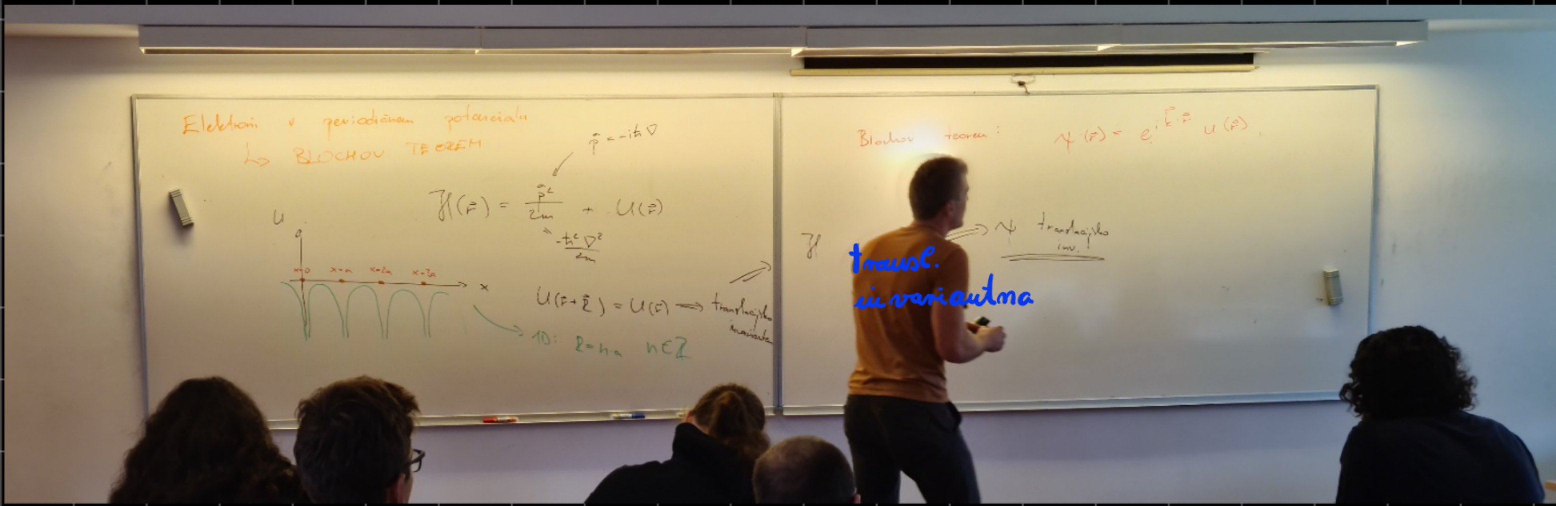



# Blochov teorem

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

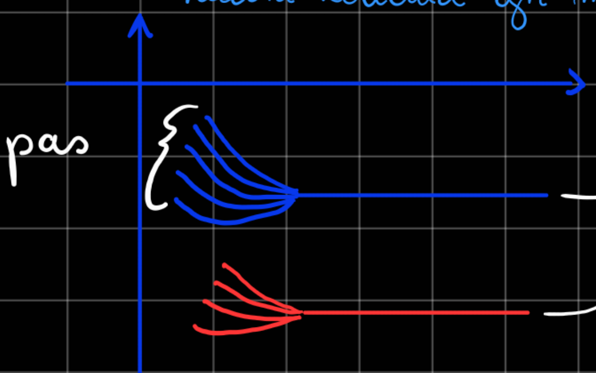
V prosti $e^-$: vsak $\vec{k}$ dovoljen

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

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

Nastanejo pasovi:

Katera količina gre na ordinato?




$r$ , $r$ ... razdalja med jedri

Orbitale se razcepijo v pas

Širina pasu odvisna od glavnega kvantnega št. (višji KŠ = širši pas).
Pas nastane kot posledica periodičnega el. pot.

