$

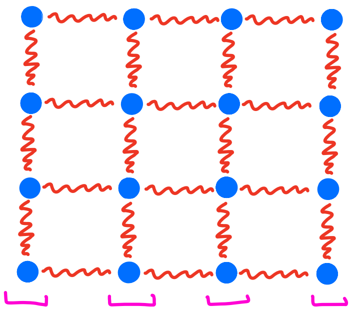
Podobno za e $J_e(V) = -(e^{\beta e V} - 1)\,J_e^{gen}$

Celoten tok $j_{el} = e\,J_h(V) - e\,J_e(V)$

$$= e\,(J_h^{gen} + J_e^{gen})(e^{\beta e V} - 1)$$



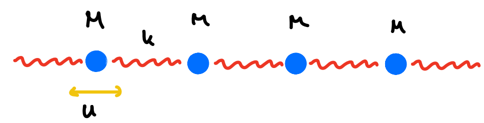
Mrežna nihanja



longitudinalno	→	←	→	←
transverzalno	↑	↓	↑	↓

Nihanje mrežnih ravnin

Mrežne ravnine združimo, z maso M →



odmik

$\vec{r}_n(t) = \vec{R}_n + \vec{u}_n(t)$

$x_n(t) = na + u_n(t)$

ravnovesna lega

$$U^{harm} = \frac{k}{2}\sum_n (u_{n+1} - u_n)^2$$

potencial $\frac{kx^2}{2}$ elastična energija

Enačba gibanja $\quad F_n = -\frac{\partial U^{harm}}{\partial u_n} = M\ddot{u}_n$

sila na n-ti delec

$$M\ddot{u}_n = k(u_{n+1} - u_n - u_n + u_{n-1})$$

$$M\ddot{u}_n = k(u_{n+1} - 2u_n + u_{n-1}) \qquad \text{Diskretna oblika val. enačbe}$$

Nastavek $\quad u_n(t) = u_0\, e^{i(kna - \omega t)}$

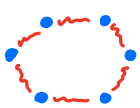
$$-M\omega^2 u_0 = k u_0 \left(e^{ika} - 2 + e^{-ika}\right)$$

$$\omega^2 = 2\frac{k}{M}(1 - \cos ka)$$

$$\omega^2 = 4\frac{k}{M}\sin^2\frac{ka}{2}$$

$$\omega = 2\sqrt{\frac{k}{M}}\left|\sin\frac{ka}{2}\right|$$

Periodični robni pogoji



N... atomov

$$u_{N+1} = u_1$$

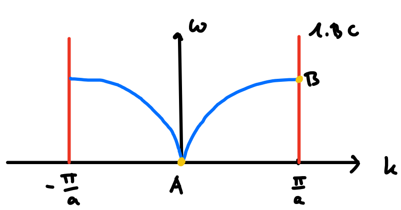
$$e^{ik(N+1)a} = e^{ika}$$

$$e^{ikNa} = 1 = e^{i2\pi n}$$

$$k = n\frac{2\pi}{Na} = n\frac{2\pi}{L} \qquad k \text{ je diskreten.}$$

Za N nihal dobimo N lastnih nihaj

1.BC $\quad -\frac{\pi}{a} < k < \frac{\pi}{a} \qquad -\frac{N}{2} < n \leq \frac{N}{2}$



v točki A $\omega = 0,\ k = 0$ translacija, ni nihanja
ničelno nihanje

B $k = \frac{\pi}{a}$ $\omega = 2\sqrt{\frac{k}{M}}$

$u_n(t) = u_0\, e^{i(n\pi - \omega t)}$ $\quad u_n(t=0) = u_0\, e^{in\pi}$

$n = \quad 0 \quad 1 \quad 2 \quad 3$

$\frac{u_n}{u_0} = \quad 1 \quad -1 \quad 1 \quad -1$

lastno nihanje $\Leftrightarrow$ v B $v_g = 0$
A $v_g = \max$

Grupna hitrost
$$v_g = \frac{d\omega}{dk} = a\sqrt{\frac{k}{M}} \cos\frac{ka}{2}$$

Vidimo $\omega(k) = \omega(k + K)$
$\uparrow$
$K = \frac{2\pi}{a}, \frac{4\pi}{a}, \dots$ vektor recipročne mreže

