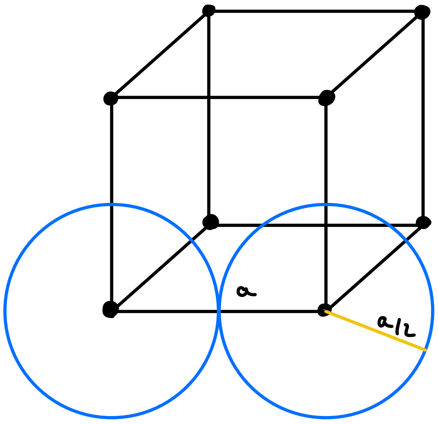
1 Navadna kubična kristalna mreža (sc, simple cubic)

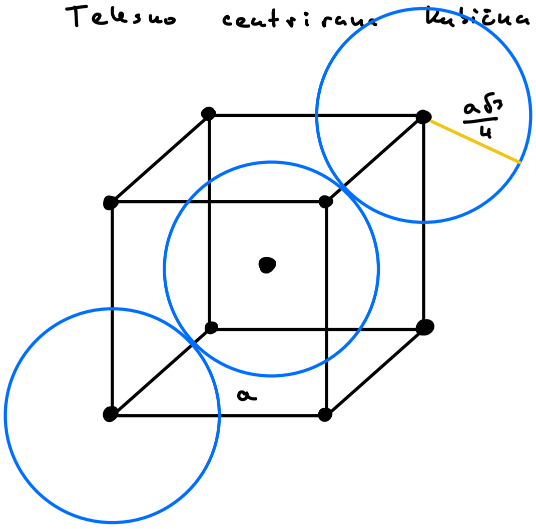


a … mrežna razdalja

η … polnitveno razmerje

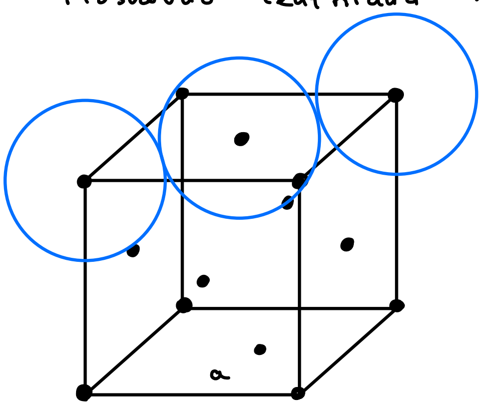
$$\eta = \frac{V_s}{V_k} = \frac{\frac{4}{3}\pi\left(\frac{a}{2}\right)^3}{a^3} = \frac{\pi}{6} \approx 52\%$$

Telesno centrirana kubična mreža (BCC, body centered cubic)



$$\eta = \frac{\left(1+8\frac{1}{8}\right)\frac{4}{3}\pi\left(\frac{a\sqrt{3}}{4}\right)^3}{a^3} = \frac{2\cdot 4\pi\ 3\sqrt{3}}{3\ 4^3} = \frac{\pi\sqrt{3}}{8} = 68\%$$

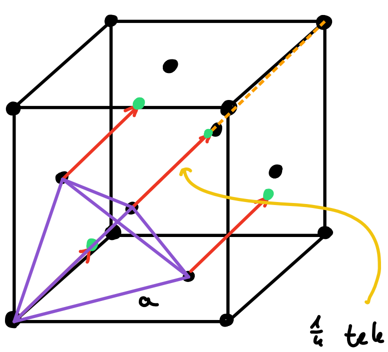
Ploskovno centrirana kubična mreža (FCC, face centered cubic)



$$r = \frac{a\sqrt{2}}{4}$$

$$\eta = \frac{\left(8\cdot\frac{1}{8} + 6\,\frac{1}{2}\right)\frac{4}{3}\pi\left(\frac{a\sqrt{2}}{4}\right)^3}{a^3} = \frac{\pi\sqrt{2}}{6} = 74\%$$

Diamantna kristalna struktura



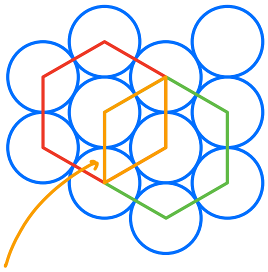
zmeraj vzamemo najmanjšo razdaljo med atomi

$$r = \frac{a\sqrt{3}}{8}$$

$$\eta = \frac{\left(4 + 8\cdot\frac{1}{8} + 6\cdot\frac{1}{2}\right)\frac{4}{3}\pi r^3}{a^3} = \frac{\pi\sqrt{3}}{16} = 34\%$$

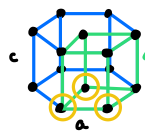
Heksagonalna kristalna struktura

- Trikotna kristalna mreža



osnovna celica

- Navadna heksagonalna mreža



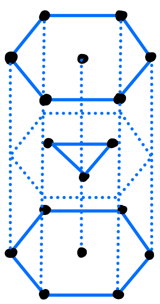
primitivna osnovna celica

$r = \frac{a}{2}$ $\qquad$ $c = a$

za max η

$$\eta = \frac{1 \cdot \pi \frac{4}{3}\left(\frac{a}{2}\right)^3}{\frac{a^2\sqrt{3}}{4} \cdot 2 \cdot a} = \frac{\pi\, 4 \cdot 4}{3 \cdot 8 \cdot \sqrt{3} \cdot 2} = \frac{\pi}{3\sqrt{3}}$$

- Heksagonalni najgostejši sklad (HCP, hexagonal close packed)

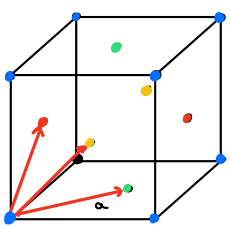


$$\eta = \frac{\left(3 + 2\cdot\frac{1}{2} + 6\cdot\frac{1}{6}\cdot 2\right)\frac{4}{3}\pi r^3}{\frac{a^2\sqrt{3}}{4}\, c}$$

$r = \frac{a}{2}$ $\qquad$ $c = 2a\sqrt{\frac{2}{3}}$

$$\eta = \frac{6 \cdot \frac{4}{3}\pi \frac{a^3}{8}}{\frac{a^2\sqrt{3}}{4}\, 2a\sqrt{\frac{2}{3}}} = \frac{\pi\sqrt{2}}{6} = 74\%$$

② FCC



$\vec{R}_n = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$

navadna kubična mreža

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

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

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

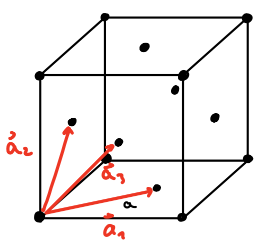
baza

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

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

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

$\vec{r}_4 = (\frac{a}{2}, 0, \frac{a}{2})$



FCC mreža

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

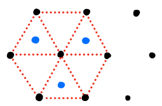
$\vec{a}_2 = (0, \frac{a}{2}, \frac{a}{2})$

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

baza

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

③ HCP – heksagonalni najgostejši sklad



• prva plastev

• druga plastev

Samo z Bravaisovo mrežo (BM) ne moremo zapisati kristala

Mreža ← zapišemo • atom

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

$\vec{a}_2 = (\frac{a}{2}, \frac{\sqrt{3}}{2} a, 0)$

$\vec{a}_3 = (0, 0, 2\sqrt{\frac{2}{3}} a)$

dve višini tetraedra

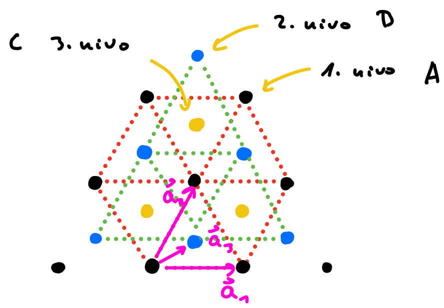
Baza

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

$\vec{r}_2 = (\frac{a}{2}, \frac{1}{3}\frac{\sqrt{3}}{2} a, \sqrt{\frac{2}{3}} a)$

opiše • delce

④



HCP ABAB

$$ABC \begin{cases} \to ABCA \begin{cases} \to ABCAB \\ \to ABCAC \end{cases} \\ \to ABCB \begin{cases} \to ABCBC \\ \to ABCBA \end{cases} \end{cases}$$

Vse strukture imajo enako gostoto

Najpogosteje se pojavlja ABC ABC struktura v naravi

ABC lahko zapišemo z BM.

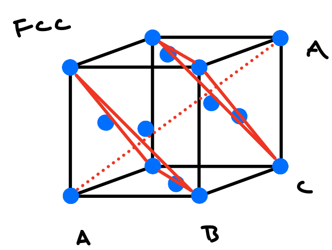
$\vec{a}_1 = (a, 0, 0)$

$\vec{a}_2 = (\frac{a}{2}, \frac{\sqrt{3}}{2} a, 0)$

$\vec{a}_3 = (\frac{a}{2}, \frac{1}{3}\frac{\sqrt{3}}{2} a, \sqrt{\frac{2}{3}} a)$

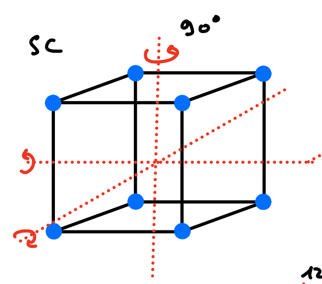
Dobimo enako mrežo kot FCC.

robovi tetraedra

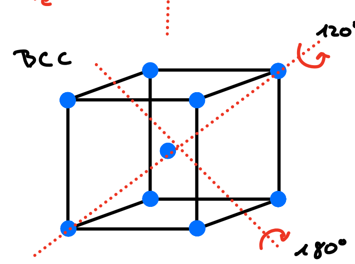


⑤ Kubična grupa

Grupa G je množica elementov (npr. $a, b \in G$)
- ima def. produkt med elementi $a \cdot b \in G$
- vsebuje enoto $a \cdot e = e \cdot a = a$
- vsebuje inverz $a a^{-1} = e$
- produkt je asociativen $a(bc) = (ab)c$

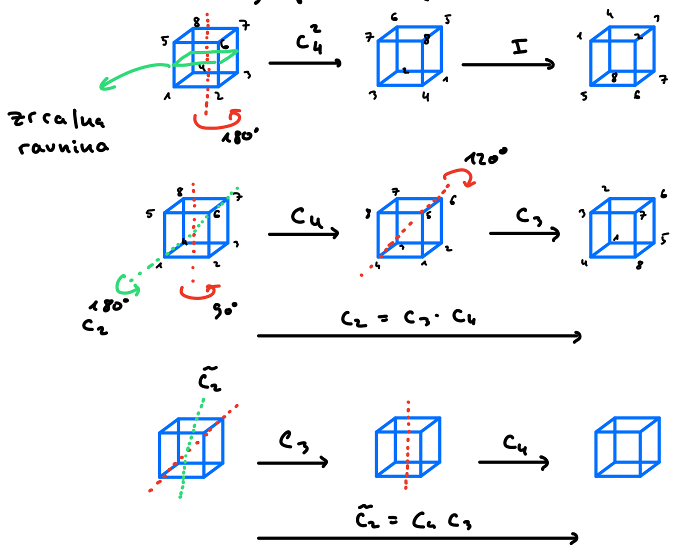


Kubična grupa
- enota je, da mreže ne zavrtimo
- 4 števna os, 3 operacije, rotacija za 90°, 180° in 270°; imamo 3 take osi. Število operacij $3 \cdot 3$
- 3 števna os, 2 operaciji, rotacije za 120° in 240°; imamo 4 take osi. Število operacij $2 \cdot 4$
- 2 števna os, 1 operacija za 180°, 6 takih osi, 6 operacij
- Skupno število rotacijskih operacij je $1 + 9 + 8 + 6 = 24$
- Operacija inverzije $\vec{r} \to -\vec{r}$. Vsako rotacijo lahko združimo z inverzijo, da dobimo novih 24 inverznih operacij



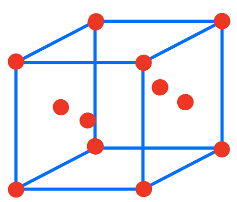
Ali te operacije tvorijo grupo?

- vsebuje enoto
- inverz imajo vse rotacije
- množenje matrik je asociativno, zato so tudi naše operacije
- produkt je definiran kot množenje matrik. Ali je produkt spet element grupe? Primeri:

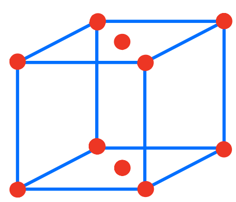


Kubična grupa je nekomutativna grupa.

⑥



Kubična mreža s centriranimi stranskimi ploskvami



Kubična mreža s centriranimi osnovnimi ploskvami.

Ni Bravaisova mreža

Je BM

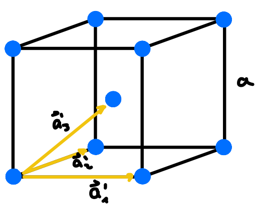
⑦ Recipročna mreža

$$\vec{R} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$$

$$\forall \vec{R} \quad e^{i\vec{k}\cdot\vec{R}} = 1 \qquad \vec{k} = m_1\vec{A}_1 + m_2\vec{A}_2 + m_3\vec{A}_3$$

$$\vec{a}_i\,\vec{A}_j = 2\pi\,\delta_{ij} \qquad \vec{A}_1 = 2\pi\,\frac{\vec{a}_2\times\vec{a}_3}{(\vec{a}_1,\vec{a}_2,\vec{a}_3)}$$

⑦ Za BCC poišči recipročno mrežo



$$\vec{a}_1 = \frac{a}{2}(-1,1,1)$$
$$\vec{a}_2 = \frac{a}{2}(1,-1,1)$$
$$\vec{a}_3 = \frac{a}{2}(1,1,-1)$$

kažejo v središča sosednjih celic.

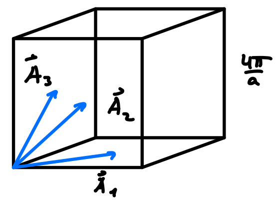
Sestavimo $\vec{a}_1, \vec{a}_2$ in $\vec{a}_3$ iz $\vec{a}_1'$, $\vec{a}_2'$ in $\vec{a}_3'$

$$\vec{a}_1' = \vec{a}_3 + \vec{a}_2$$
$$\vec{a}_2' = \vec{a}_1 + \vec{a}_2$$
$$\vec{a}_3' = \vec{a}_1 + \vec{a}_2 + \vec{a}_3$$

$$\vec A_1 = 2\pi \frac{\vec a_2\times\vec a_3}{\vec a_1\cdot(\vec a_2\times\vec a_3)} = 2\pi \frac{\frac{a^2}{4}(0,2,2)}{\frac{a^3}{8}(2+2)} = \frac{2\pi}{a}(0,1,1) = \frac{4\pi}{a}\left(0,\tfrac12,\tfrac12\right)$$

$$\vec A_2 = 2\pi \frac{\frac{a^2}{4}(2,0,2)}{a^3/2} = \frac{2\pi}{a}(1,0,1) = \frac{4\pi}{a}\left(\tfrac12,0,\tfrac12\right)$$

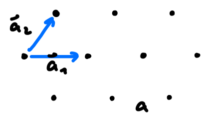
$$\vec A_3 = \frac{2\pi}{a}(1,1,0) = \frac{4\pi}{a}\left(\tfrac12,\tfrac12,0\right)$$



FCC

Recipročna mreža BCC je FCC Bravaisova mreža.