Zorko 4.3

1D kristal:

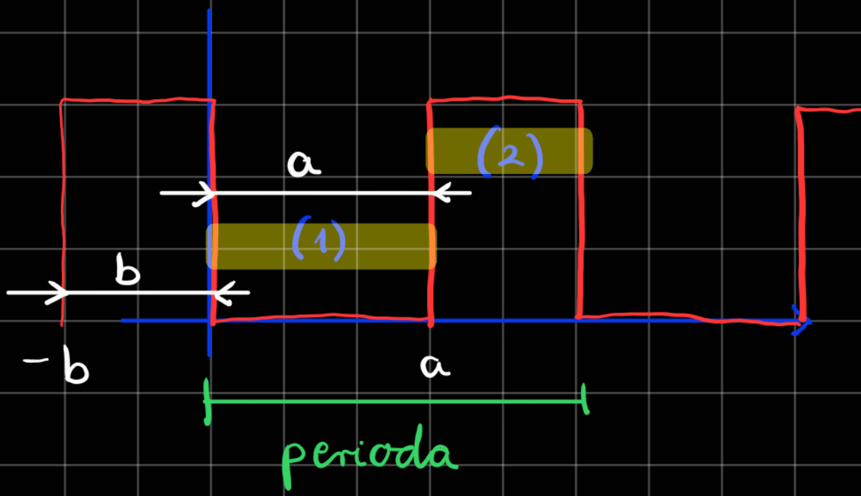
Potencial $U(x) = Ub\left[\ldots + \delta(x+a) + \delta(x) + \ldots\right]$

$a = 0{,}3\,nm$

$\Delta E = E_c - E_1$ en. reža

$Ub = 25\,meV\,nm$

$b \ll a$




Vzamemo limito: $U \to \infty$
$b \to 0$
$Ub = \text{konst.}$

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

$\mathcal{H} = -\dfrac{\hbar^2 \nabla}{2m}$, rešitev sta superpozicija ravnega valov, enega, ki se širi v levo in v desno

$\psi_1 = Ae^{ikx} + Be^{-ikx}$, $k = \sqrt{\dfrac{2mE}{\hbar^2}}$ ... ima vlogo energije

(2) tunneliranje, $E < U$

$\psi_2(x) = Ce^{Kx} + De^{-Kx}$, $K = \sqrt{\dfrac{2m(U-E)}{\hbar^2}}$

Določiti moramo A, B, C, D (BC pogoji)

MF1 mov: fja mora biti v BC zvezna in zvezno odv.

$\psi$ zvezna: $x = \emptyset \Rightarrow A + B = C + D$ #1 enačba

$\psi'$ zvezna: $\left.\frac{\partial \psi_1}{\partial x}\right|_{x=\emptyset} = k(A-B)$

$\left.\frac{\partial \psi_2}{\partial x}\right|_{x=\emptyset} = K(C-D)$

$\Rightarrow k(A-B) = K(C-D)$ #2 enačba

Isto še za $x=a$, kjer upoštevamo Blochov teorem:

(3) $x=a$: $\psi(x) = e^{ik_l x} u(x)$

$\Rightarrow \psi(x=a) = e^{ik_l a}\psi(x)$

Naša perioda je $a+b$

zveznost: $\psi_1(x=a) = Ae^{ika} + Be^{-ika}$ $\cancel{4}$

$$\psi_2(x=a) = \underbrace{\psi_2(x=-b)}\, e^{ik_l(a+b)}$$

$\vec{r} = \vec{a}$, $\vec{R} = -\vec{a} - \vec{b}$

$\vec{a} + \vec{R} = \vec{a} - \vec{a} - \vec{b} = -\vec{b}$

// uporabili smo Blochov teorem

vrednost val. fje pri $x=a$ je zaradi periodičnosti enaka kot pri $-b$

Intermezzo: • prost $e^-$: $\psi = e^{ikx}$ $\hat{p}\psi = \hbar k\psi$

• Blochov $e^-$: $\psi = e^{ikx}u(x)$ $\hat{p}\psi \cancel{=} k\psi$

(4)

$$\left.\frac{\partial \psi_1}{\partial x}\right|_{x=a} = \left.\frac{\partial \psi_2}{\partial x}\right|_{x=a} = \left.\frac{\partial \psi_2}{\partial x}\right|_{x=-b} \exp\{ik_\ell (a+b)\} \quad ✡ ✡$$

$$✡ \quad e^{ika}A + e^{-ikb}B - e^{ik_\ell(a+b)}e^{-Kb}C - e^{ik_\ell(a+b)}e^{Kb}D = \emptyset$$