Za velike λ, majhne k $\Rightarrow$ zvezna limita $\quad u_n \to u(x = na)$

$$M\ddot{u}(x) = k\,(u(x+a) - 2u(x) + u(x-a))\,\frac{a^2}{a^2}$$

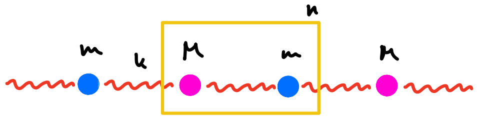
$$M\ddot{u}(x) = ka^2 \frac{d^2u}{dx^2}$$

$$\ddot{u} = \underbrace{\frac{kc^2}{M}}_{c^2} u'' \qquad c = a\sqrt{\frac{k}{M}}$$

za $ka \ll 1$ $\quad \omega = 2\sqrt{\frac{k}{M}}\left|\sin\frac{ka}{2}\right| \doteq 2\sqrt{\frac{k}{M}}\frac{ka}{2} = k\, a\sqrt{\frac{k}{M}} = k\,c$

linearna disperzija
kot zvočno valovanje

Dvoatomna veriga



$$U^{harm} = \frac{k}{2}\sum_n (u_n - v_n)^2 + (u_{n+1} - v_n)^2$$

$$F_{u_n} = -\frac{\partial U^{harm}}{\partial u_n} = -k\,(u_n - v_n + u_n - v_{n-1})$$

$$F_{v_n} = -\frac{\partial U^{harm}}{\partial v_n} = -k\,(v_n - u_n + v_n - u_{n+1})$$

$$M\ddot{u}_n = -k(2u_n - v_n - v_{n-1})$$
$$m\ddot{v}_n = -k(2v_n - u_n - u_{n+1})$$

nastavek $\begin{cases} u_n = u_0\, e^{i(\omega t - kna)} \\ v_n = v_0\, e^{i(\omega t - kna)} \end{cases}$

$$M u_0 \omega^2 = k(2u_0 - v_0 - v_0\, e^{+ika})$$
$$M v_0 \omega^2 = k(2v_0 - u_0 - u_0\, e^{-ika})$$

$$\begin{bmatrix} M\omega^2 - 2k & k(1 + e^{+ika}) \\ k(1 + e^{-ika}) & m\omega^2 - 2k \end{bmatrix} \begin{bmatrix} u_0 \\ v_0 \end{bmatrix} = 0$$

det $= 0$

$$\Rightarrow \omega_\pm^2 = k\left(\frac{1}{m} + \frac{1}{M} \pm \sqrt{\left(\frac{1}{m}+\frac{1}{M}\right)^2 - \frac{4}{mM}\sin^2\frac{ka}{2}}\right)$$

obe rešitvi sta ustrezni. Dobimo dve veji!

Limita $k \to 0$

$$\omega_-^2 = k\left(\frac{1}{m}+\frac{1}{M}\right)\left(1 - \left(1 - \frac{4}{mM\left(\frac{1}{m}+\frac{1}{M}\right)^2}\sin^2\frac{ka}{2}\right)^{1/2}\right)$$

$$\doteq k\left(\frac{1}{m}+\frac{1}{M}\right)\frac{2}{mM\left(\frac{1}{m}+\frac{1}{M}\right)^2}\sin^2\frac{ka}{2}$$

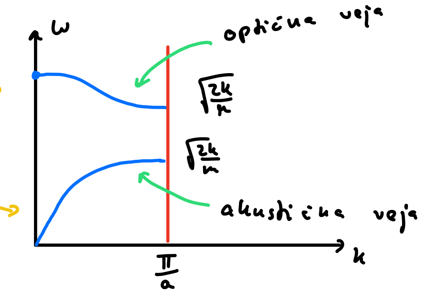
$$= \frac{2k}{m+M}\sin^2\frac{ka}{2}$$

koeficient vzmeti, valovni vektor

$$\omega_-(k\to 0) = \sqrt{\frac{2k}{m+M}}\sin\frac{ka}{2} \doteq \sqrt{\frac{k}{2(m+M)}}\,ka \quad \propto k$$

$$\Rightarrow c = \sqrt{\frac{k}{2(m+M)}}\,a$$

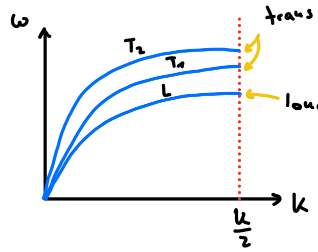
$$\omega_+(k\to 0) = \sqrt{2k\left(\frac{1}{m}+\frac{1}{M}\right)} \quad \propto \text{konst.}$$



