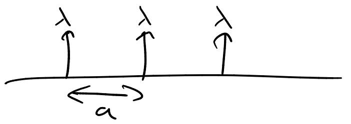
$V(x) = \lambda \sum_n \delta(x - na)$

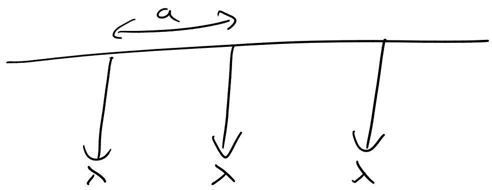


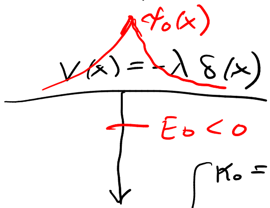
$\lambda > 0$

$\cos ka = \cos \rho a + \frac{Qa}{\rho a} \sin \rho a$ $\qquad Q = \frac{m\lambda}{\hbar^2}$ $\qquad \rho = \sqrt{\frac{2mE}{\hbar^2}}$

$Qa \ll 1$ približek skoraj prostih elektronov …

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





iz KM1
$$\begin{cases} \kappa_0 = \frac{m\lambda}{\hbar^2} \\ \psi_0(x) = \sqrt{\kappa_0}\, e^{-\kappa_0 |x|} \\ E_0 = -\frac{\hbar^2 \kappa_0^2}{2m} \end{cases}$$

$$\rho = \sqrt{\frac{2mE}{\hbar^2}} = \sqrt{-\frac{2m|E|}{\hbar^2}} = i\sqrt{\frac{2m|E|}{\hbar^2}} = i\tilde\rho$$

$$Q = -\frac{m\lambda}{\hbar^2} = -\tilde Q \qquad \tilde Q > 0$$

$$\cos ka = \cos(i\tilde\rho a) - \frac{\tilde Q a}{i\tilde\rho a} \sin(i\tilde\rho a)$$

$$\cos ka = \mathrm{ch}\, \tilde\rho a - \frac{\tilde Q a}{i\tilde\rho a}\, i\, \mathrm{sh}\, \tilde\rho a$$

$$\boxed{\cos ka = \mathrm{ch}\, \tilde\rho a - \tilde Q a \frac{\mathrm{sh}\, \tilde\rho a}{\tilde\rho a}}$$

$k \in 1BC$ $\qquad \tilde\rho = \sqrt{\frac{2m|E|}{\hbar^2}}$ $\qquad \tilde Q = \frac{m\lambda}{\hbar^2} = \kappa_0$

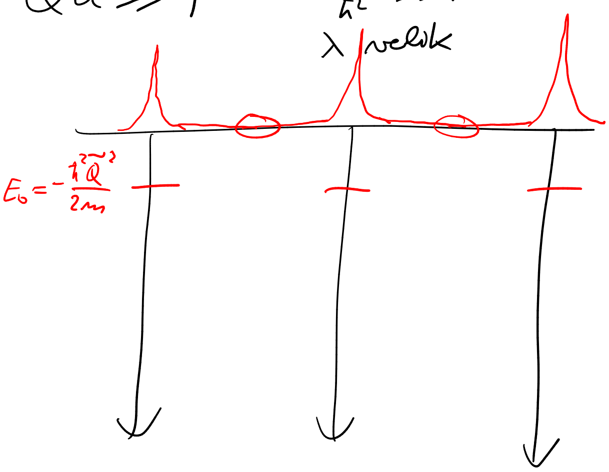
$\tilde\rho a \sim \tilde Q a$

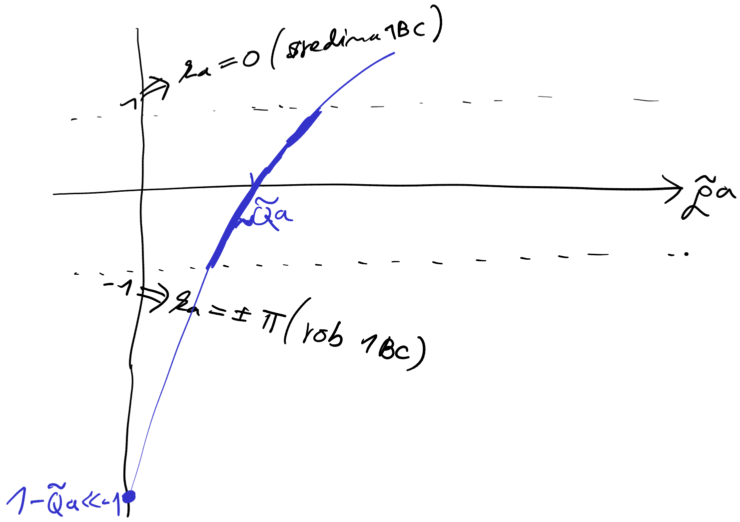
$\mathrm{ch}\, \tilde Q a - \mathrm{sh}\, \tilde Q a \sim 0$

