

$$V(x) = \lambda \sum_m \delta(x - ma) \quad \lambda > 0$$

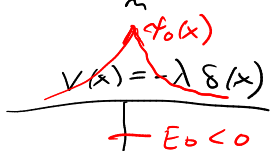

$$\cos ka = \cos pa + \frac{Qa}{pa} \sin pa$$

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

$$p = \sqrt{\frac{2mE}{\hbar^2}}$$

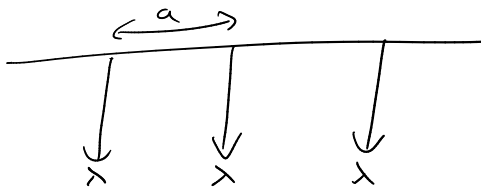
$Qa \ll 1$ približek sluzaj, protiv elektronov ...

$$V(x) = -\lambda \sum_m \delta(x - ma) ; \lambda > 0$$



iz KPII

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



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

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

$$\cos za = \cos(i\tilde{p}a) - \frac{\tilde{Q}a}{i\tilde{p}a} \sin(i\tilde{p}a)$$

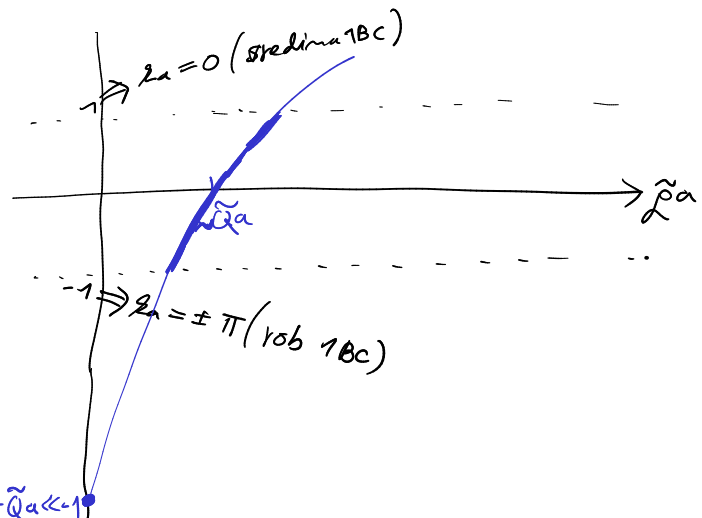
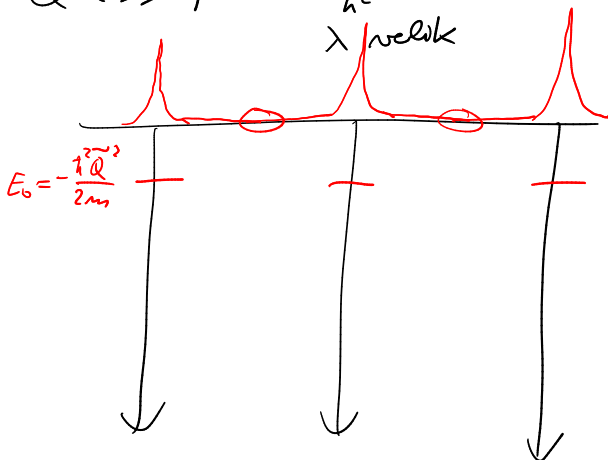
$$\cos za = \text{ch } \tilde{p}a - \frac{\tilde{Q}a}{i\tilde{p}a} i \text{sh } \tilde{p}a$$

$$\cos za = \text{ch } \tilde{p}a - \tilde{Q}a \frac{\text{sh } \tilde{p}a}{\tilde{p}a}$$

$z = iBC$ $\tilde{p} = \sqrt{\frac{2m|E|}{\hbar^2}}$ $\tilde{Q} = \frac{m\lambda}{\hbar^2} = \kappa_0$

$\tilde{p}a \sim \tilde{Q}a$
 $\text{ch } \tilde{Q}a - \text{sh } \tilde{Q}a \sim 0$
 $\tilde{Q}a \gg 1$

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



$$\cos 2a = \cosh \tilde{\rho} a - \tilde{Q} a \frac{\sinh \tilde{\rho} a}{\tilde{\rho} a} \quad \tilde{\rho} = \sqrt{\frac{2m(-E)}{\hbar^2}} \quad \tilde{Q} = \frac{m\lambda}{\hbar^2}$$