Limita $k \to \frac{\pi}{a}$

$$\omega_\pm^2\left(k=\frac{\pi}{a}\right) = k\left(\frac{1}{m}+\frac{1}{M} \pm \sqrt{\left(\frac{1}{m}+\frac{1}{M}\right) - \frac{4}{mM}}\right) = \begin{cases} k\frac{2}{M} & \omega^+ \\ k\frac{2}{m} & \omega^- \end{cases}$$

3D enoatomski kristal

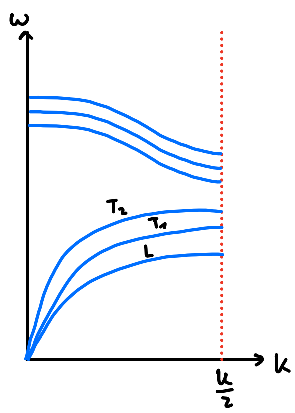


3 akustične veje

N - celic

3N - število različnih načinov nihanja

Če imamo še bazo (npr. 2 tipa atomov)



št. delcev v bazi

Število načinov nihanj $3N \cdot 2$

Kvantizacija mrežnih nihanj

1D kristal brez baze

koeficient vzmeti

$$\hat{H} = \sum_n \frac{\hat{p}_n^2}{2M} + \frac{k}{2}(\hat{u}_n - \hat{u}_{n+1})$$

$[\hat{u}, \hat{p}] = i\hbar$
$[\hat{u}_n, \hat{p}_m] = i\hbar\,\delta_{nm}$

Gremo v k prostor

$$u_n = \frac{1}{\sqrt{N}} \sum_k Q_k e^{ikna} \qquad Q_k = \frac{1}{\sqrt{N}} \sum_n u_n e^{-ikna}$$

$$p_n = \frac{1}{\sqrt{N}} \sum_k P_k e^{-ikna} \qquad P_k = \frac{1}{\sqrt{N}} \sum_n p_n e^{ikna}$$

Periodični RP $\quad u_{N+1} = u_1 \quad \Rightarrow \quad k = \frac{2\pi}{Na} j$

$$[Q_k, P_{k'}] = \frac{1}{N} \sum_n \sum_{n'} \underbrace{[u_n, p_{n'}]}_{i\hbar\delta_{nn'}} e^{-ikna} e^{ik'n'a}$$

$$= \frac{i\hbar}{N} \sum_n e^{i(k'-k)na}$$

$$= \frac{i\hbar}{N} \sum_{n=0}^{N-1} e^{i\frac{2\pi}{Na}(j'-j)na} \qquad \text{geometrijska vsota}$$

$$= \frac{i\hbar}{N} \frac{1 - e^{i\frac{2\pi}{N}(j'-j)N}}{1 - e^{i\frac{2\pi}{N}(j'-j)}}$$

$$= i\hbar \begin{cases} 1 & j'=j \\ 0 & j' \neq j \end{cases} = i\hbar\,\delta_{jj'} = i\hbar\,\delta_{kk'}$$

Vstavimo v H

$$\sum_n p_n^2 = \frac{1}{N} \sum_{n k k'} \overbrace{e^{-i(k+k')na}}^{\delta_{k,-k'}} P_k P_{k'} = \sum_k P_k P_{-k}$$

$$\sum_n (u_n - u_{n+1})^2 = \frac{1}{N} \sum_{n k k'} \overbrace{e^{i(k+k')na}}^{\delta_{k,-k'}} (1 - e^{ika})(1 - e^{ik'a})\, Q_k Q_{k'}$$

$$= \sum_k (1 - e^{ika})(1 - e^{-ika})\, Q_k Q_{-k}$$

$$= \sum_k Q_k Q_{-k}\; 2(1 - \cos ka)$$

$$H = \sum_k \frac{1}{2M} P_k P_{-k} + \frac{1}{2} M \omega_k^2 Q_k Q_{-k} \qquad \omega_k^2 = \frac{2K}{M}(1 - \cos ka)$$

kot harmonski oscilator

Za realne odmike velja $\quad Q_k = Q_{-k}^*$

$a|n\rangle = \sqrt{n}\,|n-1\rangle \qquad a^\dagger|n\rangle = \sqrt{n+1}\,|n+1\rangle \qquad a^\dagger a\,|n\rangle = n\,|n\rangle$