8



$$\begin{bmatrix}\vec a_1\\ \vec a_2\end{bmatrix}\cdot\begin{bmatrix}\vec A_1 & \vec A_2\end{bmatrix} = 2\pi\begin{bmatrix}1&0\\0&1\end{bmatrix}$$

$$\begin{bmatrix}\vec A_1 & \vec A_2\end{bmatrix} = 2\pi\begin{bmatrix}\vec a_1\\ \vec a_2\end{bmatrix}^{-1}$$

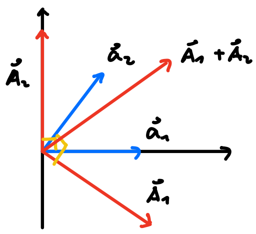
$\vec a_1 = a(1,0)$

$\vec a_2 = a\left(\frac12, \frac{\sqrt3}{2}\right)$

$$= 2\pi\begin{bmatrix}a & 0\\ a/2 & \frac{a\sqrt3}{2}\end{bmatrix}^{-1}$$

$$= 2\pi\frac{1}{\frac{a^2\sqrt3}{2}}\begin{bmatrix}\frac{a\sqrt3}{2} & 0\\ -a/2 & a\end{bmatrix}$$

$$= \frac{4\pi}{\sqrt3 a}\begin{bmatrix}\sqrt3/2 & 0\\ -1/2 & 1\end{bmatrix}$$



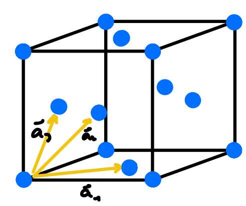
$A_1 = \frac{4\pi}{a\sqrt3}\left(\frac{\sqrt3}{2}, -\frac12\right)$ $\qquad$ $A_2 = \frac{4\pi}{\sqrt3 a}(0,1)$

$$\vec k = m_1\vec A_1 + m_2\vec A_2$$
$$= (m_1-m_2)\vec A_1 + m_1(\vec A_1+\vec A_2) \leftarrow$$ zasukana recipročna mreža (za 30°)

7 Geometrijski strukturni faktor

$$S_{\vec K} = \sum_n e^{-i\vec k\cdot\vec r_n}$$
↑ po vektorjih baze

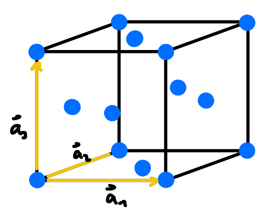
9 FCC



a $\vec R = n_1\vec a_1 + n_2\vec a_2 + n_3\vec a_3$

Baza $\vec r_0 = (0,0,0)$

$\Rightarrow$ $S_{\vec k} = 1$



b SC + baza

Baza
$\vec r_1 = (0,0,0)$
$\vec r_2 = a\left(\frac12,\frac12,0\right)$
$\vec r_3 = a\left(\frac12,0,\frac12\right)$
$\vec r_4 = a\left(0,\frac12,\frac12\right)$

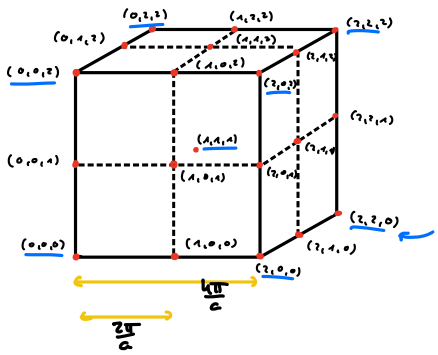
$\vec A_1 = \frac{2\pi}{a}(1,0,0)$
$\vec A_2 = \frac{2\pi}{a}(0,1,0)$
$\vec A_3 = \frac{2\pi}{a}(0,0,1)$

$\vec k = m_1\vec A_1 + m_2\vec A_2 + m_3\vec A_3$
↑ Millerjevi indeksi

$\vec k = \frac{2\pi}{a}(m_1, m_2, m_3)$

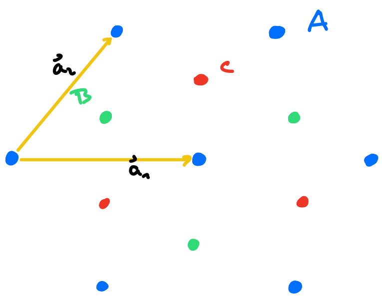
$$S_{\vec k} = \sum_n e^{-i\vec k\cdot\vec r_n} = 1 + e^{-i\frac{\pi}{a}(m_1+m_2)a} + e^{-i\pi(m_1+m_3)} + e^{-i\pi(m_2+m_3)}$$

			delež
m_1, m_2, m_3 vsi sodi		$S_{\vec k} = 4$	1/4
vsi lihi		$S_{\vec k} = 4$	
dva soda en lih		$S_{\vec k} = 2-2 = 0$	3/4
dva liha en sod		$S_{\vec k} = 0$	



strukturni faktor $\neq 0$
enako kot SC recipročna mreža

ⓒ ABC heksagonalna mreža



$$\vec{a}_3 = 3a\sqrt{\tfrac{2}{3}}\,(0,0,1)$$

$$\vec{r}_A = (0,0,0)$$

$$\vec{r}_B = \tfrac{1}{3}(\vec{a}_1 + \vec{a}_2 + \vec{a}_3)$$

$$\vec{r}_C = \tfrac{2}{3}(\vec{a}_1 + \vec{a}_2 + \vec{a}_3)$$

$$\vec{k} = m_1 \vec{A}_1 + m_2 \vec{A}_2 + m_3 \vec{A}_3$$

$$\vec{k}\cdot\vec{r}_A = 0$$

$$\vec{k}\cdot\vec{r}_B = \tfrac{2\pi}{3}(m_1+m_2+m_3)$$

$$\vec{k}\cdot\vec{r}_C = \tfrac{4\pi}{3}(m_1+m_2+m_3)$$

$$S_{\vec{k}} = 1 + e^{-i\frac{2\pi}{3}(m_1+m_2+m_3)} + e^{-i\frac{4\pi}{3}(m_1+m_2+m_3)}$$

$m_1+m_2+m_3 = 3N$ $\quad S_{\vec{k}} = 3$

$m_1+m_2+m_3 = 3N+1$ $\quad S_{\vec{k}} = 1 + e^{-i\frac{2\pi}{3}} + e^{-i\frac{4\pi}{3}} = 0$

$m_1+m_2+m_3 = 3N+2$ $\quad S_{\vec{k}} = 1 + e^{-i\frac{4\pi}{3}} + e^{-i\frac{8\pi}{3}} = 0$

⑩ Diamantna mreža (SC z bazo)

$$\vec{r}_1 = (0,0,0) \qquad \vec{r}_5 = \vec{r}_1 + \overbrace{\tfrac{a}{4}(1,1,1)}^{\vec{d}}$$

$$\vec{r}_2 = (\tfrac{a}{2},\tfrac{a}{2},0) \qquad \vec{r}_6 = \vec{r}_2 + \tfrac{a}{4}(1,1,1)$$

$$\vec{r}_3 = (\tfrac{a}{2},0,\tfrac{a}{2}) \qquad \vec{r}_7 = \vec{r}_3 + \tfrac{a}{4}(1,1,1)$$

$$\vec{r}_4 = (0,\tfrac{a}{2},\tfrac{a}{2}) \qquad \vec{r}_8 = \vec{r}_4 + \tfrac{a}{4}(1,1,1)$$

FCC premaknjena za četrtino diagonale.

$$
\begin{aligned}
S_{\vec{k}} &= e^{-i\vec{k}\vec{r}_1} + e^{-i\vec{k}(\vec{r}_1+\vec{d})} + \dots \\
&= e^{-i\vec{k}\vec{r}_1}(1 + e^{-i\vec{k}\vec{d}}) + \dots \\
&= (1 + e^{-i\vec{k}\vec{d}})(e^{-i\vec{k}\vec{r}_1} + \dots) \\
&= (1 + e^{-i\vec{k}\vec{d}})\, S_{\vec{k}}^{FCC}
\end{aligned}
$$

$$\vec{k} = \tfrac{2\pi}{a}(m_1, m_2, m_3)$$

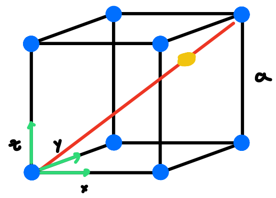
večkratnik $\overset{=4}{k}$ če m_1, m_2, m_3 sodi / lihi

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

$m_1+m_2+m_3 = kN$ $\quad S_{\vec{k}} = 8$

$m_1+m_2+m_3 = kN+2$ $\quad S_{\vec{k}} = 0$

11



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

$\vec{r}_2 = b(1,1,1)$

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

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

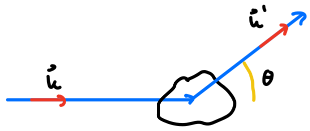
$\vec{a}_3 = a(0,0,1)$

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

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

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

$\vec{k} = \sum_i m_i \vec{A}_i$



Z rendgensko svetlobo $\lambda = 2\,\mathring{A}$, svetimo na vzorec in gledamo ojačitve

(i) praškast vzorec, pojavita se dva vrhova pri $\theta_1 = 87{,}6°$ in $\theta_2 = 141{,}1°$. Ogromno št. majhnih kristalčkov

(ii) metoda rotacije kristala (monokristal) pri sipalnem kotu θ_2 dosimo dva različna vrhova, katerih intenziteti sta v razmerju $\frac{I_1}{I_2} = 1/4$

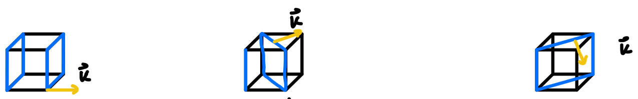
razdalje med mrežnimi ravninami

Braggov pogoj $\quad 2d \sin\frac{\theta}{2} = n\lambda$

Von Laue $\quad |\vec{k}| = |\vec{k}'| = \frac{2\pi}{\lambda} \qquad \vec{k} - \vec{k}' = \vec{K}$

vektor recipročne mreže

$d = \frac{2\pi}{|K|}$ vzamemo najkrajšega, ki je $\perp$ na mrežno ravnino



$d = a$	$d = \frac{a}{\sqrt{2}}$	
$\vec{K}_{min} = \vec{A}_1$	$\vec{K}_{min} = \vec{A}_1 + \vec{A}_2$	$\vec{K}_{min} = \vec{A}_1 - \vec{A}_2$
Millerjevi indeksi (100)	(110)	$(1\bar{1}0)$, $\bar{1}$: -1

$\underbrace{\text{Lahko konstruiramo tudi } (010) \text{ in } (001)}$

$\{100\} = \{(100),(010),(001)\}$

nova notacija

so med seboj povezani z rotacijo

$$I \propto |S_{\vec{k}}|^2 f(\theta)$$

(i) $\quad S_{\vec{k}} = \sum_n e^{-i\vec{K}\cdot\vec{r}_n} = 1 + e^{-i\frac{2\pi}{a}b(m_1+m_2+m_3)}$

• $\theta_1 \rightarrow \quad d = \frac{\lambda}{2\sin\theta/2} = a = \frac{2\cdot 10^{-10}\,\mathrm{m}}{2\sin\theta_1/2} = 1{,}5\,\mathring{A}$

$\theta_2 \rightarrow \quad \sqrt{2}\frac{a}{\sqrt{2}} = \sqrt{2}\frac{2\cdot 10^{-10}}{2\sin\theta_2/2} = 1{,}5\,\mathring{A}$

$\{100\} \quad S_{\vec{k}} = 1 + e^{-2\pi i\frac{b}{a}} = 0$ če je $b = \frac{a}{2}$ BCC

$\{110\} \quad S_{\vec{k}} = 1 + e^{-2\pi i\frac{b}{a}2} = 0$ če je $b = \frac{a}{4}$

$\{1\bar{1}0\} \quad S_{\vec{k}} = 2$

Če je kristal BCC

Na $\{100\}$ se ne sipje

$\{110\}, \{1\bar{1}0\}$ $\Rightarrow$ $\frac{a}{\sqrt{2}} = d = \frac{\lambda}{2\sin\theta_1/2}$ $\Rightarrow$ $a = 2{,}13\,\text{Å}$

Za BCC $S_G = 1 + e^{-i\pi(m_1+m_2+m_3)}$ $\quad S_G = 0$ za $m_1+m_2+m_3 =$ liho

$\Rightarrow$ naslednji odboj pri $m_1 = 2$. $\Rightarrow$ $d = \frac{a}{2}$

$\Rightarrow$ $\frac{a}{2} = \frac{\lambda}{2\sin\theta_1/2}$ $\Rightarrow$ $a = 2{,}13\,\text{Å}$ ✓

(ii) Če $s \neq \frac{a}{2}$ $\quad a = 1{,}5\,\text{Å}$

θ_1: $\{100\}$ $\rightarrow$ $S_G = 1 + e^{-i2\pi\frac{s}{a}2}$

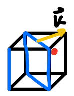
θ_2: $\underbrace{\{110\}\,\{1\bar{1}0\}}_{2\times}$ $\rightarrow$ $S_G = 2$ ✓

Če $s = \frac{a}{2}$ $\quad a = 2{,}13\,\text{Å}$

θ_1: $\{110\}\,\{1\bar{1}0\}$

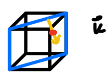
θ_2: $\underbrace{\{200\}}_{1\times}$ ✗

$\{110\}$



- ne leži na mrežni ravnini
- atom destruktivno interferira zato je I manjša

$\{1\bar{1}0\}$



- leži na mrežni ravnini
- je enak kot ostali na meži

$I_1 < I_2$

$$\frac{I_1}{I_2} = \frac{|S_G^{(1)}|^2}{|S_G^{(2)}|^2} = \frac{1}{4} = \frac{(1+e^{-i4\pi\frac{s}{a}})^2}{4}$$

$$1 = 4\cos^2 2\pi\frac{s}{a} \qquad \cos 2\pi\frac{s}{a} = \pm\frac{1}{2}$$

$$s = \left\{\frac{a}{6}, \frac{a}{3}, \frac{2a}{3}, \frac{5a}{6}\right\}$$

12 Svetloba pada na kovino

$\vec{E} = \vec{E}_0 e^{-i\omega t}$

$\vec{v} = \vec{v}_0 e^{-i\omega t}$ $\quad\rightarrow\quad$ $\vec{j} = \vec{j}_0 e^{-i\omega t}$

Drude

$m\vec{a} = e\vec{E} - \frac{m\vec{v}}{\tau}$

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

$\vec{j} = \sigma\vec{E}$ $\qquad \underbrace{\sigma = \frac{ne^2\tau}{m}}_{\text{za statično polje } E}$

$$m\vec{a} = \left(e\vec{E}_0 - \frac{m\vec{v}_0}{\tau}\right)e^{-i\omega t} = m(-i\omega)\vec{v}_0\, e^{-i\omega t}$$

$$e\vec{E}_0 = \left(\frac{1}{\tau} - i\omega\right)m\vec{v}_0$$

$$\vec{v}_0 = \frac{e\vec{E}_0}{m(\frac{1}{\tau} - i\omega)} \quad\rightarrow\quad \vec{j}_0 = \frac{ne^2}{m(\frac{1}{\tau} - i\omega)}\vec{E}_0$$

$$= \underbrace{\frac{ne^2\tau}{m}}_{\sigma_0}\frac{1}{1 - i\omega\tau}\vec{E}_0 = \sigma(\omega)\vec{E}_0$$

za $\omega\tau \ll 1$ $\Rightarrow$ $\sigma(\omega) = \sigma_0$ ohmski režim $\qquad$ so ohmske izgube $\vec{j}\cdot\vec{E}$

za $\omega\tau \gg 1$ $\Rightarrow$ $\sigma(\omega) = i\frac{\sigma_0}{\omega\tau}$ $\qquad$ ohmskih izgub ni

$$\vec{j} = ne\vec{v} = ne\dot{\vec{r}} = (\underbrace{ne\vec{r}}_{\text{gostota dipolnega momenta}})^{\cdot} = \dot{\vec{P}}$$

polarizacija

$$\vec{D} = \varepsilon_0 \vec{E} + \vec{P} = \varepsilon\varepsilon_0 \vec{E}$$

$$\vec{P} = \int \vec{j}\, dt = \vec{j}_0 \int e^{-i\omega t}\, dt = \frac{\vec{j}_0 i}{\omega} e^{-i\omega t} = \vec{P}_0 e^{-i\omega t}$$

$$\varepsilon_0 \vec{E}_0 + \vec{P}_0 = \varepsilon\varepsilon_0 \vec{E}_0$$

$$\varepsilon = 1 + \varepsilon_0 \frac{\vec{P}_0}{\vec{E}_0} = 1 + \frac{j_0\, i/\omega}{\varepsilon_0 E_0} = 1 + \frac{\sigma(\omega)\, i\, E_0}{\varepsilon_0\, \omega\, E_0} = 1 - \frac{\sigma(\omega)}{i\omega\varepsilon_0}$$

za Drudejev model $\quad \varepsilon = 1 - \left(\frac{1}{1 - i\omega\tau}\right) \frac{\sigma_0}{i\omega\varepsilon_0}$

za vidno svetlobo $\quad \omega\tau \gg 1$

$$\varepsilon = 1 - \frac{\sigma_0}{\varepsilon_0 \tau \omega^2} = 1 - \frac{ne^2\tau}{m\varepsilon_0\tau\omega^2} = 1 - \underbrace{\frac{ne^2}{m\varepsilon_0}}_{\omega_p^2} \frac{1}{\omega^2} = 1 - \frac{\omega_p^2}{\omega^2}$$

plazemska frekvenca

Ocenimo ω_p

$$n \sim 10^{28} - 10^{30} \ \frac{1}{m^3}$$

$$\omega_p \approx \sqrt{\frac{10^{30} e_0}{m_e \varepsilon_0}} \approx 10^{15}\,\mathrm{Hz} \qquad (\text{UV svetloba})$$

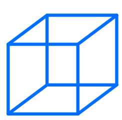
prehod ε se zgodi pri UV svetlobi.

