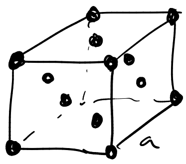
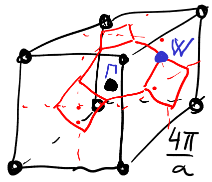
v približku skoraj prostih elektronov izračunaj razcep pasov v oglišču 1. BC za FCC kristalno mrežo

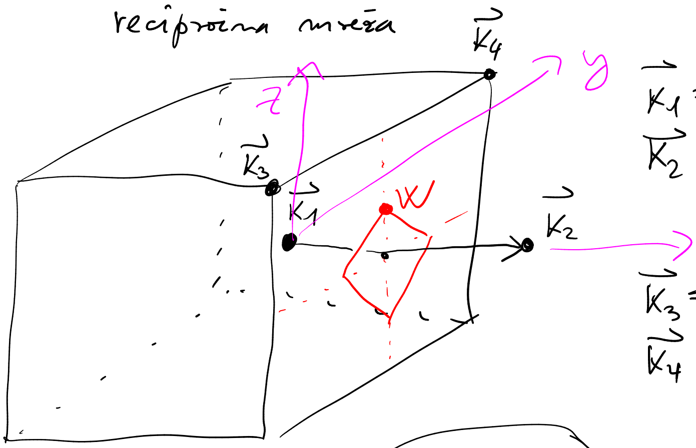


BM



recipročna mreža

1BC = Wigner-Seitzova osnovna celica recipročne mreže



$\vec{K}_1 = 0 \qquad |\vec{W}-\vec{K}_1| = d$

$\vec{K}_2 = \frac{4\pi}{a}(1,0,0) \qquad |\vec{W}-\vec{K}_2| = d$

$\vec{K}_3 = \frac{4\pi}{a}\left(\frac{1}{2},-\frac{1}{2},\frac{1}{2}\right) \qquad |\vec{W}-\vec{K}_3| = d$

$\vec{K}_4 = \frac{4\pi}{a}\left(\frac{1}{2},\frac{1}{2},\frac{1}{2}\right) \qquad |\vec{W}-\vec{K}_4| = d$

prosti elektroni: $V(\vec{r}) = 0$

$$\varepsilon(\vec{k}) = \frac{\hbar^2 k^2}{2m}, \quad \vec{k} \in \mathbb{R}^3, \quad \psi_{\vec{k}}(\vec{r}) \propto e^{i\vec{k}\cdot\vec{r}} \longrightarrow \varepsilon_{\vec{K}}(\vec{k}) = \frac{\hbar^2(\vec{k}-\vec{K})^2}{2m}, \quad \vec{k} \in 1BC \;\&\; \vec{K}, \quad \psi_{\vec{K},\vec{k}}(\vec{r}) \propto e^{i(\vec{k}-\vec{K})\cdot\vec{r}}$$

v periodičnem potencialu: $\psi_{\vec{k}}(\vec{r}) = \sum_{\vec{K}} C_{\vec{k}-\vec{K}} e^{i(\vec{k}-\vec{K})\cdot\vec{r}}$

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

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

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

v šibkem periodičnem potencialu, 1. redu perturbacije dobimo popravek samo v točkah $\vec{k}$, kjer so pasovi v odsotnosti periodičnega potenciala degenerirani

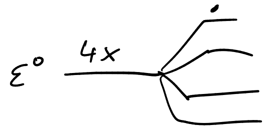
v $\vec{W}$ 4x degeneracija v odsotnosti periodičnega potenciala

$$\forall \vec{K} \in \{\vec{K}_1, \vec{K}_2, \vec{K}_3, \vec{K}_4\} \quad (\varepsilon^0_{\vec{W}-\vec{K}_n} - E) C_{\vec{W}-\vec{K}_n} + \sum_{m=1}^{4} V_{\vec{K}_m-\vec{K}_n} C_{\vec{W}-\vec{K}_m} = 0$$

$m \in \{1,2,3,4\}$

$\varepsilon^0_{\vec{W}-\vec{K}_m} = \varepsilon^0$ za $\forall m$

?