$[a_k, a_{k'}^\dagger] = \delta_{kk'}$
$[a_k, a_{k'}] = 0$
$a_k a_{k'} = a_{k'} a_k$

$$Q_k = \sqrt{\frac{\hbar}{2M\omega_k}}\,(a_k + a_{-k}^\dagger) \qquad P_k = i\sqrt{\frac{M\omega_k\hbar}{2}}\,(a_k^\dagger - a_{-k})$$

$$H = \sum_k -\frac{\hbar\omega_k}{4}(a_k^\dagger - a_{-k})(a_{-k}^\dagger - a_k) + \frac{\hbar\omega_k}{4}(a_k + a_{-k}^\dagger)(a_{-k} + a_k^\dagger)$$

$$= \sum_k \frac{\hbar\omega_k}{4}\left[- a_k^\dagger a_{-k}^\dagger + a_k^\dagger a_k + a_{-k} a_{-k}^\dagger - a_{-k} a_k + a_k a_{-k} + a_k a_k^\dagger + a_{-k}^\dagger a_{-k} + a_{-k}^\dagger a_k^\dagger\right]$$

$$= \sum_k \hbar\omega_k \left(a_k^\dagger a_k + \frac{1}{2}\right) \qquad \text{harmonski oscilator za posamezen način nihanja.}$$

Posplošitev na 3D z bazo (p vektorjev baze)

$$H = \sum_{\vec k, s} \hbar\, \omega_s(\vec k) \left(a^\dagger_{s\vec k} a_{s\vec k} + \frac{1}{2} \right)$$

velja $s = 3 \cdot p$

Def. $\quad f = \ln \mathrm{Tr}\left(e^{-\beta H} \right)$

$$-\frac{\partial f}{\partial \beta} = \frac{\mathrm{Tr}\left(H e^{-\beta H}\right)}{\mathrm{Tr}\left(e^{-\beta H}\right)} = \bar E \qquad \text{povprečna notranja energija}$$

$$f = \ln \mathrm{Tr}\left(e^{-\beta \sum \hbar \omega_s(k) \left(\hat n_s(k) + 1/2 \right)} \right) \qquad \hat n_s = a^\dagger_{s\vec k} a_{s\vec k}$$

$$= \sum_{\vec k, s} \ln \sum_{n_{sk}=0}^{\infty} e^{-\beta \hbar \omega_s(\vec k) \left(n_s(k) + 1/2 \right)} \qquad \hat n_s(\vec k) \,|n_s(\vec k)\rangle = n_s(\vec k)\, |n_s(\vec k)\rangle$$

$$= \sum_{k,s} \ln e^{-\beta \frac{\hbar \omega_s(\vec k)}{2}} \left(1 + e^{-\beta \hbar \omega_s(\vec k)} + e^{-2\beta \hbar \omega_s(\vec k)} + \dots \right) = \qquad \text{geo. vrsta}$$

$$= \sum_{k,s} \ln \left(e^{-\beta \frac{\hbar \omega_s(\vec k)}{2}} \frac{1}{1 - e^{-\beta \hbar \omega_s(\vec k)}} \right) =$$

$$= \sum_{k,s} -\beta \frac{\hbar \omega_s(\vec k)}{2} - \ln\left(1 - e^{-\beta \hbar \omega_s(\vec k)} \right)$$

gostota notranje energije

$$u = \frac{1}{V}\left(-\frac{\partial f}{\partial \beta} \right) = \frac{1}{V} \sum_{k,s} \frac{\hbar \omega_s(\vec k)}{2} + \frac{\hbar \omega_s(\vec k)\, e^{-\beta \hbar \omega_s(\vec k)}}{1 - e^{-\beta \hbar \omega_s(\vec k)}}$$