$\omega = ck \qquad c = \frac{c_0}{\sqrt{\varepsilon}}$

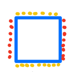
Če je $\quad \varepsilon > 0 \Rightarrow c \in \mathbb{R} \Rightarrow k \in \mathbb{R} \qquad e^{i(\vec{k}\cdot\vec{r} - \omega t)}$ ravni val

$\varepsilon < 0 \Rightarrow c \in \mathbb{C} \Rightarrow k \in \mathbb{C} \qquad e^{-\vec{k}\vec{r} - i\omega t}$ eksponentni padec ldsoj

13 Elektroni v neskončni pot. jami s periodičnimi robnimi pogoji

3D 
L

e^- ujeti v škatli

2D 
L

1D
L

za želimo periodične robne pogoje: dosimo telo — torus — krog

$\psi(\vec{r}) = \frac{1}{\sqrt{L^3}} e^{i\vec{k}\cdot\vec{r}}$, $\quad L^3 = V$

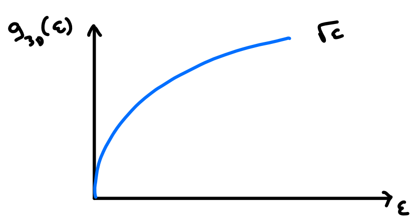
$\psi(\vec{r}) = \frac{1}{\sqrt{L^2}} e^{i\vec{k}\cdot\vec{r}}$

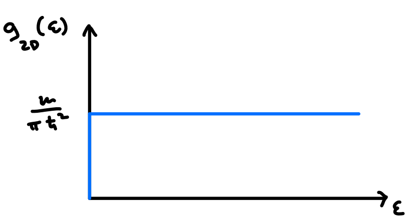
$\psi(\vec{r}) = \frac{1}{\sqrt{L}} e^{i\vec{k}\cdot\vec{r}}$

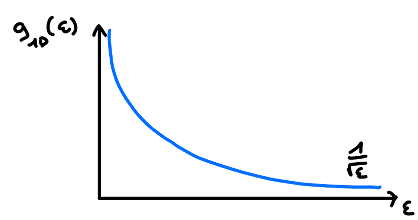
energija $\quad \varepsilon(k) = \frac{\hbar^2 k^2}{2m}$

gostota stanj $\quad g(\varepsilon) = \frac{1}{V} \frac{dN}{d\varepsilon}$

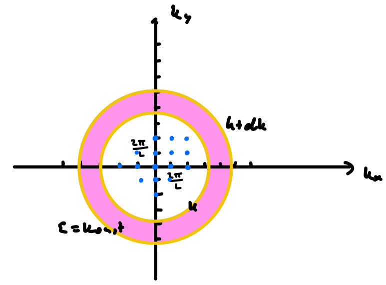
za 3D $\quad g(\varepsilon) \propto \sqrt{\varepsilon}$







Iščemo $g_{2D}(\varepsilon)$



Periodični robni pogoji:

$e^{ik_xL}=1 \qquad k_x=\frac{2\pi}{L}n_x$

$e^{ik_yL}=1 \qquad k_y=\frac{2\pi}{L}n_y$

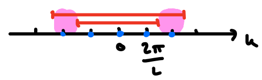
$$g(\varepsilon)=\frac{1}{V}\frac{dN(\varepsilon,\varepsilon+d\varepsilon)}{d\varepsilon}$$

$$g_{2D}(\varepsilon)=\frac{1}{L^2}\frac{d}{d\varepsilon}\left(\pi\left((k+dk)^2-k^2\right)/\left(\frac{2\pi}{L}\right)^2\right)\cdot \overset{\text{spin}}{2}$$

$$\doteq\frac{1}{L^2}\frac{d}{d\varepsilon}2\pi k\,dk\Big/\left(\frac{2\pi}{L}\right)^2\cdot 2 \qquad \varepsilon=\frac{\hbar^2k^2}{2m}$$

$$=\frac{k}{\pi}\frac{dk}{d\varepsilon}=\frac{k}{\pi}\frac{d}{d\varepsilon}\sqrt{\frac{2m\varepsilon}{\hbar^2}}=\frac{m}{\pi\hbar^2}$$

Iščemo $g_{1D}(\varepsilon)$



$$g_{1D}(\varepsilon)=\frac{1}{L}\frac{2dk/\frac{2\pi}{L}\cdot 2}{d\varepsilon}=\frac{4}{L}\frac{L}{2\pi}\frac{dk}{\frac{\hbar^2k}{m}dk}=\frac{2m}{\pi\hbar^2k}=\frac{2m}{\pi\hbar^2}\sqrt{\frac{\hbar^2}{2m\varepsilon}}=\frac{1}{\pi}\sqrt{\frac{2m}{\hbar^2}}\frac{1}{\sqrt{\varepsilon}}$$

$$\Rightarrow g(\varepsilon)=A_d\,\varepsilon^{1-d/2} \qquad d\text{... dimenzija}$$

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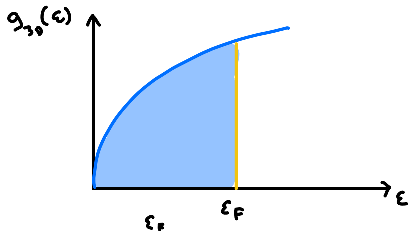
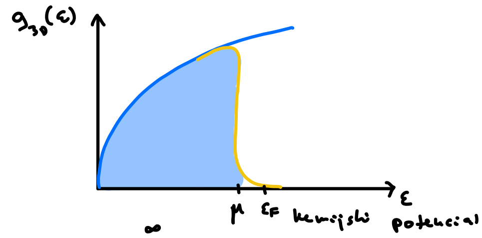
Pri $T=0$



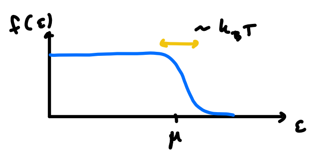
$$n=\frac{N}{V}=\int_{-\infty}^{\varepsilon_F}g(\varepsilon)\,d\varepsilon$$

Pri $T>0$



$$n=\int_{-\infty}^{\infty}g(\varepsilon)f(\varepsilon)\,d\varepsilon$$

Fermijeva porazdelitev $\quad f(\varepsilon)=\frac{1}{1+e^{\beta(\varepsilon-\mu)}} \qquad \beta=\frac{1}{k_BT}$



Iščemo $\mu(T)$

Ker želimo $n(T=0)=n(T>0)$ se mora μ premakniti

V 3D $\quad \mu\leftarrow\varepsilon_F \qquad \mu$ se premakne v levo

2D $\quad \mu=\varepsilon_F \qquad$ v 2D $\mu\neq\mu(T)$

1D $\quad \varepsilon_F\rightarrow\mu$

Sommerfeldov razvoj $\quad \mu(T)=\varepsilon_F-\frac{\pi^2}{6}(k_BT)^2\frac{g'(\varepsilon_F)}{g(\varepsilon_F)}$

$$\mu(T) = \varepsilon_F - \frac{\pi^2}{6}(k_B T)^2 \frac{A_d\left(-1+d/2\right)\varepsilon_F^{-2+d/2}}{A_d\, \varepsilon_F^{-1+d/2}}$$

$$= \varepsilon_F - \frac{\pi^2}{6}(k_B T)^2 \left(\frac{d}{2}-1\right)\frac{1}{\varepsilon_F}$$

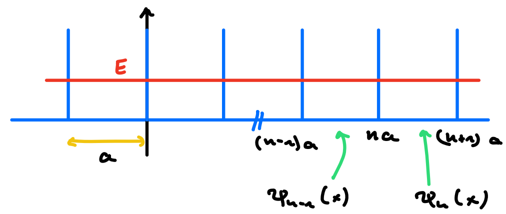
$$= \varepsilon_F\left(1 - \frac{\pi^2}{6}\underbrace{\left(\frac{d}{2}-1\right)}_{\begin{cases} -1/2 & d=1 \\ 0 & d=2 \\ 1/2 & d=3\end{cases}}\left(\frac{k_B T}{\varepsilon_F}\right)^2\right)$$

Ocenimo $\frac{k_B T}{\varepsilon_F} = \frac{1/40 \text{ eV}}{10 \text{ eV}} \approx 10^{-2} - 10^{-3}$ eV

popravki so zelo majhni

(15) Kronig-Penneyev model kristala

$$V(x) = \sum_n \lambda\, \delta(x - na) \qquad \lambda > 0$$



$$H = \frac{p^2}{2m} + V(x)$$

Iščemo ψ da $H\psi = E\psi$ $\qquad E > 0$

valovni vektor (povsod k)

Nastavek
$$\psi_n = A_n e^{iqx} + B_n e^{-iqx}, \qquad q = \sqrt{\frac{2mE}{\hbar^2}}$$
$$\psi_{n-1} = A_{n-1} e^{iqx} + B_{n-1} e^{-iqx}$$

Robni pogoji pri $x = na$ za ψ_n in ψ_{n-1}

- zveznost $\quad A_n e^{iqna} + B_n e^{-iqna} = A_{n-1} e^{iqna} + B_{n-1} e^{-iqna}$
- odvod $\quad \psi_n'(na) - \psi_{n-1}'(na) = \frac{2m\lambda}{\hbar^2}\psi(na)$

$$iq A_n e^{iqna} - iq B_n e^{-iqna} - iq A_{n-1} e^{iqna} + iq B_{n-1} e^{-iqna} = \frac{2m\lambda}{\hbar^2}\left(A_n e^{iqna} + B_n e^{-iqna}\right)$$

Za reševanje enačb bomo uporabili diskretno translacijsko simetrijo

Naj bo $\quad T\psi(x) = \psi(x+a)$ operator translacije.

$$T(H\psi(x)) = T\left(\left(\frac{p^2}{2m} + V\right)\psi\right) = \left(\frac{p^2}{2m} + V\right)T\psi = HT\psi$$ ker $V(x) = V(x+a)$ in $\frac{d}{dx} = \frac{d}{d(x+a)}$

$$\Rightarrow TH = HT \quad \Rightarrow \quad [T, H] = 0$$

Iščemo lastne funkcije T

$$T\psi(x) = \psi(x+a) = c\,\psi(x)$$

Periodični robni pogoj:

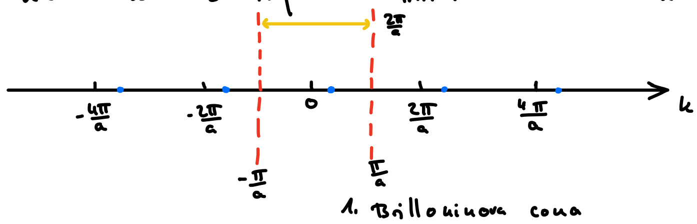
$$\psi(x + Na) = \psi(x)$$
$$T^N \psi(x) = \underbrace{c^N}_{1}\psi(x) = e^{iN\alpha}\psi(x) \Rightarrow N\alpha = 2\pi m$$
$$\Rightarrow |c| = 1 \Rightarrow c = e^{i\alpha}$$

Def $e^{ih} = e^{ika}$ $\Rightarrow$ $kaN = 2\pi n$ $\Rightarrow$ $k = \frac{2\pi n}{Na}$

Če $k \to k + K$ $K = \frac{2\pi}{a} n$ vektor recipročne mreže

$c \to e^{i(k+K)a} = e^{ika} = c$

Ker lahko s k' in $k+K$ dosimo enako energijo, se omejimo na k znotraj 1. Brillouinove cone. k je Blochov valovni vektor



1. Brillouinova cona

• pri teh je enaka lastna vrednost / energija

$\psi(x+a) = c\psi(x) = e^{ika}\psi(x)$ $k \in (-\frac{\pi}{a}, \frac{\pi}{a}]$ $k = \frac{2\pi n}{Na}$ $n \in \mathbb{Z}$

$A_n e^{iq(x+a)} + B_n e^{-iq(x+a)} = e^{ikx}(A_{n-1} e^{iqx} + B_{n-1} e^{-iqx})$

$A_n e^{iqa} = A_{n-1} e^{ikx}$ $B_n e^{-iqa} = B_{n-1} e^{ikx}$

$A_{n-1} = A_n e^{i(qa-kx)}$ $B_{n-1} = B_n e^{-i(qa+kx)}$

Vstavimo v robna pogoja

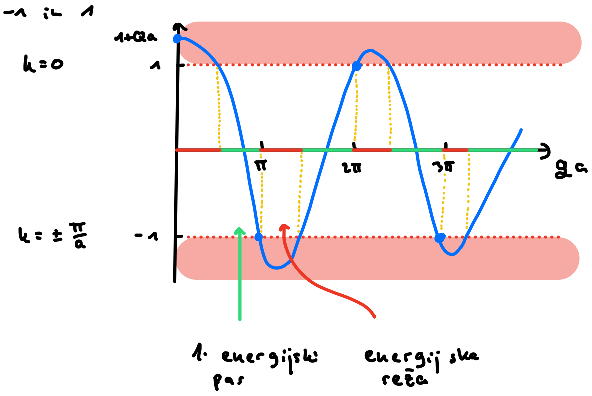
- $A_n e^{iqna} + B_n e^{-iqna} = A_n e^{i(qa-kx)} e^{iqx} + B_n e^{-i(qa+kx)} e^{-iqx}$
- odvod

Dobimo 2x2 homogen sistem $A \begin{bmatrix} A_n \\ B_n \end{bmatrix} = 0$ rešitev je $\det A = 0$

$\Rightarrow$ $\boxed{\cos ka = \cos qa + Qa\frac{\sin qa}{qa}}$ $q = \sqrt{\frac{2mE}{\hbar}}$ $Q = \frac{m\lambda}{\hbar^2}$

omejen z -1 in 1

Če k in q zadoščata enačbi to stanje obstaja.



