

Blochov teoreme

$$\psi(\vec{r}) = e^{i\vec{k}\vec{r}} u(\vec{r}), \quad u(\vec{r} + \vec{R}) = u(\vec{r})$$

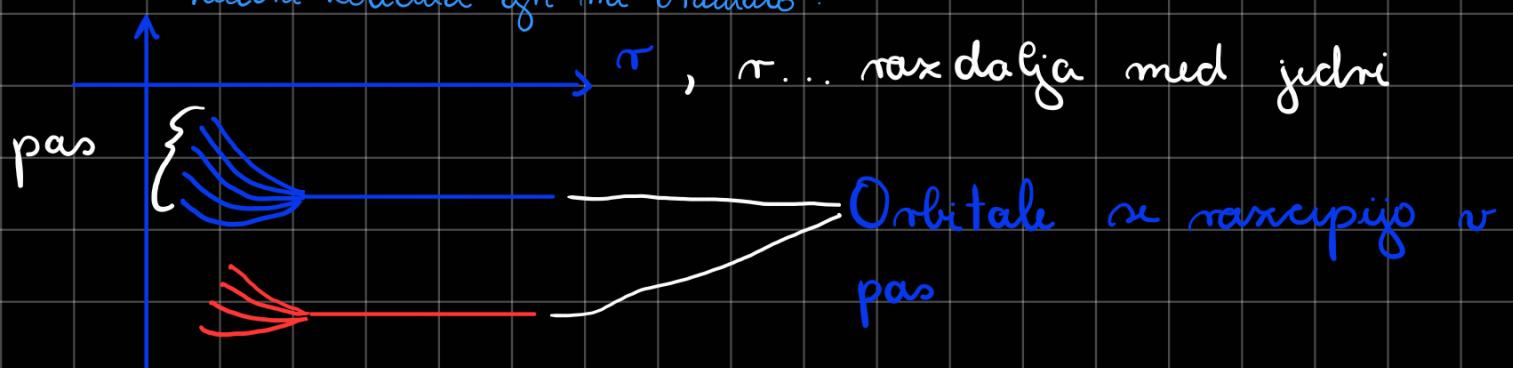
V prosti e^- : vsak \vec{k} dovoljen

V kristalu e^- : samo določeni \vec{k}

$$1D: k_l = \frac{2\pi}{N a} l, \quad l \in \mathbb{Z}, \quad N \text{ št. gradnikov, a perioda}$$

Nastanjojo pasovi:

Katera količina gre na ordinato?



Tirina paru odvisna od glavnega kvantnega št. (vsih $k \bar{s} = \text{štev pas}$).

Pas nastane kot posledica periodičnega el. pot.

Zadatak 9.3

10) Kristal:

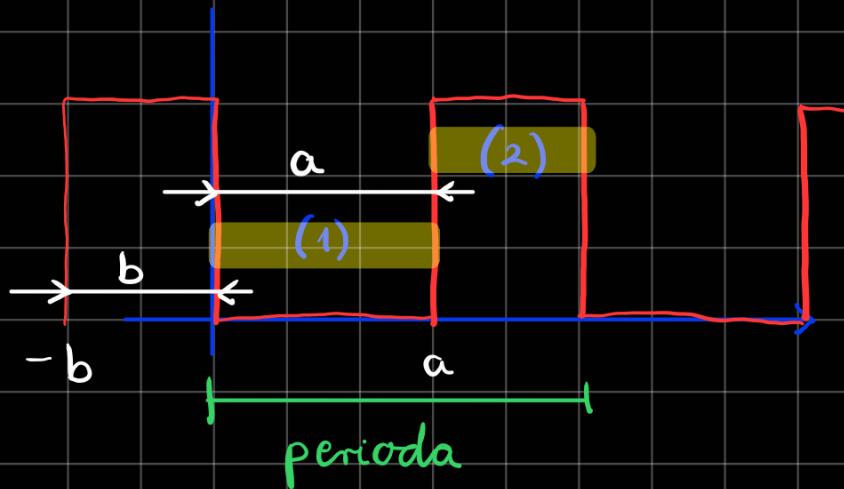
$$\text{Potencijal } U(x) = U_0 b \left[\dots + \delta(x+a) + \delta(x) + \dots \right]$$