$$= \frac{1}{V} \sum_{k,s} \hbar \omega_s(\vec k) \left(n_{s\vec k} + \frac{1}{2} \right) \qquad n_{s\vec k} = \frac{1}{e^{\beta \hbar \omega_s(\vec k)} - 1}$$

$$c_V = \frac{\partial u}{\partial T} = \frac{1}{V} \frac{\partial}{\partial T} \sum_{k,s} \hbar \omega_s(\vec k) \frac{1}{e^{\beta \hbar \omega_s(\vec k)} - 1}$$

Limita $\quad T \to \infty, \quad c_V(T \to \infty) = ?$

$$x = \beta \hbar \omega_s(\vec k) \qquad \frac{1}{e^x - 1} = \frac{1}{x + \frac{x^2}{2} + \frac{x^3}{6}} = \frac{1}{x}\left(1 + \frac{x}{2} + \frac{x^2}{6} \right)^{-1} =$$

$$= \frac{1}{x}\left(1 - \frac{x}{2} - \frac{x^2}{6} + \frac{x^2}{4} - \dots \right) = \frac{1}{x} - \frac{1}{2} + \frac{x}{12} + \dots$$

$$c_V(T \to \infty) = \frac{1}{V} \frac{\partial}{\partial T} \sum_{k,s} \hbar \omega_s(\vec k) \left(\frac{k_B T}{\hbar \omega_s(\vec k)} + \frac{\hbar \omega_s(\vec k)}{12\, k_B T} \right) = \frac{1}{V} k_B \sum_{k,s} 1 - \frac{(\hbar \omega_s(\vec k))^2}{12\, (k_B T)^2}$$

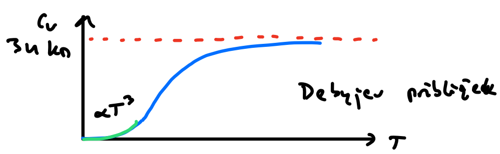
$$= \frac{3 N \cdot p}{V} k_B - \mathcal{O}\left(\frac{1}{T^2} \right) = 3 n k_B - \mathcal{O}\left(\frac{1}{T^2} \right)$$

N ... št. os. celic

s ... $1, \dots, 3p$

p ... št. atomov baze

$N \cdot p$ ... št. vseh atomov



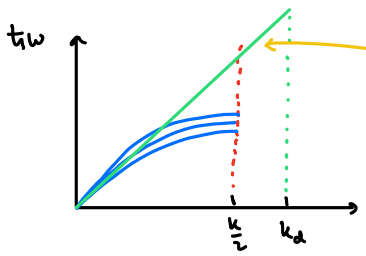
Limita $\quad T \to 0 \qquad x = \beta \hbar c_s(k)\, k$

$$c_V = \frac{1}{V} \frac{\partial}{\partial T} \sum_{k,s} \frac{\hbar\, c_s(\vec k)\, k}{e^{\beta \hbar c_s(\vec k) k} - 1} = \frac{1}{V} \frac{V}{8\pi^3} \frac{\partial}{\partial T} \sum_s \int d\Omega \int_0^\infty k^2\, dk \frac{\hbar \omega_s(\vec k)\, k}{e^{\beta \hbar c_s(\vec k) k} - 1} =$$

$$= \frac{1}{8\pi^3} \frac{\partial}{\partial T} \frac{(k_B T)^4}{\hbar^3} \underbrace{\sum_s \int \frac{d\Omega}{c_s^3(\vec k)}}_{3 \cdot 4\pi \frac{1}{\bar c^3}} \underbrace{\int_0^\infty \frac{x^3\, dx}{e^x - 1}}_{\pi^4/15} = \frac{2\pi^2}{5} k_B^4 \frac{T^3}{\hbar^3 \bar c^3}$$

$\bar c$ ... povprečna hitrost

Debyev približek za c_v



$$\omega_s(\vec k) = c k$$

$$\frac{4\pi k_d^3}{3}\,\frac{V}{8\pi^3} = N \qquad \Delta k^3 = \left(\frac{2\pi}{a}\right)^3 = \frac{8\pi^3}{V}$$