Spodnji robovi energijskih rež $qa = n\pi$

Iščemo zgornje meje rež.
Taylorjev razvoj okoli $qa = n\pi$ do drugega reda, $Qa \ll 1$

$(-1)^n \approx (-1)^n\left(1-\frac{\varepsilon^2}{2}\right) + Qa\,\frac{(-1)^n\varepsilon}{n\pi}$ $\qquad qa = n\pi+\varepsilon$

$\varepsilon_1 = \frac{2Qa}{n\pi} \qquad \varepsilon_2 = 0$

Desni rob $\quad qa = n\pi + \frac{2Qa}{n\pi}$

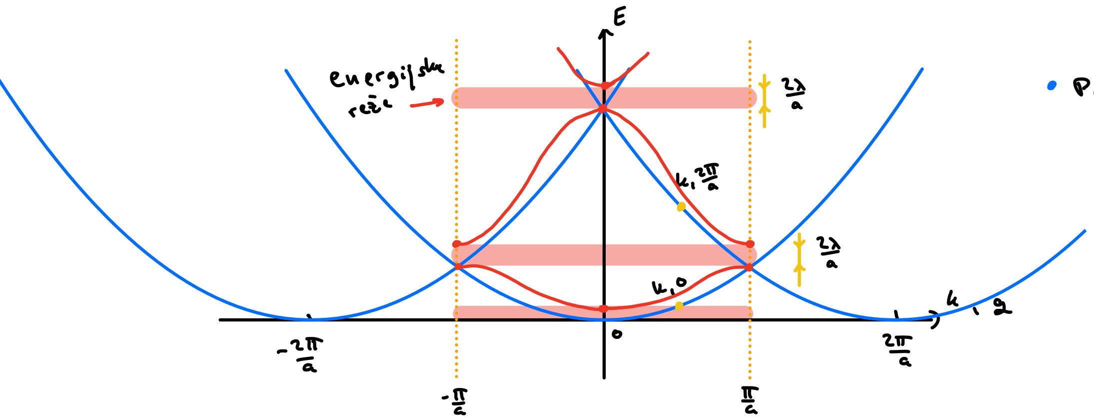
Kaj pa energija $\quad E = \frac{\hbar^2 q^2}{2m}$

Levi rob $\quad E_L = \frac{\hbar^2}{2m}\left(\frac{n\pi}{a}\right)^2$

Desni rob $\quad E_D = \frac{\hbar^2}{2m}\left(\frac{n\pi}{a}+\frac{2Q}{n\pi}\right)^2 = E_L + \frac{\hbar^2}{m}\frac{2Q}{a} + \frac{\hbar^2}{2m}\underbrace{\left(\frac{2Q}{n\pi}\right)^2}_{\approx 0}$

$$E_D = E_L + \frac{2\hbar^2}{ma}\frac{m\lambda}{\hbar^2} = E_L + \frac{2\lambda}{a}$$

Energijska reža $\quad \boxed{\Delta E = \frac{2\lambda}{a}} \quad$ konstantna



- Pri $V=0$ $(\lambda=0)$ $\quad E = \frac{\hbar^2 q^2}{2m}$

  $\cos ka = \cos qa$

  $\Rightarrow k = q$

  ali $\quad q = k + \frac{2\pi}{a}n \quad n \in \mathbb{Z}$

- $V \neq 0$ $(\lambda > 0)$

  analiziraj [illegible] graf

Ⓣ $\quad V(\vec r) = \sum_{\vec K} V_{\vec K}\, e^{i\vec K\cdot\vec r} \qquad V_{\vec K} = \frac{1}{V_{oc}}\int_{oc} V(\vec r)\, e^{-i\vec K\cdot\vec r}$

$\vec K$ vektorji recipročne mreže $\qquad$ vol. os. celice

$$\psi_{\vec k}(\vec r) = \sum_{\vec K} c_{\vec k-\vec K}\, e^{i(\vec k-\vec K)\cdot\vec r}$$

$$\varepsilon^\circ(\vec r) = \frac{\hbar^2 q^2}{2m}$$

$$(\varepsilon^\circ(\vec k-\vec K) - E)\, c_{\vec k-\vec K} + \sum_{\vec K'} V_{\vec K'-\vec K}\, c_{\vec k-\vec K'} = 0 \qquad \forall \vec K$$

lastne energije ki jo iščemo

- izberemo $\vec k \in 1BC$
- rešimo problem lastnih vrednosti

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Iščemo energije na robu BC

$k_1 = 0 \qquad k_2 = \frac{2\pi}{a}$

$k_1: \quad (\varepsilon^0(k-k_1) - E)\, c_{k-k_1} + \underbrace{V_{k_1-k_1} c_{k-k_1} + V_{k_2-k_1} c_{k-k_2}}_{\text{vzamemo le najbližja člena}} = 0$

$k_2: \quad (\varepsilon^0(k-k_2) - E)\, c_{k-k_2} + V_{k_1-k_2}\, c_{k-k_1} + V_{k_2-k_2}\, c_{k-k_1} = 0$

Matrična oblika $\qquad \varepsilon^0(k-k_1) = \varepsilon^0(k-k_2) = \varepsilon^0$

$$\begin{bmatrix} \varepsilon^0 + V_{k_1-k_1} - E & V_{k_2-k_1} \\ V_{k_1-k_2} & \varepsilon^0 + V_{k_2-k_2} - E \end{bmatrix} \begin{bmatrix} c_{k-k_1} \\ c_{k-k_2} \end{bmatrix} = 0$$

det $= 0 \qquad V_{k_2-k_2} = V_{k_1-k_1} = V_0$

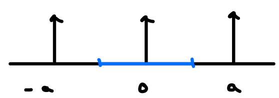
$$(\varepsilon^0 + V_0 - E)^2 - |V_{k_1-k_2}|^2 = 0 \qquad \text{Velja } V_{-k} = V_k^*$$

$$E_\pm = \varepsilon^0 + V_0 \pm |V_{k_1-k_2}|$$

$$\Delta E = E_+ - E_- = 2\,|V_{k_1-k_2}|$$

Do sedaj je bilo vse za poljuben periodičen potencial. Sedaj je pot. delta funkcij

Fourierove komponente



$$V_k = \frac{1}{a}\int_{-a/2}^{a/2} \lambda\,\delta(x)\, e^{-ikx}\, dx$$

lahko si izbrali poljubno o.c.

$$V_k = \frac{\lambda}{a}$$

$$\Rightarrow \Delta E = \frac{2\lambda}{a} \quad ✓$$

Iščemo lastne vektorje

E_+
$$\begin{bmatrix} \varepsilon^0 + \frac{\lambda}{a} - (\varepsilon^0 + \frac{\lambda}{a} + \frac{\lambda}{a}) & \frac{\lambda}{a} \\ \frac{\lambda}{a} & \varepsilon^0 + \frac{\lambda}{a} - (\varepsilon^0 + \frac{\lambda}{a} + \frac{\lambda}{a}) \end{bmatrix} = \frac{\lambda}{a}\begin{bmatrix} -1 & 1 \\ 1 & -1 \end{bmatrix}$$

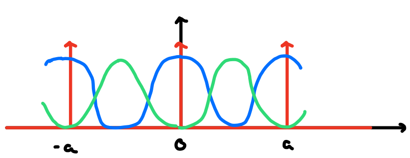
$$\frac{\lambda}{a}(-c_{k-k_1} + c_{k-k_2}) = 0 \Rightarrow c_{k-k_1} = c_{k-k_2} \overset{c_+}{} \Rightarrow \vec{v}_+ = \frac{1}{\sqrt{2}}[1, 1]$$

E_-
$$\frac{\lambda}{a}\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}[c] = 0 \Rightarrow \overset{c_-}{c_{k-k_1}} = -c_{k-k_2} \Rightarrow \vec{v}_- = \frac{1}{\sqrt{2}}(1, -1)$$

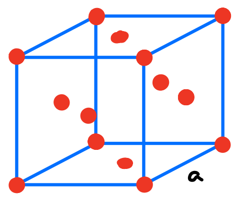
$$\psi_+ = c_+\left(e^{i\frac{\pi}{a}x} + e^{i(\frac{\pi}{a} - \frac{2\pi}{a})x}\right) = 2c_+ \cos\frac{\pi}{a}x$$

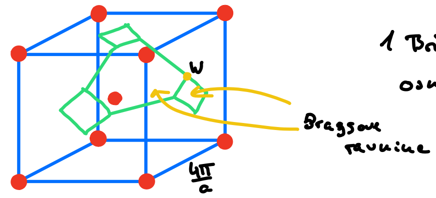
$$\psi_- = c_-\left(e^{i\frac{\pi}{a}x} - e^{-i\frac{\pi}{a}x}\right) = 2i c_- \sin\frac{\pi}{a}x$$

- $\varphi_+(x) \propto \cos^2\frac{\pi}{a}x$
- $\varphi_-(x) \propto \sin^2\frac{\pi}{a}x$



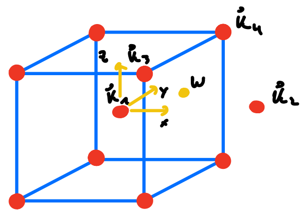
(17) V približku skoraj prostih e^- izračunaj razcep pasov v ogliščih 1BC za FCC kristalno mrežo





1 Brillouinova cona je Wigner-Seitzova osnovna celica recipročne mreže

FCC $\longrightarrow$ Recipročna celica BCC



Velja $|\vec k_i - \vec W| = d \quad i = 1, \dots, 4$

$$\vec W = \frac{4\pi}{a}\left(\frac{1}{2}, 0, \frac{1}{4}\right)$$

Prosti elektroni $V(\vec r) = 0$

$$\varepsilon(\vec k) = \frac{\hbar^2 k^2}{2m} \longrightarrow \varepsilon_{\vec K}(\vec k) = \frac{\hbar^2 (\vec k - \vec K)^2}{2m}$$

$\vec k \in \mathbb{R}^3$ $\qquad$ $\vec k \in$ 1BC in $\vec K$

$\psi_{\vec k}(\vec r) \propto e^{i\vec k\cdot\vec r}$ $\qquad$ $\psi_{\vec K, \vec k}(\vec r) \propto e^{i(\vec k - \vec K)\cdot\vec r}$

en. 4x deg. v $\vec W$

V periodičnem pot. $\quad \psi_{\vec k} = \sum_{\vec K} c_{\vec k - \vec K}\, e^{i(\vec k - \vec K)\cdot\vec r} \qquad V(\vec r) = \sum_{\vec K} V_{\vec K}\, e^{i\vec K\cdot\vec r}$

$$V_{\vec K} = \frac{1}{V_{oc}}\int_{oc} d\vec r\, V(\vec r)\, e^{-i\vec K\cdot\vec r}$$

$$\forall \vec K: \quad \varepsilon^0_{\vec q - \vec K}\, c_{\vec q - \vec K} + \sum_{\vec K'} V_{\vec K' - \vec K}\, c_{\vec q - \vec K'} = E\, c_{\vec q - \vec K}$$

V šibkem potencialu, v 1. redu perturbacije, dobimo popravke le v točkah degeneracije.

$\vec W$ je 4x deg. pri $V = 0$

$$\forall \vec K \in \{\vec K_1, \vec K_2, \vec K_3, \vec K_4\} \qquad (\varepsilon^0_{\vec W - \vec K_n} - E)\, c_{\vec W - \vec K_n} + \sum_{m=1}^{4} V_{\vec K_m - \vec K_n}\, c_{\vec W - \vec K_m} = 0$$

$n = 1, \dots, 4$

Ker $|\vec W - \vec K_i| = d \Rightarrow \varepsilon^0_{\vec W - \vec K_i} = \varepsilon^0$

$$\begin{bmatrix} \varepsilon^0 + V_{K_1 - K_1} - E, & V_{\vec K_2 - \vec K_1}, & V_{K_3 - K_1}, & V_{\vec K_4 - \vec K_1} \\ V_{\vec K_1 - \vec K_2}, & \varepsilon^0 + V_{K_2 - K_2} - E & & \\ & & \ddots & \\ & & & \end{bmatrix} \begin{bmatrix} c_{\vec W - \vec K_1} \\ c_{\vec W - \vec K_2} \\ c_{\vec W - \vec K_3} \\ c_{\vec W - \vec K_4} \end{bmatrix} = 0$$

Rešujemo za poljuben $V(\vec r)$ za FCC

Periodični pot. $V(\vec r) \rightarrow V(\underset{\text{simetrijske operacije}}{R}\,\vec r) = V(\vec r)$

$$V_{\vec k} = \frac{1}{V_{oc}} \int_{oc} d\vec r\; V(\vec r)\; e^{-i\vec k \vec r}$$

- $V_0 = \frac{1}{V_{oc}} \int_{oc} d\vec r\; V(\vec r) = \overline{V(\vec r)}$ povprečna vrednost $= 0$ (umeritev potenciala)

- $V_{\vec k} = \left(\frac{1}{V_{oc}} \int_{oc} d\vec r\; V(\vec r)\, e^{i\vec k \cdot \vec r}\right)^* = V_{-\vec k}^*$

$\Rightarrow V_{-k}^* = V_{-k} \Rightarrow V_{\vec k} \in \mathbb{R}$

- $V_{\vec k} \underset{\vec r \to -\vec r}{=} \frac{1}{V_{oc}} \int d\vec r\; V(-\vec r)\, e^{i\vec k \vec r} = \frac{1}{V_{oc}} \int d\vec r\; V(\vec r)\, e^{i\vec k \vec r} = V_{-\vec k}$

če $V(\vec r) = V(-\vec r)$

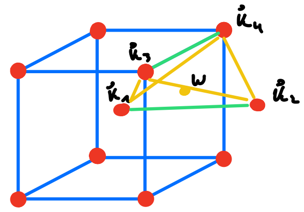
$\Rightarrow$ Imamo le še 6 prostih parametrov v 4×4 matriki

- $V_{R\vec k} = \frac{1}{V_{oc}} \int d\vec r\; V(\vec r)\, e^{-iR\vec k \vec r} = \frac{1}{V_{oc}} \int d\vec r\, V(\vec r)\, e^{-iR\vec k \overbrace{RR^{-1}}^{I} \vec r} = \frac{1}{V_{oc}} \int d\vec r\; V(\vec r)\, e^{-i\vec k R^{-1} \vec r} = \dots$

velja $(R\vec a)\cdot(R\vec b) = \vec a \cdot \vec b$

naj bo $R^{-1}\vec r = \vec u$ $\quad \vec r = R\vec u \quad \int d\vec r = \int d\vec u$

$$\dots = \frac{1}{V_{oc}} \int d\vec u\; V(R\vec u)\, e^{-i\vec k \vec u} \underset{V(R\vec u) = V(\vec u)}{=} \frac{1}{V_{oc}} \int d\vec u\; V(\vec u)\, e^{-i\vec k \vec u} = V_{\vec k}$$



$\Rightarrow$ • $V_{\vec k_2 - \vec k_1} = V_{\vec k_4 - \vec k_3} = V_1 \in \mathbb{R}$

rotacija za 90° okoli z osi

- $V_{\vec k_3 - \vec k_1} = V_{k_4 - k_1} = V_{k_3 - k_2} = V_{k_4 - k_2} = V_2$ (zrcaljenje)

$$\begin{bmatrix} \varepsilon^0 - E & V_1 & V_2 & V_2 \\ V_1 & \varepsilon^0 - E & V_2 & V_2 \\ V_2 & V_2 & \varepsilon^0 - E & V_1 \\ V_2 & V_2 & V_1 & \varepsilon^0 - E \end{bmatrix} \begin{bmatrix} c_{\vec k - \vec k_1} \\ c_{\vec k - \vec k_2} \\ c_{\vec k - \vec k_3} \\ c_{\vec k - \vec k_4} \end{bmatrix} = 0$$