✡✡

Imamo sistem enačb $M\vec{v} = \emptyset$, $\vec{v} = \begin{bmatrix} A \\ B \\ C \\ D \end{bmatrix}$

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

Ena enolična rešitev: $\vec{x} = A^{-1}b \iff \det(A) \neq \emptyset$

Crammerjevo pravilo

Numerična rešitev (iz Mathematica):

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

Spomnimo se definicij in limit

$b \to 0$

$U \to \infty$

$Ub = \text{konst.}$

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

$$K = \sqrt{\frac{2m(U-\cancel{E})}{\hbar^2}} \qquad U \gg E \qquad k_\ell = \frac{2\pi}{N(a+b)}\ell$$

$$Kb \propto \sqrt{U}\, b = \underbrace{\sqrt{Ub}}_{\text{konst.}} \sqrt{b}$$

$$Kb \sim \emptyset$$

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Uporabimo Taylorja na sinh in cosh

$$\sinh(x) = \frac{e^{x} - e^{-x}}{2} \qquad \cos(x) = \frac{e^{x} + e^{-x}}{2}$$

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

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

$$\Rightarrow \sinh(x) = x, \quad \cos(h) = 1$$

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Rešitev postane, upoštevajoč $K \gg k$

$$\frac{Ka}{2ka} Kb \sin(ka) + \cos(ka) = \cos(k_\ell a)$$

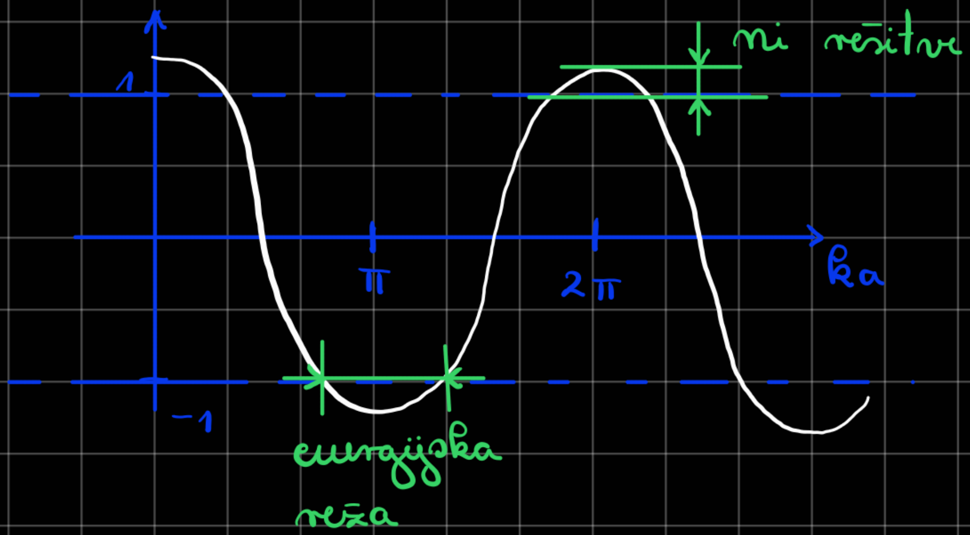
$$P \frac{\sin(ka)}{ka} + \cos(ka) = \cos(k_\ell a), \quad P = \frac{K^2 ab}{2} = \frac{\cancel{2} m a U b}{\cancel{2} \hbar^2}$$

$$= 0{,}098,$$

$$m = m_e = 9{,}1 \cdot 10^{-31}$$

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

Leva stran enačbe




V en. reži so vrednosti, ki jih $e^-$ v kristalu ne more zasesti.