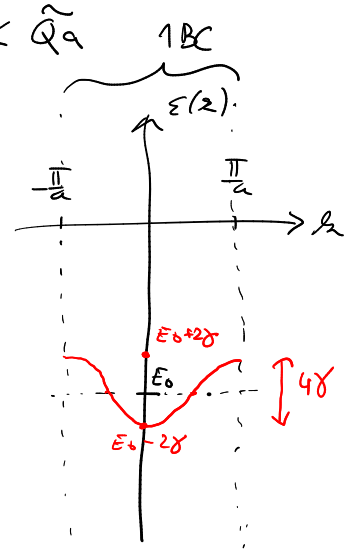
$$\begin{aligned} \tilde{\rho} a &= \tilde{Q} a + u \\ \cos 2a &= \frac{e^{\tilde{Q} a + u} + e^{-\tilde{Q} a + u}}{2} - \frac{\tilde{Q} a}{\tilde{Q} a + u} \left(\frac{e^{\tilde{Q} a + u}}{2} - \frac{e^{-\tilde{Q} a + u}}{2} \right) = \\ &= \frac{e^{\tilde{Q} a + u}}{2} \left(1 - \frac{1}{1 + \frac{u}{\tilde{Q} a}} \right) = \\ &= \frac{e^{\tilde{Q} a + u}}{2} \left(1 - \left(1 - \frac{u}{\tilde{Q} a} \right) \right) = \\ &= \frac{e^{\tilde{Q} a + u}}{2} \cdot \frac{u}{\tilde{Q} a} = \\ &= \frac{1}{2} e^{\tilde{Q} a} \frac{u}{\tilde{Q} a} \rightarrow u = 2 \tilde{Q} a e^{-\tilde{Q} a} \cos 2a \ll \tilde{Q} a \end{aligned}$$

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

$$E = \varepsilon(z) = -\frac{\hbar^2 (\tilde{\rho} a)^2}{2ma^2} = -\frac{\hbar^2 (\tilde{Q} a)^2}{2ma^2} (1 + 4 e^{-\tilde{Q} a} \cos 2a)$$

$$\varepsilon(z) = E_0 - 2 \frac{\hbar^2 \tilde{Q}^2}{m} e^{-\tilde{Q} a} \cos 2a$$

$$\varepsilon(z) = E_0 - 2\gamma \cos 2a \quad \text{prokrivajući integral}$$



Približek kesne vezi

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

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

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

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

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

1 orbitalis na om. celico

$\psi_0(\vec{r}) \rightarrow$ orbitala izolirana atoma
 $\Delta V(\vec{r}) = V(\vec{r}) - V_{at}(\vec{r}) = \sum_{\vec{R} \neq 0} V_{at}(\vec{r} - \vec{R})$
 ↑ periodičan potencijal
 potencijal atoma u izolaciji

$$k_0 = \tilde{Q} \quad \tilde{Q} a \gg 1$$

→ KP model:

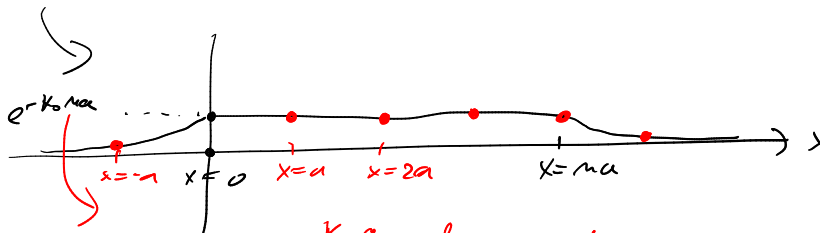
$$\beta = - \int_{-\infty}^{\infty} \sqrt{k_0} e^{-k_0|x|} \left(\sum_{m \neq 0} -\lambda \delta(x - ma) \right) \sqrt{k_0} e^{-k_0|x|} dx =$$

$$= k_0 \lambda \sum_{m \neq 0} \int_{-\infty}^{\infty} dx e^{-2k_0|x|} \delta(x - ma) = 2k_0 \lambda \sum_{m > 0} e^{-2k_0 a \cdot m} = 2k_0 \lambda e^{-2k_0 a}$$