$$\begin{bmatrix} \varepsilon^0 - E + \cancel{V_{\vec{K}_1-\vec{K}_1}}, & V_{\vec{K}_2-\vec{K}_1}, & \cdots \\ V_{\vec{K}_1-\vec{K}_2}, & \varepsilon^0 - E + \cancel{V_{\vec{K}_2-\vec{K}_2}}, & \cdots \\ \vdots & \vdots & \ddots \end{bmatrix} \begin{bmatrix} C_{\vec{W}-\vec{K}_1} \\ C_{\vec{W}-\vec{K}_2} \\ C_{\vec{W}-\vec{K}_3} \\ C_{\vec{W}-\vec{K}_4} \end{bmatrix} = 0$$

Hamiltonjan

$$V_{\vec{K}_1-\vec{K}_1} = \dots = V_{\vec{K}_4-\vec{K}_4} = V_{\vec{0}} = \frac{1}{V_{oc}} \int_{oc} d\vec{r}\, V(\vec{r}) = \overline{V(\vec{r})} \longrightarrow \emptyset$$

če je v točkah BM center inverzije $V(-\vec{r}) = V(\vec{r})$

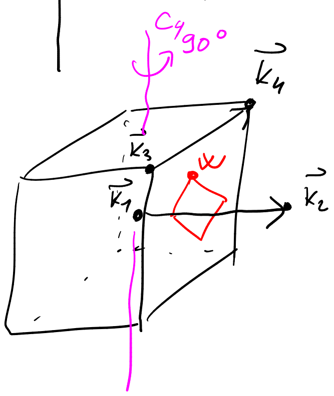
$$V_{-\vec{K}} = \frac{1}{V_{oc}} \int_{oc} d\vec{r}\, V(\vec{r}) e^{+i\vec{K}\cdot\vec{r}} = V^*_{\vec{K}}$$

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

$V_{\vec{K}} \in \mathbb{R}$

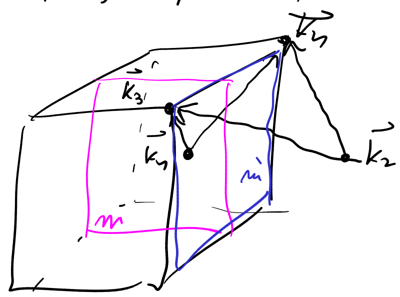
$$\begin{vmatrix} \varepsilon^0 - E, & V_{\vec{k}_2-\vec{k}_1}, & V_{\vec{k}_3-\vec{k}_1}, & V_{\vec{k}_4-\vec{k}_1} \\ V_{\vec{k}_2-\vec{k}_1}, & \varepsilon^0 - E, & V_{\vec{k}_3-\vec{k}_2} & \\ & & \ddots & \end{vmatrix} = 0$$

6 prostih realnih parametrov



$$\vec{k}_4-\vec{k}_3 = C_4(\vec{k}_2-\vec{k}_1)$$

simetrijska operacija kubične grupe



$$\vec{k}_4-\vec{k}_1 = m(\vec{k}_3-\vec{k}_1)$$
$$\vec{k}_3-\vec{k}_2 = m'(\vec{k}_3-\vec{k}_1)$$
$$\vec{k}_4-\vec{k}_2 = m\,m'(\vec{k}_3-\vec{k}_1)$$

poljubna simetrijska operacija

$V_{\vec{k}}$, $V_{R\vec{k}}$ $\qquad R = C_4, m, m', mm', \dots$

$$R\vec{k}\cdot R(R^{-1}\vec{r}) = \vec{k}\cdot R^{-1}\vec{r}$$

I

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

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

$R^{-1}\vec{r} = \vec{r}' \rightarrow \vec{r} = R\vec{r}'$

$d\vec{r} = d\vec{r}'(\pm 1)$

$$V(R\vec{r}') = V(\vec{r}')$$

$$V = V_{\vec{k}_2-\vec{k}_1} = V_{\vec{k}_4-\vec{k}_3}$$
$$V' = V_{\vec{k}_3-\vec{k}_1} = V_{\vec{k}_3-\vec{k}_2} = V_{\vec{k}_4-\vec{k}_1} = V_{\vec{k}_4-\vec{k}_2}$$