Iščemo E, $\det = 0$

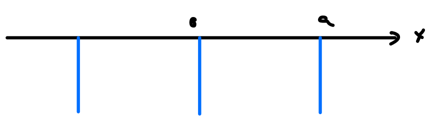
$$\begin{vmatrix} \varepsilon^0 - E & V_1 & V_2 & V_2 \\ V_1 & \varepsilon^0 - E & V_2 & V_2 \\ V_2 & V_2 & \varepsilon^0 - E & V_1 \\ V_2 & V_2 & V_1 & \varepsilon^0 - E \end{vmatrix} \sim \begin{vmatrix} \varepsilon^0 - E - V_1 & V_1 - \varepsilon^0 + E & 0 & 0 \\ V_1 & \varepsilon^0 - E & V_2 & V_2 \\ V_2 & V_2 & \varepsilon^0 - E & V_1 \\ 0 & 0 & V_1 - \varepsilon^0 + E & \varepsilon^0 - E - V_1 \end{vmatrix} \sim \begin{vmatrix} \varepsilon^0 - E - V_1 & 0 & 0 & 0 \\ V_1 & \varepsilon^0 - E + V_1 & 2V_2 & V_2 \\ V_2 & 2V_2 & V_1 + \varepsilon^0 - E & V_1 \\ 0 & 0 & 0 & \varepsilon^0 - E - V_1 \end{vmatrix} = (\varepsilon^0 - E - V_1)^2 \left((\varepsilon^0 - E + V_1)^2 - 4V_2^2 \right) = 0$$

$E_{1,2} = \varepsilon^0 - V_1$ $\quad$ 2x degeneriran

$E_3 = \varepsilon^0 + V_1 - 2V_2$

$E_4 = \varepsilon^0 + V_1 + 2V_2$

18 Kronig-Penneyev model v približku tesne vezi



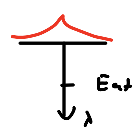
$V(x) = \sum -\tilde\lambda\, \delta(x - na)$

$\tilde\lambda > 0$

Izoliran atom

$V(x) = -\tilde\lambda\, \delta(x)$

$E_{at} = -\frac{m\tilde\lambda^2}{2\hbar^2}$



$\psi_{at}(x) = \sqrt{\kappa_0}\, e^{-\kappa_0 |x|}$

$\kappa_0 = \frac{m\lambda}{\hbar^2}$

ψ_{at} se šibko prekrivajo

$E_{at} \to E_n$ pas

Točna rešitev

$$\cos ka = \cos qa + Qa \frac{\sin qa}{qa} \qquad k \in [-\tfrac{\pi}{a}, \tfrac{\pi}{a}] \qquad q = \sqrt{\frac{2mE}{\hbar^2}} \qquad Q = \frac{m\lambda}{\hbar^2}$$

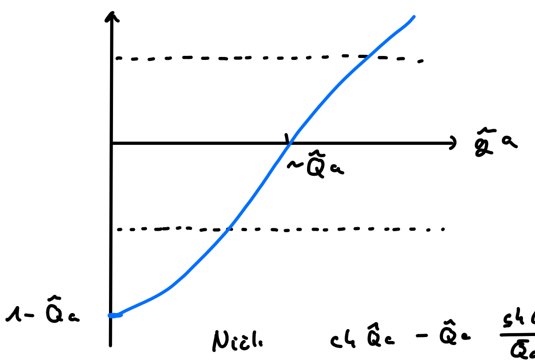
$$\hat{Q} = \frac{m\hat{\lambda}}{\hbar^2} \qquad Q = -\hat{Q}$$

$$E \text{ je neg} \Rightarrow \quad \tilde{q} = \sqrt{\frac{2m(-E)}{\hbar^2}} \qquad q = i\tilde{q}$$

$$\cos ka = \cos i\tilde{q}a - \hat{Q}a \frac{\sin i\tilde{q}a}{i\tilde{q}a} \qquad \cos ix = \operatorname{ch} x, \quad \sin ix = i \operatorname{sh} x$$

$$\cos ka = \operatorname{ch}\tilde{q}a - \hat{Q}a \frac{\operatorname{sh}\tilde{q}a}{\tilde{q}a}$$

Rešujemo grafično



Pri $\hat{Q}a \gg 1$ hitro padajoči repi
šibko prekrivanje

$\tilde{q}a \to 0 \quad \operatorname{ch}\tilde{q}a - \hat{Q}a\frac{\operatorname{sh}\tilde{q}a}{\tilde{q}a} = 1-\hat{Q}a$

$\tilde{q}a \to \infty \quad \underbrace{\operatorname{ch}\tilde{q}a}_{\gg} - \hat{Q}a\frac{\operatorname{sh}\tilde{q}a}{\tilde{q}a} = \infty$

Ničla $\operatorname{ch}\hat{Q}a - \hat{Q}a \frac{\operatorname{sh}\hat{Q}a}{\hat{Q}a} = 0$

ker za $\hat{Q}a \gg 1 \Rightarrow \operatorname{ch}\hat{Q}a \approx \operatorname{sh}\hat{Q}a$

$$\tilde{q}a = \hat{Q}a + \varepsilon \qquad \varepsilon \text{ majhen}$$

$$\cos ka = \operatorname{ch}(\hat{Q}a+\varepsilon) - \hat{Q}a \frac{\operatorname{sh}(\hat{Q}a+\varepsilon)}{\hat{Q}a+\varepsilon}$$

$$\doteq \frac{1}{2} e^{(\hat{Q}a+\varepsilon)} - \frac{\hat{Q}a}{\hat{Q}a+\varepsilon} \frac{1}{2} e^{(\hat{Q}a+\varepsilon)} =$$

$$= \frac{1}{2} e^{(\hat{Q}a+\varepsilon)} \left(1 - \frac{1}{1+\frac{\varepsilon}{\hat{Q}a}}\right) \doteq \qquad \varepsilon \ll Qa$$

$$\doteq \frac{1}{2} e^{(\hat{Q}a+\varepsilon)} \frac{\varepsilon}{\hat{Q}a} \doteq \frac{1}{2} e^{\hat{Q}a} \frac{\varepsilon}{\hat{Q}a}$$

$$\varepsilon = 2\hat{Q}a\, \underbrace{e^{-\hat{Q}a}}\, \cos ka$$

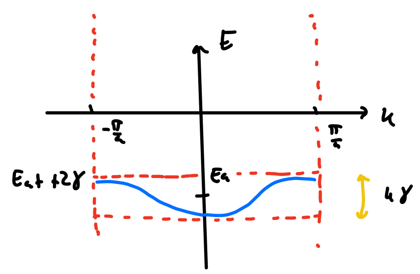
ker je to majhno
je res $\varepsilon \ll \hat{Q}a$

$$\tilde{q}a = \hat{Q}a \left(1 + 2e^{-\hat{Q}a} \cos ka\right.$$

$$E = -\frac{\hbar^2}{2m}\tilde{q}^2 = -\frac{\hbar^2(\hat{Q}a)^2}{2ma^2} - \frac{\hbar^2}{2m}\hat{Q}^2\, 4e^{-\hat{Q}a} \cos ka$$

$$= \underbrace{-\frac{\hbar^2\hat{Q}^2}{2m}}_{E_{at}} - \underbrace{\frac{2\hbar^2}{m}\hat{Q}^2 e^{-\hat{Q}a}}_{\gamma} \cos ka$$

$$E(k) = E_{at} - 2\gamma \cos ka$$



Približek tesne vezi

$$E(\vec{k}) = E_{at} - \frac{\beta + \sum_{\vec{R}\neq 0} \gamma(\vec{R})\, e^{i\vec{k}\cdot\vec{R}}}{1 + \sum_{\vec{R}\neq 0} \alpha(\vec{R})\, e^{i\vec{k}\cdot\vec{R}}}$$

Ta izraz velja za upoštevano eno orbitalo na osnovno celico.

$$\beta = -\int d\vec{r}\; \psi^*_{at}(\vec{r})\, \Delta V(\vec{r})\, \psi_{at}(\vec{r})$$

cel potencial brez tistega v centru.

$$\Delta V(\vec{r}) = \sum_{\vec{R}\neq 0} V_{at}(\vec{r}-\vec{R})$$

Prekrivalni integrali

$$\gamma(\vec{R}) = -\int d\vec{r}\; \psi^*_{at}(\vec{r})\, \Delta V(\vec{r})\, \psi_{at}(\vec{r}-\vec{R})$$

$$\alpha(\vec{R}) = \int d\vec{r}\; \psi^*_{at}(\vec{r})\, \psi(\vec{r}-\vec{R})$$

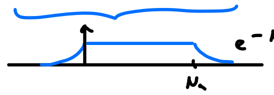
$$E_{at} = -\frac{\hbar^2 \hat{Q}^2}{2m} \qquad \psi_{at} = \sqrt{\hat{Q}}\, e^{-\hat{Q}|x|}$$

$$\beta = -\int dx\, \sqrt{\hat{Q}}\, e^{-\hat{Q}|x|}\Big(\sum_{n\neq 0} -\hat{\lambda}\,\delta(x-na)\Big)\sqrt{\hat{Q}}\, e^{-\hat{Q}|x|}$$

$$= \hat{Q}\hat{\lambda}\int dx\, e^{-2\hat{Q}|x|}\sum_{n\neq 0}\delta(x-na) = \hat{Q}\hat{\lambda}\, e^{-2\hat{Q}a} + \dots$$

$$\gamma(Na) = -\int dx\, \hat{Q}\, e^{-\hat{Q}|x|}\sum_{n\neq 0} -\hat{\lambda}\,\delta(x-na)\, e^{-\hat{Q}|x-Na|} =$$

$$= \hat{Q}\hat{\lambda}\int dx\, \underbrace{e^{-\hat{Q}(|x|+|x-Na|)}}_{e^{-N\hat{Q}a}}\sum_n \delta(x-na)$$



obdržimo samo $|N|=1$, ostali $\gamma(Na)$ so manjši za exp. faktor

$$\gamma(a) = \gamma(-a) = \underset{n=\pm 1}{\hat{Q}\hat{\lambda}}\, e^{-\hat{Q}a} + \mathcal{O}\big(\hat{Q}\hat{\lambda}\, e^{-2\hat{Q}a}\big)$$

$$\alpha(Na) = \int dx\, \hat{Q}\, e^{-\hat{Q}(|x|+|x-Na|)}$$

obdržimo samo $|N|=1$ $\quad \alpha(a) = \alpha(-a) = \mathcal{O}\big(\hat{Q}\, e^{-\hat{Q}a}\, a\big)$

majhen

$$E(k) = E_{at} - \frac{\beta + \gamma(a)\, e^{ika} + \gamma(-a)\, e^{-ika}}{1 + \alpha(a)\, e^{ika} + \alpha(-a)\, e^{-ika}}$$

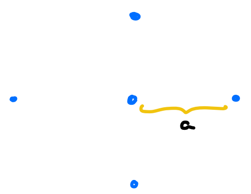
upoštevamo najbližje sosede

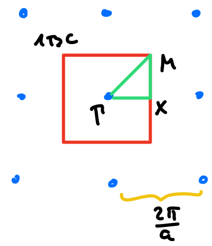
$$= E_{at} - 2\gamma\cos ka\,(1 - 2\underset{\ll}{\alpha}\cos ka) = E_{at} - 2\gamma\cos ka$$

$$\gamma = \hat{Q}\hat{\lambda}\, e^{-\hat{Q}a} = \frac{\hbar^2}{m}\hat{Q}^2 e^{-\hat{Q}a} \qquad \hat{Q} = \frac{m\hat{\lambda}}{\hbar^2} \qquad \hat{\lambda} = \frac{\hat{Q}\hbar^2}{m}$$

19 Kvadratna mreža

Iščemo $E(\vec k)$ v 1.BZ in gostoto stanj, 1s





simetrično

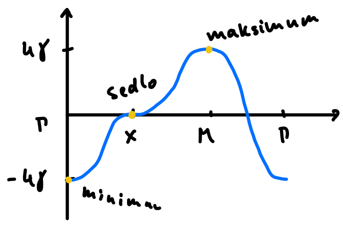
$$E(\vec k) = \underbrace{E_0 - \beta}_{=0 \text{ umeritev}} - \sum_{\substack{\vec R \neq 0 \\ \text{n.s.}}} \gamma(\vec R)\, e^{i\vec k \vec R}, \qquad \gamma(\vec R) = \gamma$$

$$= -\gamma \sum e^{i\vec k \vec R}$$

$$= -\gamma\left(e^{ik_x a} + e^{-ik_x a} + e^{ik_y a} + e^{-ik_y a}\right)$$

$$= -2\gamma\left(\cos k_x a + \cos k_y a\right)$$

Narišimo $E(\vec k)$



$\Gamma \to X \qquad k_y = 0 \qquad k_x \in [0, \frac{\pi}{a}]$

$X \to M \qquad k_x = \frac{\pi}{a} \qquad k_y \in [0, \frac{\pi}{a}]$

$-2\gamma\,(-1 + \cos k_y a)$

$M \to \Gamma \qquad k_x = k_y = k \qquad k_x \in [0, \frac{\pi}{a}]$

$-4\gamma \cos ka \qquad k^2 = k_x^2 + k_y^2$

Razvoj okoli:

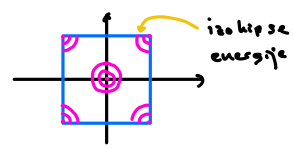
$\Gamma: \quad E = -2\gamma\left(2 - \frac{(k_x a)^2}{2} - \frac{(k_y a)^2}{2}\right) = -4\gamma + \gamma a^2 k^2 \qquad$ minimum

$\quad = -4\gamma + \frac{\hbar^2 k^2}{2m_1^*} \quad \Rightarrow \quad m_1^* = \frac{\hbar^2}{2\gamma a^2}$

$M: \quad E = -2\gamma\left(-2 + \frac{(q_x a)^2}{2} + \frac{(q_y a)^2}{2}\right) = 4\gamma - \gamma a^2 q^2 \qquad k_{x,y} a = \pi + q_{x,y} a$

$\quad = 4\gamma - \frac{\hbar^2 q^2}{2m_2^*} \quad \Rightarrow \quad m_2^* = \frac{\hbar^2}{2\gamma a^2}$

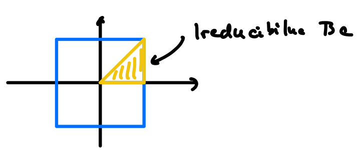
$X: \quad E = -2\gamma\left(-1 + \frac{(q_x a)^2}{2} + 1 - \frac{(k_y a)^2}{2}\right) = \gamma a^2 (k_y^2 - q_x^2) \qquad$ sedlo



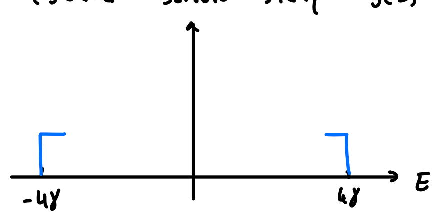
$$E(\vec k) = -\gamma \sum e^{i\vec k \vec R}$$

$$E(A\vec k) = -\gamma \sum e^{iA\vec k \vec R} = -\gamma \sum e^{iA\vec k\, A A^{-1} \vec R} = -\gamma \sum e^{i\vec k A^{-1} \vec R} = E(\vec k)$$

sim. operacije



Iščemo gostoto stanj $g(E)$



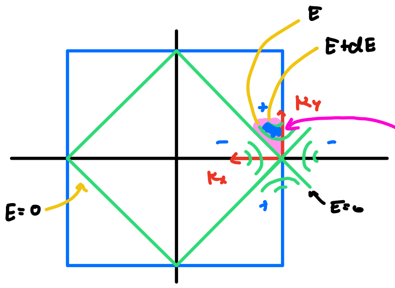
Pri $E = \pm 4\gamma$ se en. obnaša kot pri prostih elektronih, kjer je g konst (v 2D)

$$E(k_x, k_y) = -2\gamma(\cos k_x a + \cos k_y a)$$

$$E\left(\tfrac{\pi}{a} - k_x, \tfrac{\pi}{a} - k_y\right) = -2\gamma\left(\cos(\pi - k_x a) + \cos(\pi - k_y a)\right) = 2\gamma(\cos k_x a + \cos k_y a) = -E(k_x, k_y)$$

Naprej lahko računamo le za poz. energije. $g(E)$ je sodo.