$$a = 0.3 \text{ nm}$$

$$\Delta E = E_c - E_i \text{ ev. razza}$$

$$U_0 b = 25 \text{ meV nm}$$

$$b \ll a$$



Vidimo u limitu: $U \rightarrow \infty$

$$b \rightarrow 0$$

$$U_0 b = \text{konst.}$$

(1) $U=0$, e^- proti,

$\mathbf{k} = -\frac{\hbar^2 \nabla}{2m}$, rezultuju superpozicija ravnega valov, enega, ki se siri v levu in v desno

$$\Psi_1 = A e^{ikx} + B e^{-ikx}, \quad k = \sqrt{\frac{2mE}{\hbar^2}} \dots \text{imena vlogo enega}$$

(2) tuneliranje, $E < U$

$$\Psi_2(x) = C e^{Kx} + D e^{-Kx}, \quad K = \sqrt{\frac{2m(U-E)}{\hbar^2}}$$

Določiti moramo A, B, C, D (BC pogoj)

MF1 nov: ūja mora biti $\propto BC$ rôvnaa eiu rôvnuu odu.

Ψ rôvnaa: $x = \emptyset \Rightarrow A + B = C + D$ #1 euacba

$$\left. \begin{array}{l} \Psi' \text{ rôvnaa: } \frac{\partial \Psi_1}{\partial x} \Big|_{x=\emptyset} = k(A-B) \\ \frac{\partial \Psi_2}{\partial x} \Big|_{x=\emptyset} = K(C-D) \end{array} \right\} \Rightarrow k(A-B) = K(C-D)$$

#2 euacba

Isto nô ka $x=a$, kôj upôstevamo Blochov teoreum:

$$(3)_{x=a}: \Psi(x) = e^{ikx} u(x)$$

$$\Rightarrow \Psi(x=a) = e^{ika} \Psi(x)$$

Nôsa perioda je $a+b$

$$\text{rôvnuost: } \Psi_1(x=a) = Ae^{ika} + Be^{-ika} \quad \cancel{x}$$

$$\Psi_2(x=a) = \underbrace{\Psi_2(x=-b)}_{e^{ik(-b)}} e^{ika}(a+b) \quad // \text{uporabili smo Blochov}$$

rôdovost val. ūj pri $x=a$ teoreum
je xaraktri periodičnosti euaka
kot pri $-b$

Intermazuco: • pravt e^- : $\Psi = e^{ikx}$ $\hat{p}\Psi = \hbar k \Psi$

• Blochov e^- : $\Psi = e^{ikx} u(x)$ $\hat{p}\Psi \neq \hbar k \Psi$

$$(4) \quad \frac{\partial \Psi_1}{\partial x} \Big|_{x=a} = \frac{\partial \Psi_2}{\partial x} \Big|_{x=a} = \frac{\partial \Psi_2}{\partial x} \Big|_{x=b} \exp \{ i k_\ell (a+b) \} \quad \cancel{\times} \quad \cancel{\times}$$

$$\cancel{\times} \quad e^{ika} A + e^{ikb} B - e^{ik_\ell(a+b)} e^{-kb} C - e^{ik_\ell(a+b)} e^{kb} D = 0$$