$$\begin{vmatrix} \varepsilon^0-E, & V, & V', & V' \\ V, & \varepsilon^0-E, & V', & V' \\ V', & V', & \varepsilon^0-E, & V \\ V', & V', & V & \varepsilon^0-E \end{vmatrix} = 0 \rightarrow \begin{vmatrix} \varepsilon^0-E-V, & -(\varepsilon^0-E-V), & 0, & 0 \\ V, & \varepsilon^0-E, & V', & V' \\ V', & V', & \varepsilon^0-E, & V \\ 0, & 0, & -(\varepsilon^0-E-V), & \varepsilon^0-E-V \end{vmatrix} = 0$$

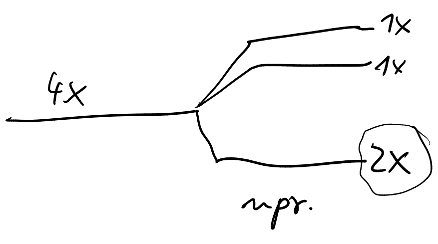
$$\begin{vmatrix} \varepsilon^0-E-V, & 0, & 0, & 0 \\ V, & \varepsilon^0-E+V, & 2V', & V' \\ V', & 2V', & \varepsilon^0-E+V, & V \\ 0, & 0, & 0, & \varepsilon^0-E-V \end{vmatrix} = 0$$

$$(\varepsilon^0-E-V)(\varepsilon^0-E-V)\left((\varepsilon^0-E+V)^2-4V'^2\right) = 0$$

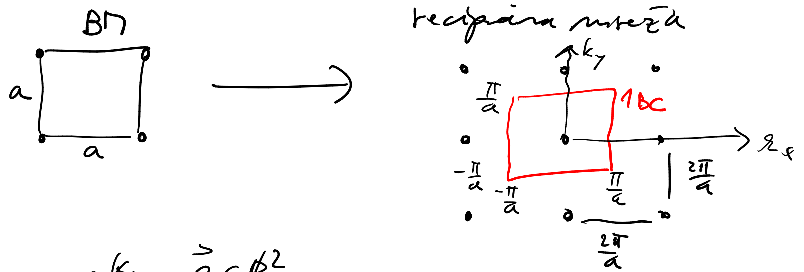
$E = \varepsilon^0 - V$ $\quad 2x$

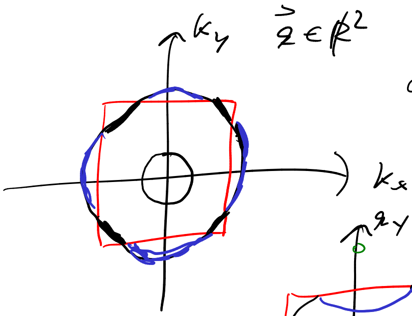
$E = \varepsilon^0 + V - 2V'$ $\quad 1x$

$E = \varepsilon^0 + V + 2V'$ $\quad 1x$



Fermijeva površina v kvadratni kristalni mreži v približku šibkega potenciala



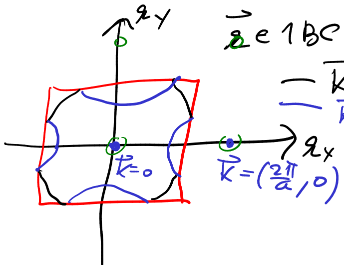


$\vec{q} \in \mathbb{R}^2$

a) prosti elektroni $V(\vec{r}) = 0$

$$\varepsilon(\vec{q}) = \frac{\hbar^2 k^2}{2m} \qquad \varepsilon_F = \frac{\hbar^2 k^2}{2m}$$