Sedlo ($E = 0$) se v BC nahaja v središču D roba



$$E(\vec{\kappa}) = \gamma a^2(\kappa_y^2 - \kappa_x^2)$$

$$= 0 \Rightarrow \kappa_x = \pm \kappa_y$$

Lahko gledamo le pot. en.
na tej sliki, da vemo, kako risati $g(E)$
Ta košček se ponovi še 7x,

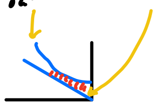
$$g(E) = \frac{1}{S}\frac{dN(E, E+dE)}{dE}$$ št. stanj med E in $E+dE$

Naj bo $G(E) = \dfrac{N(0,E)}{S} \Rightarrow g(E) = G'(E)$

$$G(E) = 2 \cdot 8 \cdot \frac{1}{S}\int_0^{\kappa_0} \left(\sqrt{\frac{E}{\gamma a^2} + \kappa_x^2} - \kappa_x\right) d\kappa_x \, \frac{1}{\left(\frac{2\pi}{L}\right)^2}$$

spin

to območje se ponovi 8x



$$E = \gamma a^2(\kappa_y^2 - \kappa_x^2)$$
$$\kappa_y = \sqrt{\frac{E}{\gamma a^2} + \kappa_x^2}$$

$\left(\frac{2\pi}{L}\right)^n$ ... ploščina 1 stanja v k prostoru za n-dim kristal

$$g(E) = \frac{dG}{dE}$$

$$g(E) = \frac{4}{\pi^2}\int_0^{\kappa_0} \frac{1}{\sqrt{\frac{E}{\gamma a^2} + \kappa_x^2}} \, \frac{1}{2} \, \frac{1}{\gamma a^2} \, d\kappa_x$$

$$= \frac{2}{\pi^2 \gamma a^2}\int_0^{\kappa_0} \frac{1}{\sqrt{1 + \frac{\kappa_x^2 \gamma a^2}{E}}} \sqrt{\frac{\gamma a^2}{E}} \, d\kappa_x \qquad u = \kappa_x \sqrt{\frac{\gamma a^2}{E}}$$

$$= \frac{2}{\pi^2 \gamma a^2}\int_0^{u_0} \frac{1}{\sqrt{1+u^2}} \, du$$

$$= \frac{2}{\pi^2 \gamma a^2} \operatorname{arcsinh} \kappa_0 \sqrt{\frac{\gamma a^2}{E}}$$

pri $E \to 0$ nas zanima $u_0 \gg 1$

$$= \frac{2}{\pi^2 \gamma a^2} \ln 2\kappa_0 \sqrt{\frac{\gamma a^2}{E}}$$

$$y = \operatorname{sh} x = \frac{e^x - e^{-x}}{2}$$

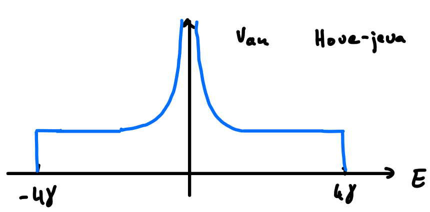
$y \gg 1 \qquad e^{-x} \approx 0$

$y = \frac{e^x}{2} \Rightarrow x = \ln 2y$

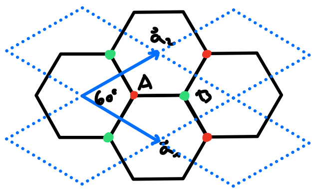
$$= \frac{2}{\pi^2 \gamma a^2}\left(\ln 2\kappa_0 \sqrt{\gamma a^2} - \frac{1}{2}\ln E\right)$$

$E \to 0$

$$\doteq -\frac{1}{\pi^2 \gamma a^2} \ln E$$



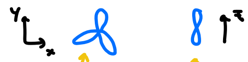
20 Disperzija v grafenu



$$\vec r_A = \frac{1}{3}(\vec a_1 + \vec a_2)$$
$$\vec r_B = \frac{2}{3}(\vec a_1 + \vec a_2)$$

Potrebujemo 2 orbitali, ker sta 2 atoma v os. celici

$$C:\ \cancel{1s^2}\ \underbrace{2s^2\ 2p^2}_{2sp_2^3\ \ 2p_z^1}$$



niso blizu fermijeve en.

uporabimo te orbitale

Najbližji sosedi na poziciji:

- $\vec R, A$:
  - $\vec R, B$
  - $\vec R - \vec a_1, B$
  - $\vec R - \vec a_2, B$
- $\vec R, B$:
  - $\vec R, A$
  - $\vec R + \vec a_1, A$
  - $\vec R + \vec a_2, A$

$$\gamma(\vec R B, \vec R A) = \gamma(\vec R - a_1 B, \vec R A) = \gamma(\vec R - a_2 B, \vec R A) =$$
$$= \gamma(\vec R A, \vec R B) = \gamma(\vec R + a_1 A, \vec R B) = \gamma(\vec R + a_2 B, \vec R A) = \gamma$$

zaradi simetrij

$$\beta(\vec R A) = \beta(\vec R B) = \beta$$

$$\beta = -\int d\vec r\ \psi^*_{at}(\vec r)\, \Delta V(\vec r)\, \psi_{at}(\vec r)$$

$$\gamma(\vec R) = -\int d\vec r\ \psi^*_{at}(\vec r)\, \Delta V(\vec r)\, \psi_{at}(\vec r - \vec R)$$

$$E(\vec k) = E_{at} - \beta + \sum_{\vec R = ns\phi} \gamma(\vec R) e^{i\vec k\cdot\vec R}$$

Velja le za en orbitalo na os. celico

Recept za vse orbital)

$$H|\psi\rangle = E|\psi\rangle$$

$$|\psi\rangle = \sum_{\vec R \alpha} c_{\vec R \alpha} |\vec R\, \alpha\rangle \qquad \alpha \in [A, B]$$

orbitala p_z

približek tesne vezi (vzeli smo le p_z orbitale)

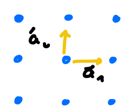
energija e^- v izolirani orbitali

popravek

$$-\gamma c_{\vec R B} - \gamma c_{\vec R - \vec a_1 B} - \gamma c_{\vec R - \vec a_2 B} + (E_0 - \beta) c_{\vec R A} = E c_{\vec R A}$$
$$-\gamma c_{\vec R A} - \gamma c_{\vec R + \vec a_1 A} - \gamma c_{\vec R + \vec a_2 A} + (E_0 - \beta) c_{\vec R B} = E c_{\vec R B}$$

Preverimo, da se to sklada s prvotnim receptom

Preverimo na kvadratni mreži



$$-\gamma c_{\vec R + \vec a_1} - \gamma c_{\vec R + \vec a_2} - \gamma c_{\vec R - \vec a_1} - \gamma c_{\vec R - \vec a_2} + (E_0 - \beta) c_{\vec R} = E c_{\vec R}$$

$$c_{\vec R} = c\, e^{i\vec k\cdot\vec R} \qquad \text{nastavek}$$

$$\Rightarrow -\gamma c \sum_i e^{i\vec k\cdot\vec a_i} + (E_0 - \beta) c = E c$$

$$E(\vec k) = E_0 - \beta - \gamma \sum_i e^{i\vec k\cdot\vec a_i} \quad ✓$$

Nazaj na grafen

Nastavek $\quad c_{\vec R A} = c_A e^{i\vec k\cdot\vec R} \qquad c_{\vec R B} = c_B e^{i\vec k\vec R}$

Vstavimo v * $\qquad \beta,\gamma\in\mathbb{R}$

$$-\gamma c_B\left(e^{i\vec k\vec R} + e^{i\vec k(\vec R-\vec a_1)} + e^{i\vec k(\vec R-\vec a_2)}\right) + (\varepsilon_0-\beta)c_A e^{i\vec k\vec R} = E c_A e^{i\vec k\vec R}$$

$$-\gamma c_A\left(e^{i\vec k\vec R} + e^{i\vec k(\vec R+\vec a_1)} + e^{i\vec k(\vec R+\vec a_2)}\right) + (\varepsilon_0-\beta)c_B e^{i\vec k\vec R} = E c_B e^{i\vec k\vec R}$$

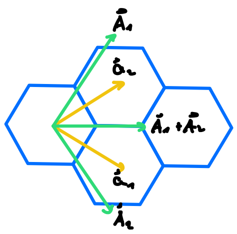
$$\begin{bmatrix} E_0-\beta & -\gamma(1+e^{-i\vec k\vec a_1}+e^{-i\vec k\vec a_2}) \\ -\gamma(1+e^{i\vec k\vec a_1}+e^{i\vec k\vec a_2}) & E_0-\beta\end{bmatrix}\begin{bmatrix}c_A\\c_B\end{bmatrix} = E\begin{bmatrix}c_A\\c_B\end{bmatrix} \qquad \Rightarrow E_1(\vec k),\ E_2(\vec k)$$

$$(E_0-\beta-E)^2 - \gamma^2\left|1+e^{ika_1}+e^{ika_2}\right|^2 = 0 \qquad a a^* = |a|^2$$

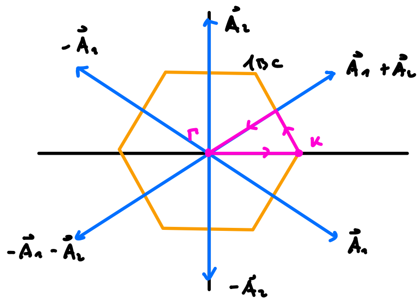
$$E_0-\beta-E = \pm\gamma\left|1+e^{i\vec k\vec a_1}+e^{i\vec k\vec a_2}\right|$$

$$E = E_0-\beta\pm\gamma\left|1+e^{i\vec k\vec a_1}+e^{i\vec k\vec a_2}\right|$$

Recipročno mrežo že poznamo (trikotna mreža) $\qquad$ k prostor in 1BC



$$\vec K = m_1\vec A_1 + m_2\vec A_2 = m_1'\vec A_1 + m_2'(\vec A_1+\vec A_2)$$



Zanima nas dogajanje v točki K

$\vec k = \vec K + \vec q \qquad |\vec q| \ll \frac{\pi}{a}$

$$\vec K = \frac23\,\frac{(\vec A_1+\vec A_2)+\vec A_1}{2} = \frac23\vec A_1 + \frac13\vec A_2$$

$$E = \pm\gamma\left|1 + e^{i\frac23 A_1a_1 + i\frac13 A_2a_1 + i\vec q\vec a_1} + e^{i\frac23 A_1a_2 + i\frac13 A_2a_2 + i\vec q\vec a_2}\right| \qquad \vec A_i\vec a_j = 2\pi\delta_{ij}$$

$$= \pm\gamma\left|1 + \underbrace{e^{i\frac23 2\pi}}_{e^{-\frac23\pi i}} e^{i\vec q\vec a_1} + e^{i\frac13 2\pi}e^{i\vec q\vec a_2}\right|$$

$$= \pm\gamma\left|1 + e^{-i\frac{2\pi}{3}}(1+i\vec q\cdot\vec a_1) + e^{i\frac{2\pi}{3}}(1+i\vec q\vec a_2)\right| \qquad 1+e^{i\frac{2\pi}{3}}+e^{-i\frac{2\pi}{3}} = 0$$

$$= \pm\gamma\left|e^{-i\frac{2\pi}{3}}\, i\vec q\vec a_1 + e^{i\frac{2\pi}{3}}\, i\vec q\vec a_2\right|$$

$$= \pm\gamma\left|i\cos\frac{2\pi}{3}\,\vec q(\vec a_1+\vec a_2) + \sin\frac{2\pi}{3}\,\vec q(\vec a_1-\vec a_2)\right|$$

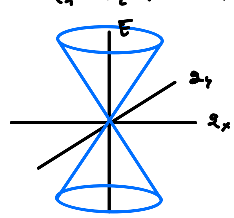
$$= \pm\gamma\sqrt{\cos^2\frac{2\pi}{3}\left|\vec q(\vec a_1+\vec a_2)\right|^2 + \sin^2\frac{2\pi}{3}\left|\vec q(\vec a_1-\vec a_2)\right|^2}$$

$\vec a_1+\vec a_2 = 3a(1,0,0)$

$\vec a_1-\vec a_2 = \sqrt3 a(0,-1,0)$

$$= \pm\gamma\sqrt{\frac14 9a^2q_x^2 + \frac34 3a^2 q_y^2}$$

$$= \pm\frac{3\gamma a}{2}\sqrt{q_x^2+q_y^2} = \pm\frac32\gamma a q$$



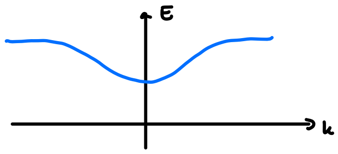
21 Ciklotronska efektivna masa

Elektroni v kristalu in mag. polju.

Uporabimo kvazi klasičen približek

$$\hbar\dot{\vec k} = \vec F = e\vec v\times\vec B \qquad \vec v = \frac{1}{\hbar}\frac{\partial E(\vec k)}{\partial \vec k} \quad \text{grupna hitrost}$$

Naj bo dan nek pas



$$m_g^* = \sqrt[3]{\det m^*}$$

Razvoj okoli minimuma

$$E(k) = \frac{\hbar^2}{2}\vec k\cdot (m^*)^{-1}\vec k + E_0 \qquad g(E) = \frac{\sqrt{2m_g^{*3}}}{\pi^2\hbar^3}\sqrt{E-E_0}$$

$$(m^*)^{-1}_{\alpha\beta} = \frac{1}{\hbar^2}\left(\frac{\partial^2 E(k)}{\partial k_\alpha \partial k_\beta}\right)_{\alpha\beta}\Bigg|_{k=0} \quad \text{tenzor ef. mase}$$

Lastne vrednosti $(m^*)^{-1} > 0$ (ker je minimum)

$$v_\alpha = \frac{1}{\hbar}\frac{\partial E}{\partial k_\alpha} \qquad E(k) = E_0 + \frac{\hbar^2}{2}\sum_{ij} k_i (m^*)^{-1}_{ij} k_j$$

$$v_\alpha = \frac{1}{\hbar}\frac{\partial}{\partial k_\alpha}\left(E_0 + \frac{\hbar^2}{2}\sum_{ij} k_i (m^*)^{-1}_{ij} k_j\right)$$

$$= \frac{\hbar}{2}\sum_{ij} \delta_{i\alpha}(m^*)^{-1}_{ij} k_j + k_i (m^*)^{-1}_{ij}\delta_{j\alpha}$$

$$= \frac{\hbar}{2}\sum_j (m^*)^{-1}_{\alpha j} k_j + \frac{\hbar}{2}\sum_i k_i (m^*)^{-1}_{i\alpha} \qquad (m^*)^{-1} \text{ simetričen}$$

$$= \hbar\sum_i (m^*)^{-1}_{\alpha i} k_i$$

$$\vec v = \hbar (m^*)^{-1}\vec k$$

$$m^*\vec v = \hbar\vec k$$

$$\hbar\dot{\vec k} = m^*\dot{\vec v}$$

$$m^*\dot{\vec v} = -e_0\vec v\times\vec B$$

Nastavek $\vec v = \vec v_0 e^{-i\omega t}$

$$-i\omega m^*\vec v_0 e^{-i\omega t} = -e_0\vec v_0 e^{-i\omega t}\times\vec B$$

$$i\omega m^*\vec v_0 = e_0\vec v_0\times\vec B \qquad \vec B = B(0,0,1) \qquad \vec v_0\times\vec B = B(v_y, -v_x, 0)$$

$$(m^*)\begin{pmatrix} v_x \\ v_y \\ v_z\end{pmatrix} = \frac{e_0B}{i\omega}\begin{pmatrix} v_y \\ -v_x \\ 0\end{pmatrix}$$

$$\begin{bmatrix} m_{xx} & m_{xy} - \frac{e_0B}{i\omega} & m_{xz} \\ m_{xy} + \frac{e_0B}{i\omega} & m_{yy} & m_{yz} \\ m_{xz} & m_{yz} & m_{zz}\end{bmatrix}\vec v = 0$$

$$0 = \det[\,] = \det m^* - \cancel{m_{xy}m_{zz}}\frac{e_0B}{i\omega} + \frac{e_0B}{i\omega}\left(\cancel{m_{xy}m_{zz}} + \frac{e_0B}{i\omega}m_{zz} - \cancel{m_{xz}m_{yz}}\right) + \cancel{m_{xz}\frac{e_0B}{i\omega}m_{yz}}$$

$$= \det m^* + \left(\frac{e_0B}{i\omega}\right)^2 m_{zz}$$

$$\omega = e_0B\sqrt{\frac{m_{zz}}{\det m^*}} \qquad \omega_c = \frac{e_0B}{m_e}$$