$\cancel{\times} \cancel{\times}$

Imams sistem euacib $M\vec{v} = \emptyset$, $\vec{v} =$

$$\begin{bmatrix} A \\ B \\ C \\ D \end{bmatrix}$$

Quick recap: $A\vec{x} = \vec{b}$

Eua euolica reiterv: $\vec{x} = A^{-1}\vec{b} \Leftrightarrow \det(A) \neq 0$

Crammerjevo pravilo

Numerica reiterv (ix Mathematica):

$$\frac{k^2 - \ell^2}{2k\ell} \sinh(kb) \sin(ka) + \cosh(kb) \cos(ka) \\ = \cos[k_\ell(a+b)]$$

Spomnino & difiničij u limit

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

$$k = \sqrt{\frac{2m(U-E)}{\hbar^2}}$$

$U \gg E$

$$\begin{aligned} b &\rightarrow 0 \\ U &\rightarrow \infty \\ Ub &= \text{konst.} \end{aligned}$$

$$k_\ell = \frac{2\pi}{N(a+b)} l$$

$$K_b \propto \sqrt{U} b = \underbrace{\sqrt{U} b}_{\text{komt.}} \sqrt{b}$$

$$K_b \sim \emptyset$$

Uporabimo Taylorja ma nih in cosh

$$\sinh(x) = \frac{e^x - e^{-x}}{2} \quad \cosh(x) = \frac{e^x + e^{-x}}{2}$$

$$e^x \doteq 1 + x$$

$$e^{-x} \doteq 1 - x$$

$$\Rightarrow \sinh(x) = x, \quad \cosh(0) = 1$$

Renitev postave, upoštevajoč $K \gg k$

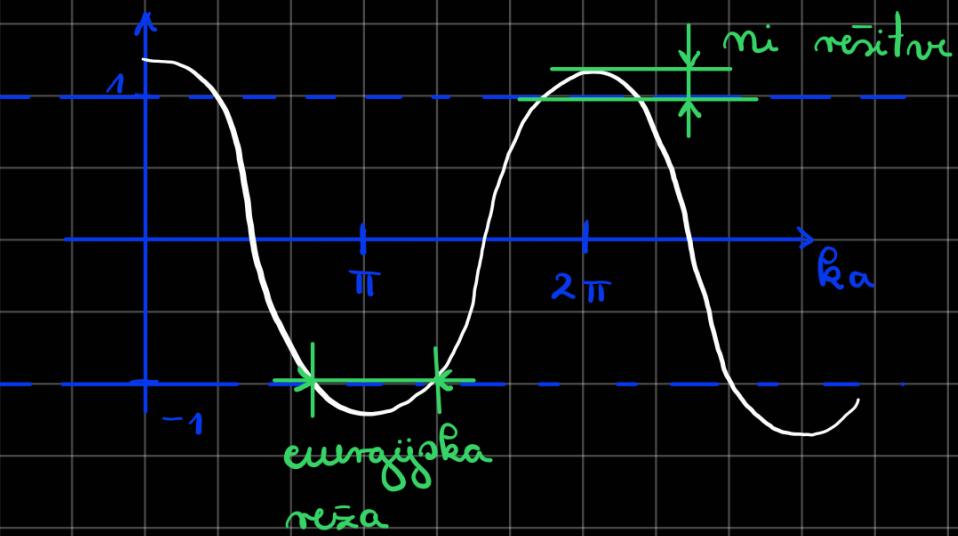
$$\frac{ka}{2k_a} K_b \sin(ka) + \cos(ka) = \cos(k_a a)$$

$$P \frac{\sin(ka)}{ka} + \cos(ka) = \cos(k_a a), \quad P = \frac{K^2 ab}{2} = \frac{2m a U b}{2 \hbar^2} \\ = 0.098,$$

$$m = m_e = 9.1 \cdot 10^{-31}$$

$$\frac{\sin(ka)}{ka} = 1, \quad ka \rightarrow 0$$

Dva strani enačbe



V en. reži so vrednosti, ki jih e- v kristalu ne more nasesti.