Fermijeva površina krožnica



$\vec{q} \in 1BC$ & $\vec{K}$

— $\vec{K} = 0$

— $\vec{K} \neq 0$

4x degeneracija $\left(\vec{K}_1 = 0,\ \vec{K}_2 = (\frac{2\pi}{a}, 0),\ \vec{K}_3 = (0, \frac{2\pi}{a}),\ \vec{K}_4 = (\frac{2\pi}{a}, \frac{2\pi}{a})\right)$

b) šibek potencial

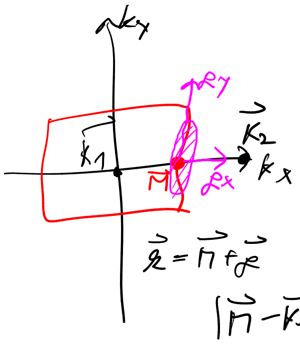
2x degeneracija $\left[\vec{K}_1 = 0,\ \vec{K}_2 = (\frac{2\pi}{a}, 0)\right]$

$$\begin{vmatrix} \varepsilon^0_{\vec{q}-\vec{K}_1} - E & V \\ V^* & \varepsilon^0_{\vec{q}-\vec{K}_2} - E \end{vmatrix} = 0$$

$$E^2 - \left(\varepsilon^0_{\vec{q}-\vec{K}_1} + \varepsilon^0_{\vec{q}-\vec{K}_2}\right)E + \varepsilon^0_{\vec{q}-\vec{K}_1} \cdot \varepsilon^0_{\vec{q}-\vec{K}_2} - |V|^2 = 0$$

$$E = \frac{\varepsilon^0_{\vec{q}-\vec{K}_1} + \varepsilon^0_{\vec{q}-\vec{K}_2}}{2} \pm \sqrt{\left(\frac{\varepsilon^0_{\vec{q}-\vec{K}_1} + \varepsilon^0_{\vec{q}-\vec{K}_2}}{2}\right)^2 - \varepsilon^0_{\vec{q}-\vec{K}_1} \cdot \varepsilon^0_{\vec{q}-\vec{K}_2} + |V|^2}$$

$$E = \frac{\varepsilon^0_{\vec{q}-\vec{K}_1} + \varepsilon^0_{\vec{q}-\vec{K}_2}}{2} \pm \sqrt{\left(\frac{\varepsilon^0_{\vec{q}-\vec{K}_1} - \varepsilon^0_{\vec{q}-\vec{K}_2}}{2}\right)^2 + |V|^2}$$



$$\varepsilon^0_{\vec{q}-\vec{K}_1} = \frac{\hbar^2(\vec{q}-\vec{K}_1)^2}{2m} = \frac{\hbar^2(\vec{\Pi}-\vec{K}_1+\vec{\rho})^2}{2m} = \varepsilon^0 + \frac{\hbar^2}{m}(\vec{\Pi}-\vec{K}_1)\cdot\vec{\rho} + \frac{\hbar^2\rho^2}{2m}$$

$$\varepsilon^0_{\vec{q}-\vec{K}_2} = \frac{\hbar^2(\vec{q}-\vec{K}_2)^2}{2m} = \frac{\hbar^2(\vec{\Pi}-\vec{K}_2+\vec{\rho})^2}{2m} = \varepsilon^0 + \frac{\hbar^2}{m}(\vec{\Pi}-\vec{K}_2)\cdot\vec{\rho} + \frac{\hbar^2\rho^2}{2m}$$

$\vec{q} = \vec{\Pi} + \vec{\rho}$

$|\vec{\Pi}-\vec{K}_1| = |\vec{\Pi}-\vec{K}_2|$

$\varepsilon^0_{\vec{\Pi}-\vec{K}_1} = \varepsilon^0_{\vec{\Pi}-\vec{K}_2} = \varepsilon^0$

$\vec{\Pi}-\vec{K}_1 = -(\vec{\Pi}-\vec{K}_2)$

$$E = \varepsilon^0 + \frac{\hbar^2\rho^2}{2m} \pm \sqrt{\left(\frac{\hbar^2}{2m}(\vec{K}_2-\vec{K}_1)\cdot\vec{\rho}\right)^2 + |V|^2} =$$

$$= \varepsilon^0 + \frac{\hbar^2\rho^2}{2m} \pm \sqrt{\left(\frac{\hbar^2}{2m}\Delta K\cdot\rho_x\right)^2 + |V|^2} =$$

$$\Delta K = |\vec{K}_2 - \vec{K}_1|$$

$$= \varepsilon^0 + \frac{\hbar^2\rho^2}{2m} \pm |V|\sqrt{1 + \left(\frac{\hbar^2\Delta K\rho_x}{2m|V|}\right)^2} =$$