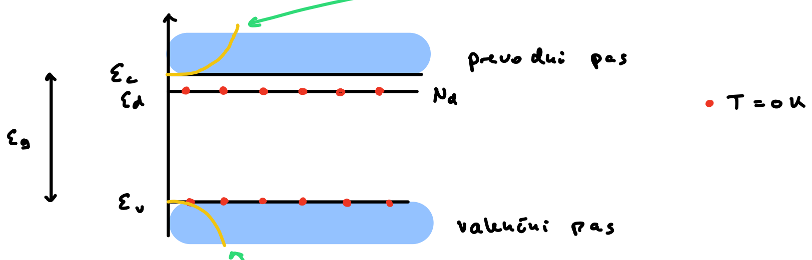
$$\omega = \frac{e_0B}{m_c^*} \qquad m_c^* = m_e\sqrt{\frac{\det m^*}{m_{zz}}}$$

$\hookrightarrow$ ciklotronska efektivna masa

(22) e^- v polprevodniku

$n_c(T) = ?$

$$g_c(\varepsilon) = \frac{\sqrt{2m_c^{*}}}{\pi^2\hbar^3}\sqrt{\varepsilon-\varepsilon_c} \qquad m_c^{*} = \sqrt[3]{\det m_c^{*}}$$



$$g_v(\varepsilon) = \frac{\sqrt{2m_v^{*}}}{\pi^2\hbar^3}\sqrt{\varepsilon_v-\varepsilon} \qquad m_v^{*} = \sqrt[3]{-\det m_v^{*}}$$

$$n_c = \int_{\varepsilon_c} g_c(\varepsilon) f(\varepsilon)\, d\varepsilon = \ldots \qquad p_v = P_v\, e^{-\beta(\mu-\varepsilon_v)}$$

$$f(\varepsilon) = \frac{1}{e^{\beta(\varepsilon-\mu)}+1} \doteq e^{-\beta(\varepsilon-\mu)} \qquad \text{za } \mu-\varepsilon_v \gg k_BT$$

za nedegeneriran polprevodnik $\quad \mu \ll \varepsilon, \quad \varepsilon-\mu \gg k_BT$

$$P_v = \frac{1}{4}\left(\frac{2m_v^{*}k_BT}{\pi\hbar^2}\right)^{3/2}$$

$$\ldots = N_c\, e^{-\beta(\varepsilon_c-\mu)}$$

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

$$N_c = \frac{1}{4}\left(\frac{2m_c^{*}k_BT}{\pi\hbar^2}\right)^{3/2}$$

Iščemo n_c

$$n_c = p_v + p_d$$

Omejimo se $p_v = 0$, torej $k_BT \ll \varepsilon_g$

$$n_c = p_d$$

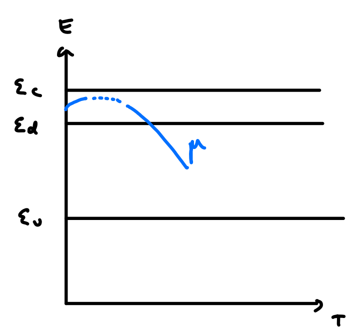
$$N_c\, e^{-\beta(\varepsilon_c-\mu)} = N_d \frac{1}{1+2e^{-\beta(\varepsilon_d-\mu)}}$$

$$\frac{N_d}{N_c} = e^{-\beta(\varepsilon_c-\mu)} + 2e^{-\beta(\varepsilon_c+\varepsilon_d-2\mu)} \qquad \mu = ?$$

$$2e^{-\beta(\varepsilon_c+\varepsilon_d)}\left(e^{\beta\mu}\right)^2 + e^{-\beta\varepsilon_c}\left(e^{\beta\mu}\right) - \frac{N_d}{N_c} = 0$$

$$e^{\beta\mu} = -\frac{1}{4}e^{\beta\varepsilon_d} \pm \sqrt{\frac{1}{16}e^{2\beta\varepsilon_d} + \frac{N_d}{2N_c}e^{\beta(\varepsilon_c+\varepsilon_d)}}$$

$$= \frac{1}{4}e^{\beta\varepsilon_d}\left(-1 \pm \sqrt{1+8\frac{N_d}{N_c}e^{\beta(\varepsilon_c-\varepsilon_d)}}\right)$$



Limite

- $8\frac{N_d}{N_c}e^{\beta(\varepsilon_c-\varepsilon_d)} \ll 1$ visokotemp. lim.

$$e^{\beta\mu} = \frac{1}{4}e^{\beta\varepsilon_d}\left(-1+1+4\frac{N_d}{N_c}e^{\beta(\varepsilon_c-\varepsilon_d)}\right) = \frac{N_d}{N_c}e^{\beta\varepsilon_c}$$

$$\mu = \varepsilon_c + k_BT\ln\frac{N_d}{N_c(T)} = \varepsilon_c + k_BT\left(\ln \text{konst} + \ln T^{-3/2}\right)$$

(konst $\ll$)

$$= \varepsilon_c - \frac{3}{2}k_BT\ln T$$

- $8\frac{N_d}{N_c}e^{\beta(\varepsilon_c-\varepsilon_d)} \gg 1$ nizkotemp. lim.

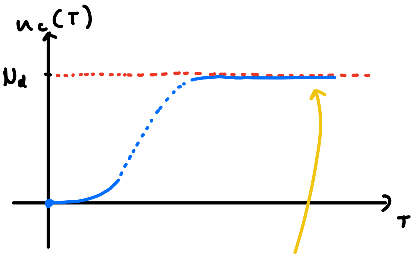
$$e^{\beta\mu} = \frac{1}{\sqrt{2}}\sqrt{\frac{N_d}{N_c}}\, e^{\frac{\beta}{2}(\varepsilon_c+\varepsilon_d)}$$

$$\mu = \frac{\varepsilon_c+\varepsilon_d}{2} + \frac{1}{2\beta}\ln\frac{N_d}{2N_c} = \frac{\varepsilon_c+\varepsilon_d}{2} + \frac{k_BT}{2}\left(\text{konst} + \ln T^{-3/2}\right)$$

$$= \frac{\varepsilon_c+\varepsilon_d}{2} - \frac{3k_BT}{4}\ln T$$

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

$n_c(T) = N_d$

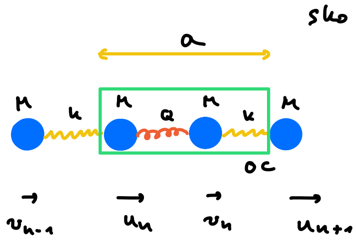


$$n_c(T) = \sqrt{\frac{N_c N_D}{2}}\, e^{-\beta\frac{\varepsilon_c-\varepsilon_d}{2}}$$

$$\propto T^{3/4}\, e^{-\frac{1}{k_BT}\frac{\varepsilon_c-\varepsilon_d}{2}}$$

vsi donorski e^- skočijo v prevodni pas

23 1D veriga



Gibalne enačbe

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

Periodični robni pogoji ⇒ upoštevamo translacijsko simetrijo

⇒ Blochov teorem ⇒ ravni valovi

Blochov val. vektor

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

$$-M\omega^2 u_0 e^{i(kna-\omega t)} = Q(v_0-u_0)e^{i(kna-\omega t)} + k(v_0 e^{-ika} - u_0)e^{i(kna-\omega t)}$$
$$-M\omega^2 v_0 = Q(u_0 - v_0) + k(u_0 e^{ika} - v_0)$$

$$0 = M\omega^2 u_0 + Q(v_0-u_0) + k(v_0 e^{-ika} - u_0)$$
$$0 = M\omega^2 v_0 + Q(u_0-v_0) + k(u_0 e^{ika} - v_0)$$

$$\begin{bmatrix} M\omega^2 - Q - k & Q + ke^{-ika} \\ Q + ke^{ika} & M\omega^2 - Q - k \end{bmatrix}\begin{bmatrix} u_0 \\ v_0 \end{bmatrix} = 0$$

$$(M\omega^2 - (Q+k))^2 - (Q + ke^{ika})(Q + ke^{-ika}) = 0$$

$$M^2\omega^4 - 2M\omega^2(Q+k) + Q^2 + 2Qk + k^2 - Q^2 - Qke^{-ika} - Qke^{ika} - k^2 = 0$$

$$M^2\omega^4 - 2M\omega^2(Q+k) - Qk(\underbrace{e^{ika} + e^{-ika}}_{2\cos ka} - 2) = 0$$

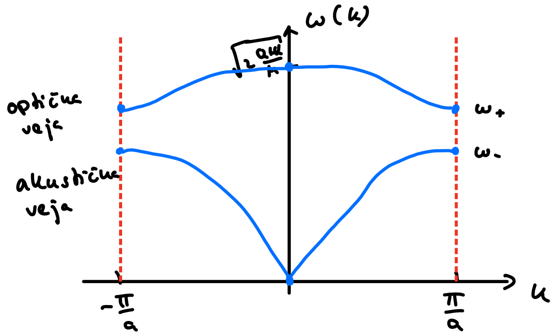
$$\omega^4 - 2\frac{Q+k}{M}\omega^2 + \frac{2Qk}{M^2}(1-\cos ka) = 0$$

$$\omega^2_{1,2} = \frac{Q+k}{M} \pm \sqrt{\left(\frac{Q+k}{M}\right)^2 - \frac{2Qk}{M^2}(1-\cos ka)}$$

$$= \frac{Q+k}{M} \pm \frac{1}{M}\sqrt{Q^2 + k^2 + 2Qk(\cos ka + 1 - 1)}$$

$$\sin^2\frac{x}{2} = 1 - \cos x$$

$$= \frac{Q+k}{M} \pm \frac{1}{M}\sqrt{(Q+k)^2 - 4Qk\sin^2\frac{ka}{2}} = \frac{Q+k}{M}\left(1 \pm \sqrt{1 - \frac{4Qk}{(Q+k)^2}\sin^2\frac{ka}{2}}\right)$$



$k = 0$ $\qquad \omega_1^2 = 0$

$$\omega_2^2 = 2\,\frac{Q+K}{M}$$

$k = \frac{\pi}{a}$

$$\omega_{1,2}^2 = \frac{Q+K}{M} \pm \frac{1}{M}\sqrt{Q^2+K^2-2QK}$$

$$= \frac{Q+K}{M} \pm \frac{|Q-K|}{M}$$

$$\omega_1^2 = \frac{2Q}{M} \quad Q>K \qquad = \frac{2K}{M} \quad K>Q$$

$$\omega_2^2 = \frac{2K}{M} \quad Q>K \qquad = \frac{2Q}{M} \quad K>Q$$

$$\Rightarrow \quad \omega_+^2 = \frac{2\max(Q,K)}{M} \qquad \omega_-^2 = \frac{2\min(Q,K)}{M}$$

k majhen $\qquad k \ll \frac{\pi}{a}$

$$\omega^2 = \frac{Q+K}{M}\left(1 - \sqrt{1 - \frac{QK}{(Q+K)^2}(ka)^2}\right) \approx \qquad \sqrt{1+\varepsilon} = 1 + \frac{\varepsilon}{2}$$

$$= \frac{Q+K}{M}\left(1 - \left(1 - \frac{1}{2}\frac{QK}{(Q+K)^2}(ka)^2\right)\right)$$

$$= \frac{Q+K}{M}\,\frac{1}{2}\,\frac{QK}{(Q+K)^2}(ka)^2 = \frac{QK}{2M(Q+K)}(ka)^2$$

$$\omega = \sqrt{\frac{QK}{2M(Q+K)}}\,|k|\,a = c\,|k|$$

$$c = \sqrt{\frac{QK}{2M(Q+K)}}\,a$$

Iščemo lastna nihanja

$$\begin{bmatrix} M\omega^2 - Q - K & Q + Ke^{-ika} \\ Q + Ke^{ika} & M\omega^2 - Q - K \end{bmatrix} \begin{bmatrix} u_0 \\ v_0 \end{bmatrix} = 0$$

$$u_0 = -\frac{Q + Ke^{-ika}}{M\omega^2 - Q - K}\,v_0$$

$$\begin{bmatrix} u_0 \\ v_0 \end{bmatrix} = \begin{bmatrix} -\frac{Q + Ke^{-ika}}{M\omega^2 - Q - K} \\ 1 \end{bmatrix}$$

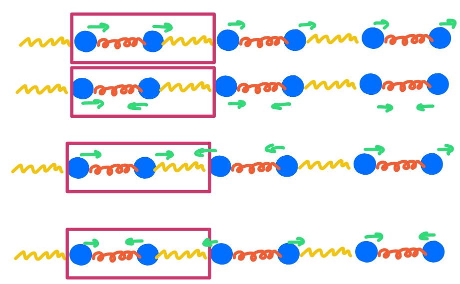
1 $\quad k = 0 \quad$ akustična $\qquad \begin{pmatrix} u_0 \\ v_0 \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$

2 $\quad k = 0 \quad$ optična $\qquad \begin{pmatrix} u_0 \\ v_0 \end{pmatrix} = \begin{pmatrix} 1 \\ -1 \end{pmatrix}$

$Q > K$ $\quad$ 3 $\quad k = \frac{\pi}{2} \quad$ akustična $\qquad \begin{pmatrix} u_0 \\ v_0 \end{pmatrix} = \left(-\frac{Q-K}{K-Q},\ 1\right) = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$

$$e^{ikan} = (1)^n$$

4 $\quad k = \frac{\pi}{2} \quad$ optična $\qquad \left(\frac{u_0}{v_0}\right) = \begin{pmatrix} 1 \\ -1 \end{pmatrix}$



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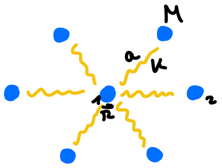
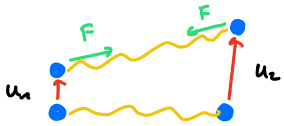


Odmik le izven ravnine lista

$a > a_0$ ⟺ prednapetost vzmeti

neraztegnjena dolžina vzmeti



$$F = k(x - a_0) = k\left(\sqrt{(u_2-u_1)^2 + a^2} - a_0\right) =$$

$$= k(a-a_0) + \mathcal{O}\left((u_2-u_1)^2\right)$$

zanemarimo

$$F_\parallel = F\cos\alpha = k(a-a_0) + \cancel{\mathcal{O}((u_2-u_1)^2)}$$

$$F_\perp = F\sin\alpha = k(a-a_0)\tan\alpha = k(a-a_0)\frac{(u_2-u_1)}{a} = \tilde{k}(u_2-u_1)$$