$\tilde Q a \gg 1$

$\tilde Q a \gg 1$ $\qquad \frac{m\lambda a}{\hbar^2} \gg 1$

λ velik





$$\cos ka = \operatorname{ch}\tilde{\rho} a - \tilde{Q}a\,\frac{\operatorname{sh}\tilde{\rho} a}{\tilde{\rho} a} \qquad \tilde{\rho} = \sqrt{\frac{2m(-\varepsilon)}{\hbar^2}} \qquad \tilde{Q} = \frac{m\lambda}{\hbar^2}$$

$$\tilde{\rho} a = \tilde{Q}a + u \qquad \tilde{Q}a \gg 1$$

$$\cos ka = \frac{e^{\tilde{Q}a+u}}{2} + \cancel{\frac{e^{-(\tilde{Q}a+u)}}{2}} - \frac{\tilde{Q}a}{\tilde{Q}a+u}\left(\frac{e^{\tilde{Q}a+u}}{2} - \cancel{\frac{e^{-(\tilde{Q}a+u)}}{2}}\right) \doteq$$

$$\doteq \frac{e^{\tilde{Q}a+u}}{2}\left(1 - \frac{1}{1+\frac{u}{\tilde{Q}a}}\right) =$$

$$\doteq \frac{e^{\tilde{Q}a+u}}{2}\left(1 - \left(1 - \frac{u}{\tilde{Q}a}\right)\right) =$$

$$= \frac{e^{\tilde{Q}a+u}}{2}\cdot\frac{u}{\tilde{Q}a} \doteq$$

$$= \frac{1}{2}e^{\tilde{Q}a}\frac{u}{\tilde{Q}a} \longrightarrow u = 2\tilde{Q}a\,e^{-\tilde{Q}a}\cos ka \ll \tilde{Q}a$$

$$\tilde{\rho} a = \tilde{Q}a\left(1 + 2e^{-\tilde{Q}a}\cos ka\right)$$

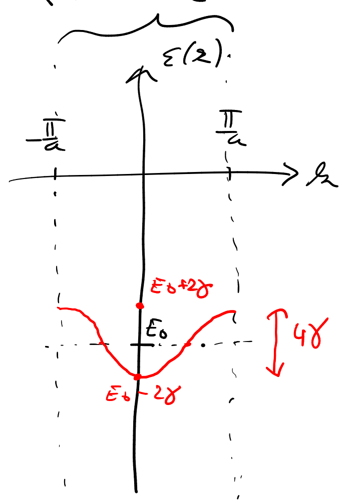
$$E = \varepsilon(k) = -\frac{\hbar^2(\tilde{\rho} a)^2}{2ma^2} \doteq \underbrace{-\frac{\hbar^2(\tilde{Q}a)^2}{2ma^2}}_{E_0}\left(1 + 4e^{-\tilde{Q}a}\cos ka\right)$$

$$\varepsilon(k) = E_0 - 2\underbrace{\frac{\hbar^2\tilde{Q}^2}{m}e^{-\tilde{Q}a}}_{\gamma}\cos ka$$

γ → prekrivalni integral

$$\varepsilon(k) = E_0 - 2\gamma\cos ka$$

1 BC



Približek tesne vezi

$$\varepsilon(\vec{k}) = E_0 - \frac{\beta + \sum_{\vec{R}\neq 0}\gamma(\vec{R})e^{i\vec{k}\cdot\vec{R}}}{1 + \sum_{\vec{R}\neq 0}\alpha(\vec{R})e^{i\vec{k}\cdot\vec{R}}}$$