↳ predpostavim $\ll 1$

$$\doteq \varepsilon^0 + \frac{\hbar^2\rho^2}{2m} \pm |V|\left(1 + \frac{1}{2}\left(\frac{\hbar^2\Delta k\rho_x}{2m|V|}\right)^2\right) =$$

šibek potencial

$$|V| \ll \frac{\hbar^2\Delta k^2}{4m}$$

$$= \varepsilon^0 \pm |V| + \frac{\hbar^2\rho_y^2}{2m} + \frac{\hbar^2\rho_x^2}{2m}\left(1 \pm \frac{\hbar^2\Delta k^2}{4m|V|}\right) =$$

$$\doteq \varepsilon^0 \pm |V| + \frac{\hbar^2\rho_y^2}{2m} \pm \frac{\hbar^2\rho_x^2}{2m}\cdot\frac{\hbar^2\Delta k^2}{4m|V|}$$

$$\varepsilon(\vec{p}) = \varepsilon^0 \pm |V| + \frac{\hbar^2}{2}\vec{p}\cdot M^{*-1}\vec{p}$$

$$M^* = \begin{bmatrix} \pm m \cdot \frac{4m|V|}{\hbar^2 \Delta k^2} & 0 \\ 0 & m \end{bmatrix}$$

↳ tenzor efektivne mase

$$M^* = \begin{bmatrix} m_x^* & 0 \\ 0 & m_y^* \end{bmatrix} \qquad m_x^* \ll m_y^*$$

prosti elektroni

$$\varepsilon(\vec{k}) = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2}{2}\vec{k}\cdot\begin{bmatrix} m^{-1} & 0 \\ 0 & m^{-1}\end{bmatrix}\vec{k}$$

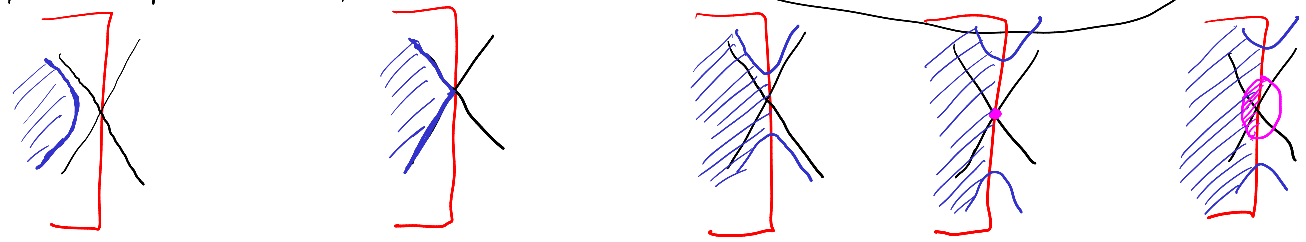
$$M^* = \begin{bmatrix} m & 0 \\ 0 & m \end{bmatrix} = m\,I$$

črte konst. energije

spodnji pas: $\varepsilon(\vec{p}) = \varepsilon^0 - |V| + \frac{\hbar^2 p_y^2}{2m} - \frac{\hbar^2 p_x^2}{2m}\cdot\frac{\hbar^2 \Delta k^2}{4m|V|}$ → hiperbole

zgornji pas: $\varepsilon(\vec{p}) = \varepsilon^0 + |V| + \frac{\hbar^2 p_y^2}{2m} + \frac{\hbar^2 p_x^2}{2m}\cdot\frac{\hbar^2 \Delta k^2}{4m|V|}$ → elipse

$\varepsilon_F < \varepsilon^0 - |V|$ $\qquad$ $\varepsilon_F = \varepsilon^0 - |V|$



$\varepsilon^0 - |V| < \varepsilon_F < \varepsilon^0 + |V|$ $\qquad$ $\varepsilon_F = \varepsilon^0 + |V|$ $\qquad$ $\varepsilon_F > \varepsilon^0 + |V|$