$$\gamma(\vec{R}) = \gamma(ma) = - \int_{-\infty}^{\infty} dx \sqrt{k_0} e^{-k_0|x|} \sum_m -\lambda \delta(x - ma) \cdot \sqrt{k_0} e^{-k_0|x - ma|} =$$

$$= k_0 \lambda \sum_m \int_{-\infty}^{\infty} dx e^{-k_0|x| - k_0|x - ma|} \delta(x - ma)$$

$$e^{-k_0|x| - k_0|x - ma|} = \begin{cases} x < 0: & e^{-k_0(x + x - ma)} = e^{-k_0 ma} e^{2k_0 x} \\ 0 < x < ma: & e^{-k_0 x + k_0(x - ma)} = e^{-k_0 ma} \\ x > ma: & e^{-k_0(2x - ma)} = e^{-k_0 ma} e^{-2k_0(x - ma)} \end{cases}$$



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

↳ may be žiji sajed atoma pri $x=0$

$$\gamma(ma) = \begin{cases} k_0 \lambda e^{-k_0 a} & ; m = \pm 1 \\ \phi & ; \text{ sicer} \end{cases}$$

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

KP

$$\epsilon(z) = E_0 - 2k_0 \lambda e^{-2k_0 a} - k_0 \lambda e^{-k_0 a} \underbrace{(e^{i\vec{k} \cdot \vec{R}} + e^{-i\vec{k} \cdot \vec{R}})}_{2 \cos za}$$

$$\epsilon(z) = E_0 - 2k_0 \lambda e^{-k_0 a} \cos za$$

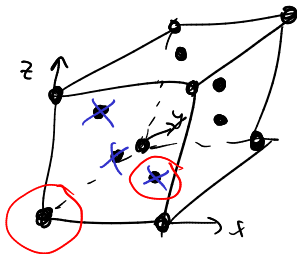
$$\epsilon(z) = E_0 - 2\gamma \cos za$$

$$\gamma = k_0 \lambda e^{-k_0 a}$$

$$k_0 = \frac{m\lambda}{\hbar^2}$$

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

V približni teoriji konne rezi obravnava el. pro, ki ga tvorijo s-orbitale atomov v FCC kristalni mreži



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

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

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

$$\vec{R} \text{ n.s. } \vec{0}$$

štri najbližjih sosedov $\Rightarrow z=12$

↑
koordinatni sistem

$$\epsilon(\vec{z}) = \underbrace{E_0 - B}_{\text{skladni produkti}} - \sum_{\vec{R} \text{ n.s. } \vec{0}} \gamma(\vec{R}) e^{i\vec{z} \cdot \vec{R}}$$

$= 0$ (izbira izhodnišča energijske skale)

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

n.s.: $\vec{R} = \frac{a}{2}(\pm 1, \pm 1, 0)$

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

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

$$\epsilon(\vec{z}) = -\gamma \left(e^{i(\pm 1 \pm 1) \frac{a}{2}} + e^{i(\pm 1 - \pm 1) \frac{a}{2}} + e^{i(-\pm 1 \pm 1) \frac{a}{2}} + e^{i(-\pm 1 - \pm 1) \frac{a}{2}} + \dots \right) =$$

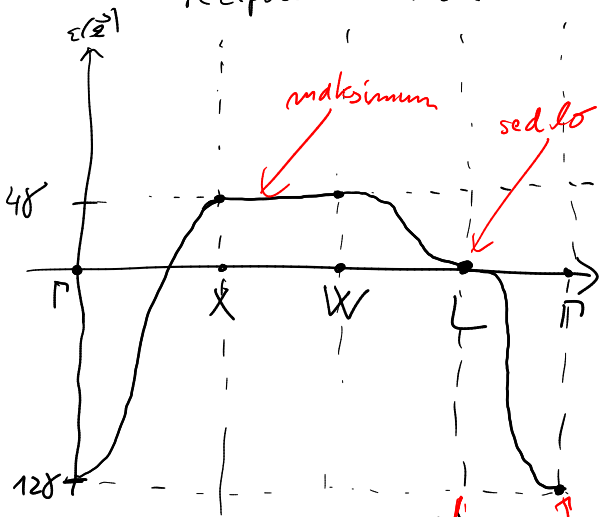
$$= -\gamma \left(e^{i2x \frac{a}{2}} \cdot 2 \cos \frac{2y \frac{a}{2}}{2} + e^{-i2x \frac{a}{2}} \cdot 2 \cos \frac{2y \frac{a}{2}}{2} + \dots \right) =$$