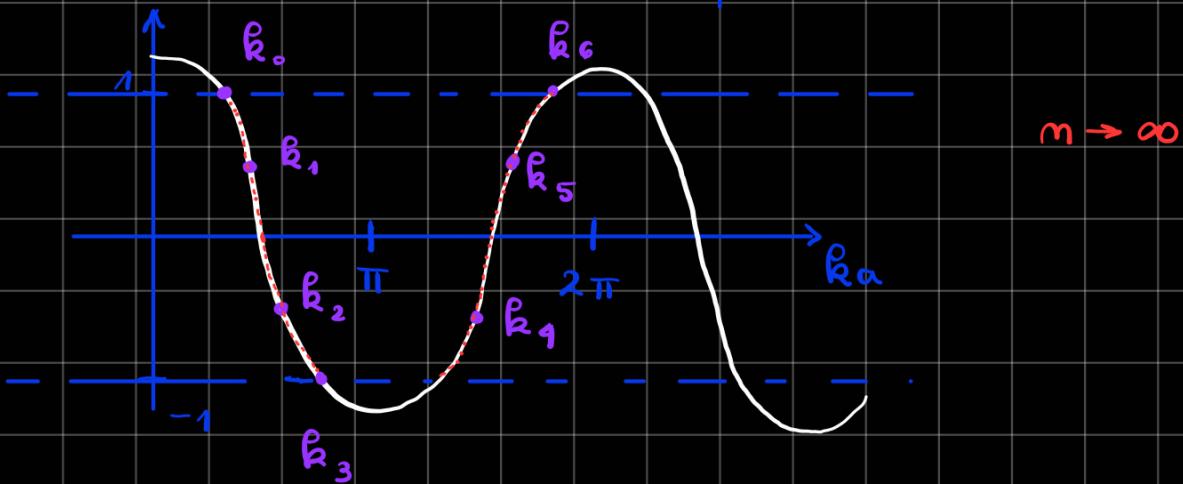
Vrednosti k_a , pri katerih $|LSE| > 1 \Rightarrow$ enačba nima rezitve