št. celic znotraj krogle s polmerom k_d

$$\Rightarrow \underset{\text{Debyev}}{k_d^3} = 6\pi^2 n \,, \qquad n = \frac{N}{V}$$

$$c_v = \frac{1}{V}\frac{\partial}{\partial T}\sum_{s\vec k}\frac{\hbar\omega_s(\vec k)}{e^{\beta\hbar\omega_s(\vec k)}-1}$$

Debyjev približek $\omega_s(\vec k) = c k$

$$= \frac{1}{V}\,3\,\frac{V}{8\pi^3}\frac{\partial}{\partial T}\int d^3k\,\frac{\hbar c k}{e^{\beta\hbar c k}-1}$$

$$= \frac{3}{8\pi^3}\,4\pi\,\frac{\partial}{\partial T}\int_0^{k_d} dk\,\frac{\hbar c k^3}{e^{\beta\hbar c k}-1}$$

$$= \frac{3}{2\pi^2}\int_0^{k_d}\frac{\hbar c k^3}{(e^{\beta\hbar c k}-1)^2}\,e^{\beta\hbar c k}\,\hbar c k\,\frac{1}{k_B T^2}\,dk$$

$$= \frac{3(\hbar c)^2}{2\pi^2 k_B T^2}\,\frac{1}{(\beta\hbar c)^5}\int_0^{\Theta_D/T}\frac{x^4 e^x}{(e^x-1)^2}\,dx$$

$$= \frac{3k_B}{2\pi^2}\left(\frac{k_B T}{\hbar c}\right)^3\int_0^{\Theta_D/T}\frac{x^4 e^x}{(e^x-1)^2}\,dx$$

$$\omega_D = c k_D$$

$$x_D = \beta\hbar c k_D = \beta\hbar\omega_D = \frac{\hbar\omega_D}{k_B T} = \frac{\Theta_D}{T}$$

$$\Theta_D = \frac{\hbar\omega_D}{k_B}$$ Debyjeva temperatura

Limite $T\to\infty$

$$c_v = \frac{3k_B}{2\pi^2}\left(\frac{k_B T}{\hbar c}\right)^3\int_0^{\Theta_D/T \ll 1} x^2\,dx = \frac{3k_B}{2\pi^2}\left(\frac{k_B T}{\hbar c}\right)^3\frac{\Theta_D^3}{3T^3}$$

$$= \frac{k_B}{2\pi^2}\,k_D^3 = \frac{k_B}{2\pi^2}\,6\pi^2 n = 3k_B n \quad ✓$$

$T\to 0$

$$c_v = \frac{3k_B}{2\pi^2}\left(\frac{k_B T}{\hbar c}\right)^3\underbrace{\int_0^{\infty}\frac{x^4 e^x}{(e^x-1)^2}\,dx}_{\frac{4\pi^4}{15}} = \frac{2\pi^2 k_B}{5}\left(\frac{k_B T}{\hbar c}\right)^3 \quad ✓$$

Θ_D je ločnica med obravnavo eksitacij kvantno ($T<\Theta_D$) ali klasično ($T>\Theta_D$)

	Θ_D [K]
NaCl	321
KCl	231
Li	400
diamant	1860

$$c_v^{el} = \frac{\pi^2}{2}\left(\frac{T}{T_F}\right) n_{el}\, k_B$$

$$n_{el} = z\, n$$

Kdaj je $c_v^{el} = c_v^{f}$ fononska

$$\Rightarrow T = 0{,}145\sqrt{\frac{z\,\Theta_D}{T_F}}\;\Theta_D$$

Gostota fononskih stanj

$$\frac{1}{V}\sum_{s,\vec k} H(\omega_s(\vec k)) = \frac{1}{8\pi^3}\sum_s\int d^3k\, H(\omega_s(\vec k)) = \int_0^\infty g(\omega)\,H(\omega)\,d\omega$$

poljubna funkcija

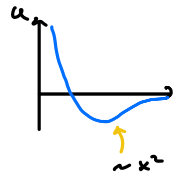
$$g(\omega) = \sum_s\int_{\omega_s(k)=\omega}\frac{dS}{8\pi^3\,|\nabla_k\,\omega_s(\vec k)|}$$