$$= -\gamma \left(2 \cos \frac{2x \frac{a}{2}}{2} \cdot 2 \cos \frac{2y \frac{a}{2}}{2} + \dots \right) =$$

$$\boxed{\epsilon(\vec{z}) = -4\gamma \left(\cos \frac{2x \frac{a}{2}}{2} \cos \frac{2y \frac{a}{2}}{2} + \cos \frac{2x \frac{a}{2}}{2} \cos \frac{2z \frac{a}{2}}{2} + \cos \frac{2y \frac{a}{2}}{2} \cos \frac{2z \frac{a}{2}}{2} \right)}$$

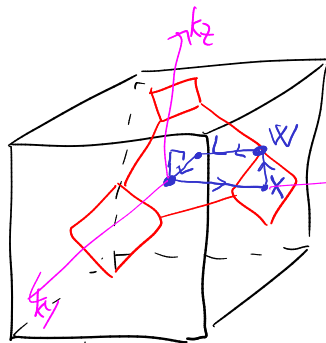
$\vec{z} \in \text{1BC}$

recipročna mreža



maksimum

sedlo



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

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

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

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

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

$$\Gamma \rightarrow X \quad \vec{z} = (2x, 0, 0)$$

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

$$\epsilon = -4\gamma \left(\cos \frac{2x \frac{a}{2}}{2} \cdot 1 + \cos \frac{2x \frac{a}{2}}{2} \cdot 1 + 1 \cdot 1 \right)$$

$$\epsilon = -4\gamma - 8\gamma \cos \frac{2x \frac{a}{2}}{2}$$

$$X \rightarrow W \quad \vec{z} = \left(\frac{2\pi}{a}, 0, 2z\right)$$

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

$$\epsilon = -4\gamma \left(-1 \cdot 1 + (-1) \cdot \cos \frac{2z \frac{a}{2}}{2} + 1 \cdot \cos \frac{2z \frac{a}{2}}{2} \right) = 4\gamma$$

$$W \rightarrow L \quad \vec{z} = \left(\frac{2\pi}{a} - 2x, 2z, \frac{\pi}{a}\right)$$

$$x \in \left[0, \frac{\pi}{a}\right]$$

$$\epsilon = -4\gamma \left(-\cos \frac{2x \frac{a}{2}}{2} \cdot \cos \frac{2z \frac{a}{2}}{2} + (-\cos \frac{2x \frac{a}{2}}{2}) \cdot 0 + 0 \right)$$

$$\epsilon = 4\gamma \cos^2 \frac{2x \frac{a}{2}}{2}$$

$$L \rightarrow \gamma \quad \vec{z} = \left(\frac{\pi}{a} - x, \frac{\pi}{a} - x, \frac{\pi}{a} - x\right)$$

$$x \in \left[0, \frac{\pi}{a}\right]$$

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

van Hove singularnost

$$g(\epsilon) \propto \frac{1}{\sqrt{4\gamma - \epsilon}}$$

$$\propto \frac{1}{\sqrt{4\gamma - \epsilon}}$$

$$-12\gamma$$

Γ

L

$X-W$

ϵ

minimum: $\epsilon(\vec{r}) = -48 \left(\cos \frac{r_x a}{2} \cos \frac{r_y a}{2} + \cos \frac{r_x a}{2} \cos \frac{r_z a}{2} + \cos \frac{r_y a}{2} \cos \frac{r_z a}{2} \right)$