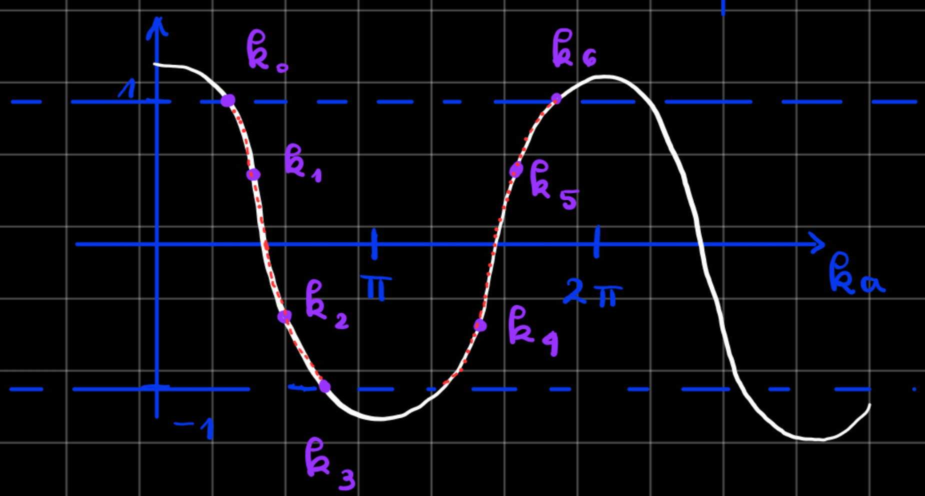
Vrednosti $ka$, pri katerih $|LSE| > 1 \Rightarrow$ enačba nima rešitve