Če je $\omega_s(\vec k) = ck$

$$\nabla_{\vec k}\, \omega_s(\vec k) = c\hat k$$
$$|\nabla_{\vec k}\, \omega_s(\vec k)| = c$$

$$g(\omega) = \frac{3}{8\pi^3}\,\frac{4\pi k^2}{c} = \frac{3}{2\pi^2}\,\frac{\omega^2}{c^3}$$

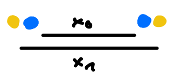
Pomen anharmonskih členov



anharmonski člen
$x^3, x^4, \ldots$

1. Fononi imajo končen τ
2. Linearni temp. raztezek
3. $c_v(T)$ ni neodvisen od T pri $T > \Theta_D$
4. Prevajanje toplote

Temperaturno raztezanje kristala



$x = x_1 - x_0$ raztezek

$$U(x) = cx^2 - gx^3 - fx^4$$
$c, g, f > 0$ za $x < x_0$

$$\langle x\rangle = \frac{\int_{-\infty}^{\infty} x e^{-\beta U(x)}dx}{\int_{-\infty}^{\infty} e^{-\beta U(x)}dx} = \frac{\int_{-\infty}^{\infty} x\, e^{-\beta c x^2}(1 + \beta g x^3 + \beta f x^4)\,dx}{\int_{-\infty}^{\infty} e^{-\beta c x^2}} = \frac{\beta g\,(\beta c)^{1/2}}{(\beta c)^{5/2}} = \frac{3g}{4c^2}k_B T \quad \propto T$$

Toplotna prevodnost mrežnih nihanj

Kovine bolje prevajajo toploto kot izolatorji.

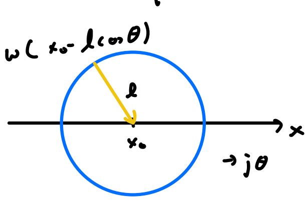
1.) Debyjeva aproksimacija $\omega = ck$

2.) Fononi se sipajo

$\omega(T(x))$ gostota energije

imajo končen življenjski čas τ

3.) Do sipanja se v hipu vzpostavi termično ravnovesje



$l = c\tau$ povprečna prosta pot

fonon se sipje na robu krogle in gre skozi x_0.

$$j_\theta = \langle c_x\, \omega(x_0 - l\cos\theta)\rangle_\Omega = \frac{1}{4\pi}\,2\pi \int_{-1}^{1} c\,\cos\theta\;\omega(x_0 - l\cos\theta)\; d\cos\theta \overset{\text{Taylor}}{=}$$

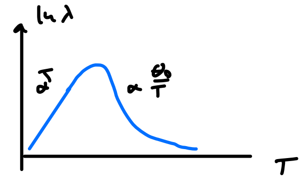
$$= \frac12 \int_{-1}^{1} dy\; c\, y\, \left(\omega(x_0) - l y \frac{d\omega}{dx}\Big|_{x_0}\right) = \frac12\,\frac23\, c\,l \left(-\frac{d\omega}{dx}\right) = -\frac13\, c\,l\, \underbrace{\frac{d\omega}{dT}}_{c_v}\, \frac{dT}{dx}\Big|_{x_0}$$

$$j_\Theta = \frac{1}{3} c \ell c_v (-\nabla T) = \underbrace{\frac{1}{3} c^2 \tau c_v}_{\lambda} (-\nabla T)$$

T limit

- $T \gg \Theta_D$ $\qquad c_v = 3 n k_B \qquad \tau = \frac{1}{\bar n} \propto \frac{1}{T^x} \qquad x \in (1,2)$ meritve

$$\bar n = \frac{1}{e^{\beta \hbar \omega_D^*} - 1} \doteq \frac{1}{\beta \hbar \omega_D} = \frac{k_B T}{\hbar \omega_D}$$

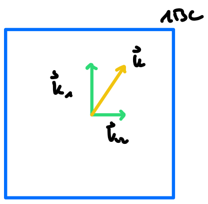


- $T \ll \Theta_D$ $\qquad j_\Theta = \lambda (-\nabla T)$

$$\hbar \vec k = \hbar \vec k_1 + \hbar \vec k_2$$

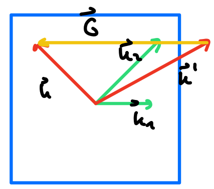
$$\sum_k \bar n_k \hbar \vec k = \sum_k \bar n'_k \hbar \vec k$$

Normalni sipalni procesi



če so k znotraj 1BC se ohranja gib. kol.