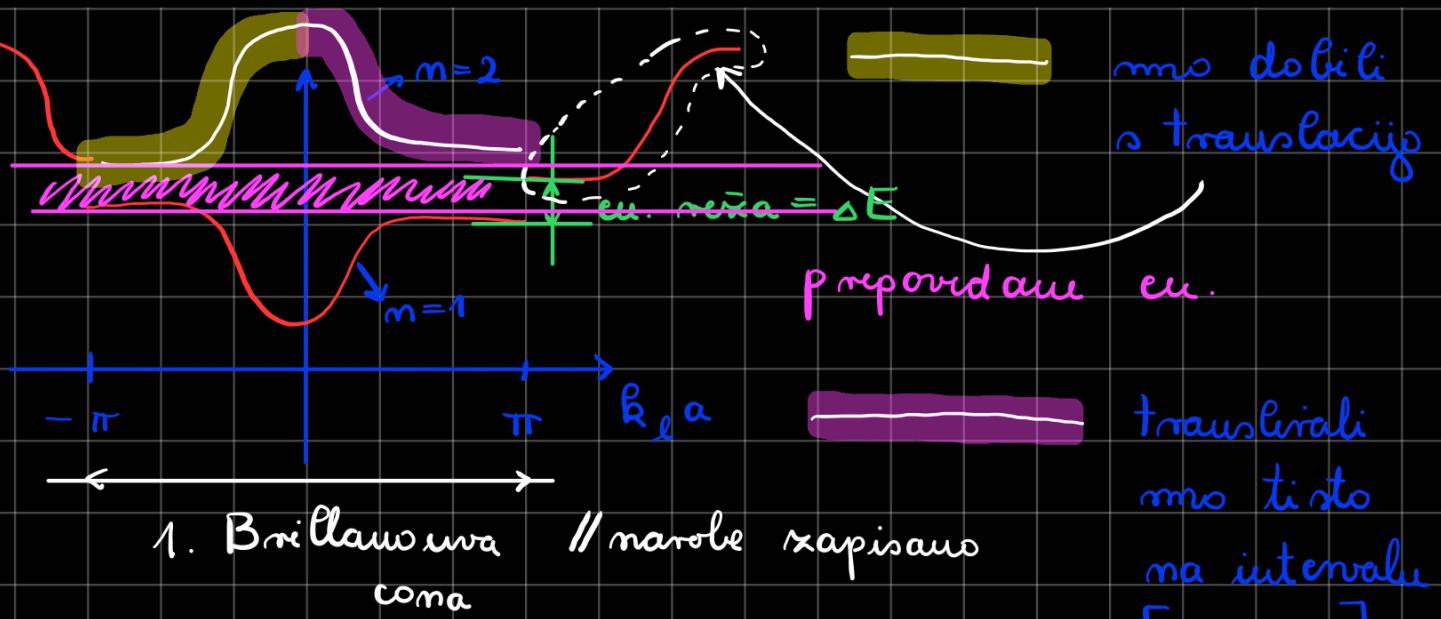
Primer: $m=6$

l	k	$\cos(k_l a)$
0	0	1
1	$\frac{\pi}{3} \cdot \frac{l}{a}$	$\frac{1}{2}$
2		$-\frac{1}{2}$
3		-1
4		$-\frac{1}{2}$
5		$+\frac{1}{2}$
6		1

$$k_l = \frac{2\pi}{Na} l$$

$$k \propto \sqrt{E}$$





$$P \ll 1$$

$$k_a = \pi + \tilde{k}_a, \tilde{k}_a \sim 0$$

$$P \frac{\sin(\tilde{k}_a)}{\tilde{k}_a} + \cos(\tilde{k}_a) = -1$$

$$\sin(\pi + \tilde{k}_a) = -\sin(\tilde{k}_a)$$

$$\cos(\pi + \tilde{k}_a) = -\cos(\tilde{k}_a)$$

$$1. \text{ eu. re\v{z}ka : } k_x a = \pi \Rightarrow \cos(k_x a) = -1$$

Razvijemo do 2. reda, ker 1. red da evo nuznimivo rezultat

$$\sin \tilde{k}_a \approx \tilde{k}_a$$

$$P \frac{\tilde{k}_a}{\tilde{k}_a + \pi} + \lambda - \frac{\tilde{k}_a^2 a^2}{2} = \lambda$$

$$\cos(\tilde{k}_a) \approx 1 - \frac{\tilde{k}_a^2 a^2}{2}$$

$$\text{dobivmo kvadratus ena\v{c}bo} + O((\tilde{k}_a)^3)$$

$$\tilde{k}_1 a = 0 \Rightarrow k_1 a = \pi$$

$$\tilde{k}_2 a = \frac{2P}{\pi} \Rightarrow k_2 a = \pi + \frac{2P}{\pi}$$

A circula ria $k_2 a = \pi \Rightarrow \cos k_2 a = -1$

$P <= 1$

$k_2 a = \pi + \hat{k}_2 a$

$P \frac{\sin(k_2 a)}{k_2 a} + \cos k_2 a = 1$

$\sin(\pi + \hat{k}_2 a) = -\sin \hat{k}_2 a$

$\cos(\pi + \hat{k}_2 a) = -\cos \hat{k}_2 a$

3 $\Rightarrow \Delta E = E_2 - E_1 \approx \frac{\hbar^2}{2m} \frac{4P}{\pi^2} = 0.17 eV$

2 \Rightarrow

1 \Rightarrow

(a) $E_2 = \frac{\hbar^2}{2m} \left(\frac{\pi}{a}\right)^2$

(b) $E_1 = \frac{\hbar^2}{2m} \left(\frac{\pi}{a} + \frac{2P}{\pi a}\right)^2$

Ergebnis: $k_2 a = \pi$ (a)
 $\hat{k}_2 a = \frac{2P}{\pi}$ (b)