$\sin\alpha \sim \tan\alpha$

$$\tilde{k} = \frac{k(a-a_0)}{a}$$

Gibalne enačbe

$$M\ddot{u}_{\vec{R}} = \tilde{k}\sum_{\vec{R}'}(u_{\vec{R}'} - u_{\vec{R}}) \qquad u_{\vec{R}} = u_0 e^{i(\vec{k}\cdot\vec{R} - \omega t)}$$

najbližji sosedje

$$-\omega^2 M e^{i\vec{k}\cdot\vec{R}} = \tilde{k}\sum_{\vec{R}'}^{6}\left(e^{i\vec{k}\cdot\vec{R}'} - e^{i\vec{k}\cdot\vec{R}}\right)$$

$$-\frac{M\omega^2}{\tilde{k}} = \sum_{\vec{R}'}^{6}\left(e^{i\vec{k}(\vec{R}'-\vec{R})} - 1\right) \qquad \text{naj bo } \vec{R} = 0$$

$$-\frac{M\omega^2}{\tilde{k}} = \sum_{\vec{R}'}^{6}\left(e^{i\vec{k}\cdot\vec{R}'} - 1\right)$$

$$-\frac{M\omega^2}{\tilde{k}} = \frac{1}{2}\sum_{\vec{R}'}\left(\underbrace{e^{i\vec{k}\cdot\vec{R}'} + e^{-i\vec{k}\cdot\vec{R}'}}_{2\cos\vec{k}\cdot\vec{R}'} - 2\right) \qquad \cos\alpha - 1 = -2\sin^2\frac{\alpha}{2}$$

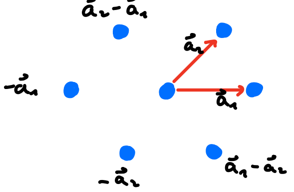
$$-\frac{M\omega^2}{\tilde{k}} = -2\sum_{\vec{R}'}\sin^2\left(\frac{\vec{k}\cdot\vec{R}'}{2}\right)$$

$$\boxed{\omega^2 = \frac{2\tilde{k}}{M}\sum_{\vec{R}'}\sin^2\frac{\vec{k}\cdot\vec{R}'}{2} \quad \text{n.s.o.}}$$

velja za poljubno prednapeto 2D mrežo za nihanje $\perp$ na ravnino mreže

Če $|\vec{k}| \ll \frac{1}{a}$

$$\Rightarrow \omega^2 = \frac{2\tilde{k}}{M}\sum_{\vec{R}'}\left(\frac{\vec{k}\cdot\vec{R}'}{2}\right)^2 = \frac{\tilde{k}}{2M}\sum_{\vec{R}'}(\vec{k}\cdot\vec{R}')^2$$



$$= \frac{2\tilde{k}}{2M}\left((\vec{k}\cdot\vec{a}_1)^2 + (\vec{k}\cdot\vec{a}_2)^2 + (\vec{k}\cdot(\vec{a}_1-\vec{a}_2))^2\right)$$

$\vec{k} = (k_x, k_y)$

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

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

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

$$= \frac{\tilde{k}}{M}\left((k_x a)^2 + \left(k_x\frac{a}{2} + k_y\frac{\sqrt{3}}{2}a\right)^2 + \left(k_x\frac{a}{2} - k_y\frac{\sqrt{3}}{2}a\right)^2\right)$$

$$= \frac{\tilde{k}}{M}\left((k_x a)^2 + 2\frac{1}{4}(k_x a)^2 + 2\frac{3}{4}(k_y a)^2\right)$$

$$= \frac{3\tilde{k}}{2M}a^2(k_x^2 + k_y^2) = \frac{3\tilde{k}}{2M}k^2a^2 = c^2k^2 \qquad k = |\vec{k}|$$

$$c = \frac{dE}{dT} \qquad E = \sum_{\vec{k}}\hbar\omega_{\vec{k}}\left(\frac{1}{e^{\beta\hbar\omega_k} - 1} + \frac{1}{2}\right)$$

↳ bo odpadlo pri odvodu

Nizka T, β velik

$$E = \frac{1}{\frac{(2\pi)^2}{S}}\int_{1BC} d\vec{k}\,\hbar\omega_{\vec{k}}\frac{1}{e^{\beta\hbar\omega_k} - 1}$$

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

2D $\Delta k = \frac{(2\pi)^2}{S}$ površina celotnega kristala

$$E \overset{\beta \text{ velik}}{=} \frac{S}{(2\pi)^2} \int \underbrace{d\vec{k}}_{\text{1BC } 2\pi k dk} \hbar c k \frac{1}{e^{\beta\hbar c k}-1} \quad \omega = ck$$

izven 1.BC je integrand skoraj 0.

$$= \frac{S}{2\pi} \int_0^\infty dk \frac{\hbar c k^2}{e^{\beta \hbar c k}-1}$$

$$= \frac{S}{2\pi \beta^3 c^2 \hbar^2} \underbrace{\int_0^\infty \frac{x^2}{e^x - 1} dx}_{\zeta(3) = 2,4}$$

$$c = \frac{dE}{dT} = \frac{3 S k_B^3 T^2}{2\pi \hbar^2 c^2} \zeta(3)$$

$$N = \frac{S}{\frac{a^2\sqrt{3}}{2}} \qquad \frac{C}{N} = \frac{3\sqrt{3}\, k_B^3 a^2 \zeta(3)}{4\pi \hbar^2 c^2} T^2$$

za $c^2 = \frac{3}{?} \frac{K}{M} a^2$

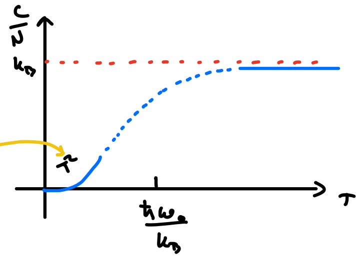
$$\frac{C}{N} = \frac{\sqrt{3}\, k_B^3 \zeta(3) M T^2}{2\pi K \hbar^2} = \frac{\sqrt{3}\,\zeta(3)}{2\pi} \left(\frac{k_B T}{\hbar \underbrace{\sqrt{\frac{K}{M}}}_{\omega_0}} \right)^2 k_B$$

β velik $\iff$ $k_B T \ll \hbar \sqrt{\frac{K}{M}}$

Visokotemperaturna limita, $\beta\hbar\omega_k \ll 1 \quad \forall \vec{k} \in$ 1BC

$$E = \sum_{k'} \hbar\omega_k \frac{1}{1+\beta\hbar\omega_k - 1} = \sum \frac{1}{\beta} = N k_B T$$

$$\frac{C}{N} = k_B$$

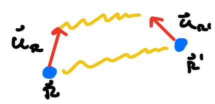


(25) 3D kristal, za splošno Bravaisovo mrežo, en atom na celico

$\vec{R}, \vec{u}_{\vec{R}}, \quad M\ddot{\vec{u}}_R = \sum \vec{F}$.

Iščemo F, Lagrangeva formulacija, $L = T - V$, $\frac{\partial L}{\partial \vec{u}_{\vec{R}}} = \frac{d}{dt}\frac{\partial L}{\partial \dot{\vec{u}}_{\vec{R}}}$

$$T = \sum_{\vec{R}} \frac{1}{2} M \dot{\vec{u}}_{\vec{R}}^2$$



$$V = \frac{1}{2}\sum_{\vec{R}} \sum_{\substack{\vec{R}' \\ n.s.\vec{R}}} \frac{1}{2} K \big(\underbrace{|\vec{R}' + \vec{u}_{R'} - \vec{R} - \vec{u}_R|}_{} - |\vec{R}' - \vec{R}| \big)^2$$

$$\sqrt{(\vec{R}' - \vec{R} + \vec{u}_{R'} - \vec{u}_R)^2} = \sqrt{(\vec{R}'-\vec{R})^2 + \cancel{(\vec{u}_{R'} - \vec{u}_R)^2} + 2(\vec{R}'-\vec{R})(\vec{u}_{R'} - \vec{u}_R)} =$$

anharmonski člen

$$= |\vec{R}' - \vec{R}| \sqrt{1 + \frac{2(\vec{u}_{R'} - \vec{u}_R)\cdot(\vec{R}'-\vec{R})}{(\vec{R}'-\vec{R})^2}}$$

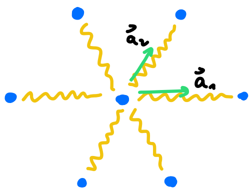
u majhen

$$= |\vec{R}' - \vec{R}| \left(1 + \frac{(\vec{u}_{R'} - \vec{u}_R)\cdot(\vec{R}'-\vec{R})}{(\vec{R}'-\vec{R})^2} \right)$$

$$= |\vec{R}' - \vec{R}| + (\vec{u}_{\vec{R}'} - \vec{u}_{\vec{R}}) \cdot \underbrace{\frac{\vec{R}'-\vec{R}}{|\vec{R}'-\vec{R}|}}_{\hat{e}_{R'-R}}$$

$$V = \frac{K}{4} \sum_{\vec{R}} \sum_{\vec{R}'} \left[(\vec{u}_{\vec{R}'} - \vec{u}_{\vec{R}}) \hat{e}_{\vec{R}'-\vec{R}} \right]^2$$

(26) Nihanje v 2D ravnini kristala



$$\frac{\partial L}{\partial \vec u_0} - \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{\vec u}_0}\right) = 0$$

$$T = \sum_{\vec R} \frac12 M \dot{\vec u}_{\vec R}^2$$

$$V = \frac12 \sum \sum \frac12 k \left((\vec u_{\vec R'} - \vec u_{\vec R}) \hat e_{\vec R'-\vec R} \right)^2 \hat e_{\vec R'-\vec R}$$

Vstavimo v Lagranže

$$-\frac12 \sum\sum k \frac12 2 \left((\vec u_{\vec R'} - \vec u_{\vec R}) \hat e_{\vec R'-\vec R}\right) \underbrace{(\delta_{\vec R',0} - \delta_{\vec R,0})}_{\frac{\partial}{\partial \vec u_0}(\vec u_{\vec R'} - \vec u_{\vec R})} - \frac{d}{dt}\left(\sum_{\vec R} \frac12 M 2 \dot{\vec u}_{\vec R} \delta_{\vec R,0}\right) = 0$$

$$-\frac12 \sum_{\vec R = n.s.0} k (\vec u_0 - \vec u_{\vec R}) \hat e_{0-\vec R} + \frac12 \sum_{\vec R = n.s.0} k (\vec u_{\vec R'} - \vec u_{\vec R}) \hat e_{\vec R'-0}\, e_{\vec R'-0} - M \ddot{\vec u}_0 = 0$$

$\vec R \leftrightarrow \vec R'$

$\hat e_{-\vec R'} = -\hat e_{\vec R'}$

$$\sum_{\vec R = n.s.\vec 0} k \left((\vec u_{\vec R} - \vec u_0) \hat e_{\vec R} \right) \hat e_{\vec R} - M \ddot{\vec u}_0 = 0$$

Zaradi translacijske simetrije mora veljati za vse atome

Nastavek $\vec u_{\vec R} = \vec u\, e^{i(\vec k\cdot\vec R - \omega t)}$

$$\sum k \left(\vec u\, e^{i(\vec k\cdot\vec R - \omega t)} - e^{-i\omega t} \right) \hat e_{\vec R}) \hat e_{\vec R} - M(-\omega^2) \vec u\, e^{-i\omega t} = 0$$

$$\sum k (\vec u\cdot\hat e_{\vec R}) (e^{i\vec k\cdot\vec R} - 1) \hat e_{\vec R} + M\omega^2 \vec u = 0$$

$$\frac12 \sum k (e^{i\vec k\cdot\vec R} + 1)(\vec u\cdot\hat e_{\vec R})\hat e_{\vec R} + \frac12 \sum k (e^{-i\vec k\cdot\vec R} + 1)(\vec u\cdot \underbrace{\hat e_{\vec R})\hat e_{-\vec R}}_{\hat e_{\vec R}\cdot\hat e_{\vec R}} + M\omega^2\vec u = 0$$

$$\frac12 \sum k (e^{i\vec k\cdot\vec R} - 1 + e^{-i\vec k\cdot\vec R} - 1) = \underbrace{\cos(\vec k\cdot\vec R) - 1}_{-2\sin^2\left(\frac{\vec k\cdot\vec R}{2}\right)}$$

$$-\sum_{\vec R} k 2 \sin^2\left(\frac{\vec k\cdot\vec R}{2}\right)(\vec u\cdot\hat e_{\vec R})\hat e_{\vec R} + M\omega^2\vec u = 0$$

$$-\sum 2k \sin^2\left(\frac{\vec k\cdot\vec R}{2}\right)(\hat e_{\vec R}\otimes\hat e_{\vec R})\vec u + M\omega^2\vec u = 0$$

Dobimo primer lastnih vrednosti → pri vsakem $\vec k$ dobimo 2 lastni vrednosti, v 3D kristalu bi dobili 3

6 sosedov, gledali bomo 2×3

$\vec R$ n.s. $\vec 0$		$\hat e_{\vec R}$	$\hat e_{\vec R}\otimes\hat e_{\vec R}$	$\sin^2\frac{\vec k\cdot\vec R}{2}$
$\vec a_1$	$a(1,0)$	$(1,0)$	$\begin{bmatrix}1&0\\0&0\end{bmatrix}$	$\sin^2\frac{k_x a}{2}$
$\vec a_2$	$a(\frac12,\frac{\sqrt3}{2})$	$(\frac12,\frac{\sqrt3}{2})$	$\frac14\begin{bmatrix}1&\sqrt3\\\sqrt3&3\end{bmatrix}$	$\sin^2\left(\frac{k_x}{4}+\frac{\sqrt3 k_y}{4}\right)a$
$\vec a_1-\vec a_2$	$a(\frac12,-\frac{\sqrt3}{2})$	$(\frac12,-\frac{\sqrt3}{2})$	$\frac14\begin{bmatrix}1&-\sqrt3\\-\sqrt3&3\end{bmatrix}$	$\sin^2\left(\frac{k_x}{4}-\frac{\sqrt3 k_y}{4}\right)a$

$\vec k = (k_x, k_y)$

$\vec k \in$ 1.B.c.

Poenostavimo, omejimo se na $\vec k = (k_x, 0)$

Vstavimo v enačbo.

$$-4k\left(\sin^2\left(\frac{ak_x}{2}\right)\begin{bmatrix}1&0\\0&0\end{bmatrix} + \sin^2\left(\frac{k_x a}{4}\right)\frac14\begin{bmatrix}1&\sqrt3\\\sqrt3&3\end{bmatrix} + \sin^2\left(\frac{k_x a}{4}\right)\frac14\begin{bmatrix}1&-\sqrt3\\-\sqrt3&3\end{bmatrix}\right)\vec u + 2M\omega^2\vec u = 0$$

$$\begin{bmatrix}4k\left(\sin^2\frac{k_x a}{2} + \frac12\sin^2\frac{k_x a}{4}\right) & 0\\ 0 & 6k\sin^2\frac{k_x a}{4}\end{bmatrix}\vec u = M\omega^2\vec u$$

Lastni vrednosti

$$\omega_1^2 = \frac{4k}{M}\left(\sin^2\frac{k_x a}{2} + \frac{1}{2}\sin^2\frac{k_x a}{4}\right)$$
$$\omega_2^2 = \frac{6k}{M}\sin^2\frac{k_x a}{4}$$

obe sta akustična

Lastni vektorji

$\vec{u}_1 = (1,0)$ longitudinalni $\parallel \vec{k}$

$\vec{u}_2 = (0,1)$ transverzalni $\perp \vec{k}$

Hitrost zvoka ?

$\omega = ck$ v dolgovalovni limiti $k_x a \ll 1$

$$\omega_1^2 = \frac{4k}{M}\left(\left(\frac{k_x a}{2}\right)^2 + \frac{1}{2}\left(\frac{k_x a}{4}\right)^2\right) = \frac{9k}{8M}(k_x a)^2 \qquad c_L = \sqrt{\frac{9ka^2}{8M}}$$

$$\omega_2^2 = \frac{3k}{8M}(k_x a)^2 \qquad c_T = \sqrt{\frac{3ka^2}{8M}} < c_L$$

velja splošno