Γ \rightarrow bližini Γ $r_x a \ll 1; r_y a \ll 1; r_z a \ll 1$

$$\begin{aligned} \epsilon(\vec{r}) &= -48 \left(\left(1 - \frac{r_x^2 a^2}{8}\right) \left(1 - \frac{r_z^2 a^2}{8}\right) + \dots \right) = \\ &= -48 \left(1 - \frac{r_x^2 a^2}{8} - \frac{r_z^2 a^2}{8} + 1 - \frac{r_x^2 a^2}{8} - \frac{r_z^2 a^2}{8} + 1 - \frac{r_y^2 a^2}{8} - \frac{r_z^2 a^2}{8} \right) = \\ &= -48 \left(3 - \frac{2(r_x^2 + r_y^2 + r_z^2) a^2}{8} \right) = -12\gamma + \gamma r^2 a^2 = \epsilon^2 = |\vec{r}|^2 \\ &= \underbrace{-12\gamma}_{\epsilon_{\min}} + \frac{\hbar^2 r^2}{2m^*} \quad m^* = \frac{\hbar^2}{2a^2\gamma} \\ &\quad \hookrightarrow \text{efektivna masa} \end{aligned}$$

\vec{r} je 3D $\rightarrow v_g(\vec{r}) \propto \sqrt{(\epsilon + 12\gamma)}$
 $\epsilon - (-12\gamma)$

L: $L = (\frac{\pi}{a}, \frac{\pi}{a}, \frac{\pi}{a})$
 $\vec{k} = L + \vec{r}$ ($|\vec{r}| \ll \frac{\pi}{a}$)

$$\begin{aligned} \epsilon(\vec{k}) &= -48 \left(\cos \frac{r_x a}{2} \cos \frac{r_z a}{2} + \dots \right) = \\ &= -48 \left(\cos \frac{r_x a}{2} \cos \frac{r_z a}{2} + \dots \right) = \\ &= -\gamma a^2 (r_x r_y + r_x r_z + r_y r_z) = \\ &= -\frac{\gamma a^2}{2} (r_x, r_y, r_z) \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix} \begin{pmatrix} r_x \\ r_y \\ r_z \end{pmatrix} = -\frac{\gamma a^2}{2} \vec{r}^T \tilde{A} \vec{r} = \quad A = U^T \tilde{A} U \\ &= \underbrace{-\frac{\gamma a^2}{2} (U \vec{r})^T \tilde{A} (U \vec{r})}_{\text{diagonal}} \end{aligned}$$

$\det \begin{pmatrix} -\lambda & 1 & 1 \\ 1 & -\lambda & 1 \\ 1 & 1 & -\lambda \end{pmatrix} = 0$ $-\lambda^3 + 2 + 3\lambda = 0$
 $\lambda_1 = -1$
 $(\lambda+1)(-\lambda^2 + 2 + \lambda) = 0$
 $\hookrightarrow \lambda_2 = -1$
 $\lambda_3 = 2$

$\tilde{A} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 2 \end{pmatrix}$

$\rightarrow = \frac{\hbar^2}{2} \vec{r} \cdot \tilde{A}^{-1} \vec{r}$

X: $X = (\frac{2\pi}{a}, 0, 0)$
 $\vec{k} = X + \vec{r}$ ($|\vec{r}| \ll \frac{\pi}{a}$)

$$\begin{aligned} \epsilon(\vec{k}) &= -48 \left(-\cos \frac{r_x a}{2} \cos \frac{r_y a}{2} - \cos \frac{r_x a}{2} \cos \frac{r_z a}{2} + \cos \frac{r_x a}{2} \cos \frac{r_z a}{2} \right) = \\ &= -48 \left(-\left(1 - \frac{r_x^2 a^2}{8} - \frac{r_y^2 a^2}{8}\right) - \left(1 - \frac{r_x^2 a^2}{8} - \frac{r_z^2 a^2}{8}\right) + \left(1 - \frac{r_x^2 a^2}{8} - \frac{r_z^2 a^2}{8}\right) \right) = \end{aligned}$$

$= 48 - \gamma a^2 r_x^2 =$

$= 48 + \frac{\hbar^2}{2} \vec{r} \cdot \tilde{A}^{-1} \vec{r}$

$\tilde{A}^{-1} = \begin{pmatrix} \frac{\hbar^2}{2\gamma a^2} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$

$\rightarrow g(\epsilon) = \frac{1}{\sqrt{48 - \epsilon}}$

1D prosti elektroni: $g(\epsilon) \propto \frac{1}{\sqrt{\epsilon}}$