1 orbitala na osn. celico

$$\beta = -\int \psi_0^*(\vec{r})\,\Delta V(\vec{r})\,\psi_0(\vec{r})\,d\vec{r}$$

$$\gamma(\vec{R}) = -\int \psi_0^*(\vec{r})\,\Delta V(\vec{r})\,\psi_0(\vec{r}-\vec{R})\,d\vec{r}$$

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

$\psi_0(\vec{r})$ → orbitala izoliranega atoma

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

↑ periodični potencial; potencial atoma v izhodišču

$$\varepsilon(\vec{k}) = E_0 - \beta - \sum_{\vec{R}\text{ n.s. }\vec{0}} \gamma(\vec{R})e^{i\vec{k}\cdot\vec{R}}$$

→ KP model:

$$K_0 = \tilde{Q} \qquad \tilde{Q}a \gg 1$$

$$\beta = -\int_{-\infty}^{\infty}\sqrt{K_0}\,e^{-K_0|x|}\left(\sum_{n\neq 0} -\lambda\,\delta(x-na)\right)\sqrt{K_0}\,e^{-K|x|}\,dx =$$

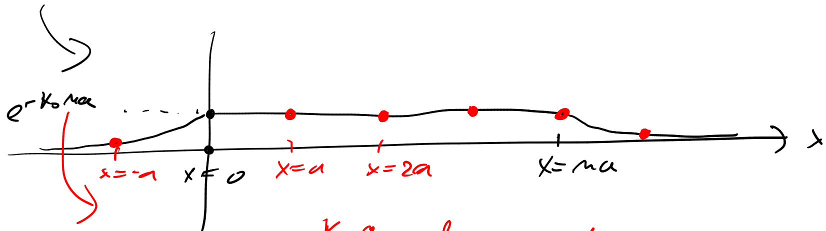
$$= K_0\lambda\sum_{n\neq 0}\int_{-\infty}^{\infty}dx\,e^{-2K_0|x|}\,\delta(x-na) = 2K_0\lambda\sum_{n>0}e^{-2K_0 a\cdot n} \doteq 2K_0\lambda e^{-2K_0 a}$$

$$\gamma(\vec{R}) = \gamma(ma) = -\int_{-\infty}^{\infty}dx\,\sqrt{K_0}\,e^{-K_0|x|}\sum_{n} -\lambda\,\delta(x-na)\cdot\sqrt{K_0}\,e^{-K_0|x-ma|} =$$

$m\neq 0$

$$= K_0\lambda\sum_{n}\int_{-\infty}^{\infty}dx\,\underline{e^{-K_0|x|-K_0|x-ma|}}\,\delta(x-na)$$

$$\underline{e^{-K_0|x|-K_0|x-ma|}} = \begin{cases} x<0: & e^{+K_0(x+x-ma)} = e^{-K_0 ma}e^{2K_0 x} \\ 0<x<ma: & e^{-K_0 x + K_0(x-ma)} = e^{-K_0 ma} \\ x>ma: & e^{-K_0(2x-ma)} = e^{-K_0 ma}e^{-2K_0(x-ma)} \end{cases}$$



$n=1 \rightarrow e^{-k_0 a}$ & $n=1$

↳ najbližji sosed atoma pri $x=0$

$$\gamma(na) = \begin{cases} k_0 \lambda e^{-k_0 a} & ; \ n = \pm 1 \\ \emptyset & ; \ \text{sicer} \end{cases}$$

$$\varepsilon(\vec{k}) = E_0 - \beta - \sum_{\vec{R}} \gamma(\vec{R}) e^{i\vec{k}\cdot\vec{R}}$$

KP

$$\varepsilon(k) = E_0 - 2k_0\lambda \cancel{e^{-2k_0 a}} - k_0\lambda e^{-k_0 a}\underbrace{\left(e^{ika} + e^{-ika}\right)}^{2\cos ka}$$

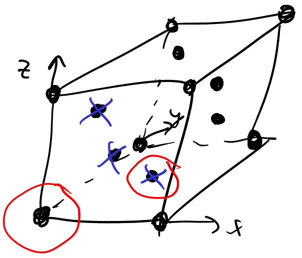
$$\varepsilon(k) = E_0 - 2k_0\lambda e^{-k_0 a}\cos ka$$

$$\varepsilon(k) = E_0 - 2\gamma\cos ka$$

$$\gamma = k_0 \lambda e^{-k_0 a} \qquad k_0 = \frac{m\lambda}{\hbar^2}$$

$$\gamma = \frac{\hbar^2 k_0^2}{m} e^{-k_0 a}$$

V približku tesne vezi obravnaj el. pas, ki ga tvorijo s-orbitale atomov v FCC kristalni mreži