Umklapp sipalni procesi



$$\vec k_1 + \vec k_2 = \vec k + \vec G = \vec k'$$

$$\hbar\omega \sim k_B T \ll \hbar \omega_D$$

$$\tau = \frac{1}{\bar n} \qquad \bar n = \frac{1}{e^{\Theta_D/T} - 1} \qquad k_B \Theta_D = \hbar \omega_D c$$

Landauovi nivoji in de Haas von Alphen oscilacije

$$\vec B = B \hat e_z \qquad \vec B = \nabla \times \vec A \qquad \vec A = (0, xB, 0) \qquad \nabla \vec A = 0$$

$$\hat p = -i\hbar\nabla \xrightarrow{B} \hat p = -i\hbar\nabla + e\vec A$$

$$\hat H = \frac{1}{2m}(-i\hbar\nabla + e\vec A)^2 = -\frac{\hbar^2}{2m}\left(\nabla^2 + 2\frac{ie}{\hbar}\vec A \cdot \nabla - \frac{e^2}{\hbar^2}A^2\right)$$

$$= -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial z^2} + \left(\frac{\partial}{\partial y} + \frac{ie}{\hbar} x B\right)^2\right)$$

$$H\psi = \varepsilon\psi \qquad \psi = u(x)\, e^{i(k_z z - \beta y)}$$

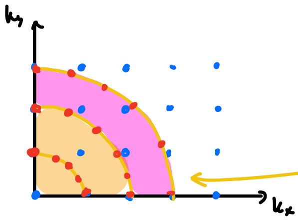
$$\varepsilon u = -\frac{\hbar^2}{2m} u''(x) + \frac{\hbar^2 k_z^2}{2m} u + \frac{\hbar^2}{2m}\left(\beta - \frac{exB}{\hbar}\right)^2 u$$

$$\varepsilon u = -\frac{\hbar^2}{2m} u''(x) + \frac{\hbar^2 k_z^2}{2m} u + \underbrace{\frac{\hbar^2}{2m}\frac{e^2B^2}{\hbar^2}\frac{m}{m}}_{\frac{m\omega_c^2}{2}}\left(x - \frac{\beta\hbar}{eB}\right)^2 u \qquad \frac{eB}{m} = \omega_c$$

Dobimo premaknjeni harmonski oscilator

$$\varepsilon = \hbar\omega_c \left(n+\frac{1}{2}\right) + \frac{\hbar^2 k_z^2}{2m}$$

kvantna števila k_z in n



k_z fiksen

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

$$\frac{\hbar^2}{2m}\left(k_x^2+k_y^2\right) = \hbar\omega_c\left(n+1/2\right)$$

Ploščina kroga $\pi\left(k_x^2+k_y^2\right) = \frac{\hbar\pi e B}{m\hbar^2}\, 2m \left(n+\frac{1}{2}\right)$

$$\parallel$$

$$A_n = \frac{2\pi e B}{\hbar}\left(n+\frac{1}{2}\right)$$

$$\Delta A_n = A_{n+1} - A_n = \frac{2\pi e B}{\hbar} = \text{konst.}$$

degeneracija n-tega nivoja $g_n = \frac{\Delta A_n}{\left(\frac{2\pi}{L}\right)^2} = \frac{eBL^2}{h} = \frac{e\,\Phi_m}{h} = \frac{\Phi_m}{\Phi_0}$

kvantiziran magnetni pretok $\Phi = \frac{h}{e}$

$$A_F = \pi k_F^2 = \frac{2\pi}{\hbar} eB\left(n+\frac{1}{2}\right)$$

$$\frac{1}{B_n} = \frac{2\pi e}{A_F\,\hbar}\left(n+\frac{1}{2}\right)$$

$$\frac{1}{B_{n+1}} - \frac{1}{B_n} = \frac{2\pi e}{A_F\hbar}$$