$Y_{lm}(\vartheta,\varphi)$

s-orbitala: $l=0 \to m=0$ $\quad Y_{00}(\vartheta,\varphi)=\frac{1}{\sqrt{4\pi}}$

$$\gamma(\vec R) = -\int \psi_0^*(\vec r)\,\Delta V(\vec r)\,\psi(\vec r-\vec R)\,d\vec r = \gamma$$

$\vec R$ n.s. $\vec 0$

št. najbližjih sosedov $\Rightarrow z = 12$

koordinacijsko število

$$\varepsilon(\vec k) = E_0-\beta - \sum_{\vec R = \text{n.s.}\vec 0} \gamma(\vec R)\, e^{i\vec k\cdot\vec R}$$

uvodni podatki

$=0$ (izbira izhodišča energijske skale)

$$\varepsilon(\vec k) = -\gamma \sum_{\vec R\ \text{n.s.}\vec 0} e^{i\vec k\cdot\vec R}$$

n.s.: $\vec R = \frac{a}{2}(\pm1,\pm1,0)$

$\vec R = \frac{a}{2}(\pm1,0,\pm1)$

$\vec R = \frac{a}{2}(0,\pm1,\pm1)$

$$\varepsilon(\vec k) = -\gamma\left(e^{i(k_x+k_y)\frac{a}{2}} + e^{i(k_x-k_y)\frac{a}{2}} + e^{i(-k_x+k_y)\frac{a}{2}} + e^{i(-k_x-k_y)\frac{a}{2}} + \dots\right) =$$

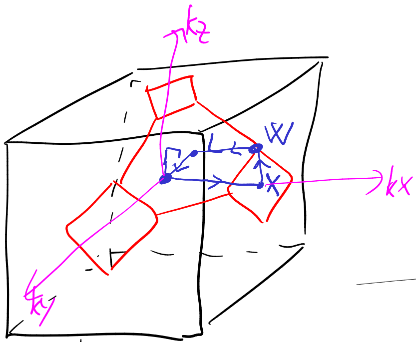
$$= -\gamma\left(e^{ik_x\frac{a}{2}}\cdot 2\cos\frac{k_ya}{2} + e^{-ik_x\frac{a}{2}}\cdot 2\cos\frac{k_ya}{2} + \dots\right) =$$

$$= -\gamma\left(2\cos\frac{k_ya}{2}\cdot 2\cos\frac{k_xa}{2} + \dots\right) =$$

$$\boxed{\varepsilon(\vec k) = -4\gamma\left(\cos\frac{k_xa}{2}\cos\frac{k_ya}{2} + \cos\frac{k_xa}{2}\cos\frac{k_za}{2} + \cos\frac{k_ya}{2}\cos\frac{k_za}{2}\right)}$$

$\vec k \in$ 1BC

recipročna mreža



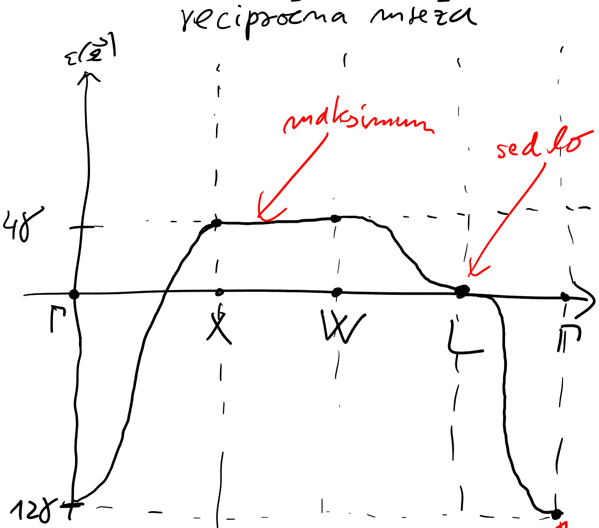
$\frac{4\pi}{a}$

$\Gamma = (0,0,0)$

$X = (\frac{2\pi}{a},0,0)$

$W = (\frac{2\pi}{a},0,\frac{\pi}{a})$

$L = (\frac{\pi}{a},\frac{\pi}{a},\frac{\pi}{a})$



$\Gamma \to X$ $\quad \vec k = (k_x,0,0)$

$0 < k_x < \frac{2\pi}{a}$

$\varepsilon = -4\gamma\left(\cos\frac{k_xa}{2}\cdot 1 + \cos\frac{k_xa}{2}\cdot 1 + 1\cdot 1\right)$

$\varepsilon = -4\gamma - 8\gamma\cos\frac{k_xa}{2}$

$X \to W$ $\quad \vec k = (\frac{2\pi}{a},0,k_z)$

$0 < k_z < \frac{\pi}{a}$

$\varepsilon = -4\gamma\left(-1\cdot 1 + (-1)\cdot\cancel{\cos\frac{k_za}{2}} + 1\cdot\cancel{\cos\frac{k_za}{2}}\right) = 4\gamma$

$W \to L$ $\quad \vec k = (\frac{2\pi}{a}-\rho, \rho, \frac{\pi}{a})$

$\rho \in [0,\frac{\pi}{a}]$

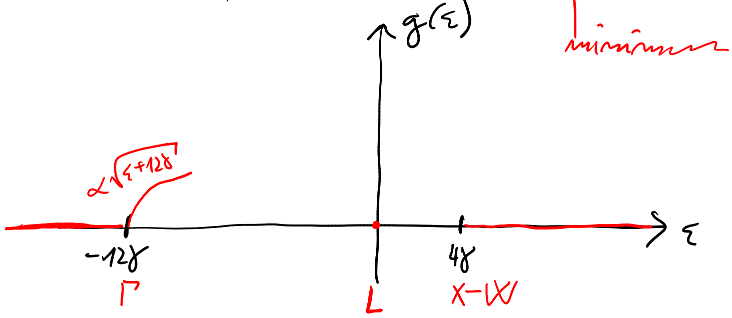
$\varepsilon = -4\gamma\left(-\cos\frac{\rho a}{2}\cdot\cos\frac{\rho a}{2} + (-\cos\frac{\rho a}{2})\cdot 0 + 0\right)$

$\varepsilon = 4\gamma\cos^2\frac{\rho a}{2}$

$L \to \Gamma$ $\quad \vec k = (\frac{\pi}{a}-\rho, \frac{\pi}{a}-\rho, \frac{\pi}{a}-\rho)$

$\rho \in [0,\frac{\pi}{a}]$

$\varepsilon = -4\gamma\left(\sin\frac{\rho a}{2}\cdot\sin\frac{\rho a}{2}\cdot 3\right) = -12\gamma\sin^2\frac{\rho a}{2}$



minimum: Γ

$$\varepsilon(\vec{q}) = -4\gamma\left(\cos\frac{q_x a}{2}\cos\frac{q_y a}{2} + \cos\frac{q_x a}{2}\cos\frac{q_z a}{2} + \cos\frac{q_y a}{2}\cos\frac{q_z a}{2}\right)$$

v bližini Γ $q_x a \ll 1$; $q_y a \ll 1$; $q_z a \ll 1$

$$\varepsilon(\vec{q}) = -4\gamma\left(\left(1-\frac{q_x^2 a^2}{8}\right)\left(1-\frac{q_y^2 a^2}{8}\right) + \dots\right) =$$

$$= -4\gamma\left(1 - \frac{q_x^2 a^2}{8} - \frac{q_y^2 a^2}{8} + 1 - \frac{q_x^2 a^2}{8} - \frac{q_z^2 a^2}{8} + 1 - \frac{q_y^2 a^2}{8} - \frac{q_z^2 a^2}{8}\right) =$$

$$= -4\gamma\left(3 - \frac{2(q_x^2 + q_y^2 + q_z^2)a^2}{8}\right) = -12\gamma + \gamma q^2 a^2 = \qquad q^2 = |\vec{q}|^2$$

$$= \underbrace{-12\gamma}_{\varepsilon_{min}} + \frac{\hbar^2 q^2}{2m^*} \qquad m^* = \frac{\hbar^2}{2a^2\gamma}$$

↳ efektivna masa

$\vec{q}$ je 3D $\longrightarrow$ $g(\varepsilon) \propto \sqrt{(\varepsilon + 12\gamma)}$

$\varepsilon - (-12\gamma)$