Primer: $n = 6$

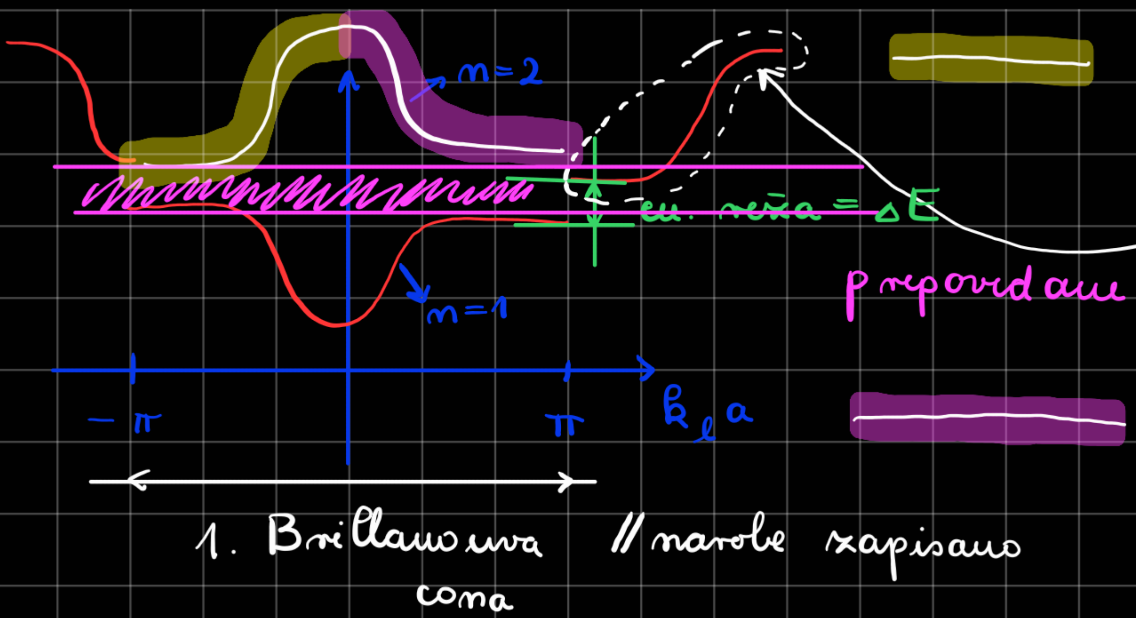
$$k_\ell = \frac{2\pi}{Na}\ell$$

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

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




$n \to \infty$




smo dobili s translacijo

translirali smo tisto na intervalu $[-2\pi, \pi]$

$P << 1$

$ka = \pi + \hat{k}a \,, \quad \hat{k}a \sim 0$

$$P \frac{\sin(ka)}{ka} + \cos(ka) = -1$$

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

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

1. en. reža: $k_l a = \pi \Rightarrow \cos(k_l a) = -1$

Razvijemo do 2. reda, ker 1. red da eno nezanimivo rešitev

$\sin \hat{k}a \doteq \hat{k}a$

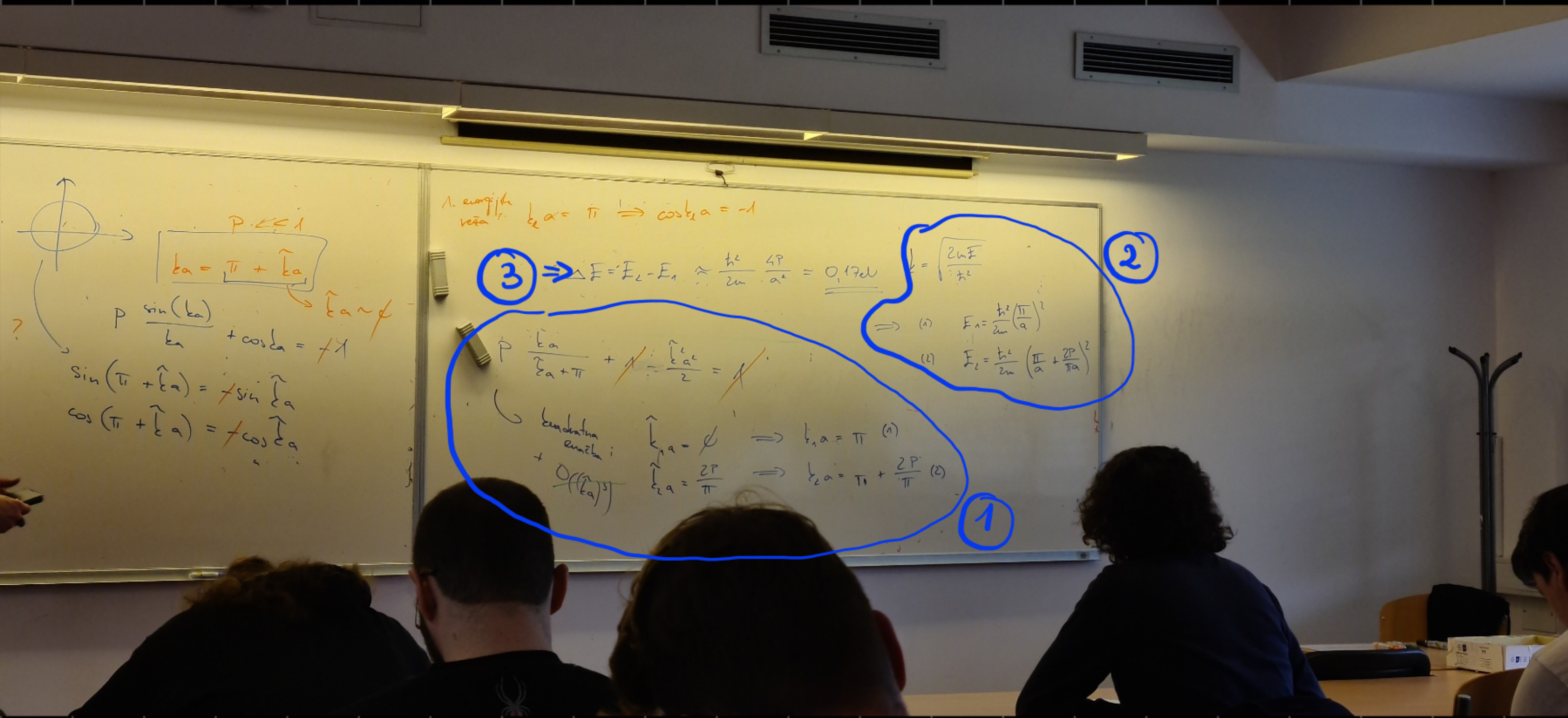
$$P \frac{\hat{k}a}{\hat{k}a + \pi} + \cancel{1} - \frac{\hat{k}^2 a^2}{2} = \cancel{1}$$

$\cos(\hat{k}a) \doteq 1 - \frac{\hat{k}^2 a^2}{2}$

dobimo kvadratno enačbo $+ O((\hat{k}a)^3)$

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

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



Vaja iz Kronnig-Penneyjevega modela: 2. izpit 19/20
3 b) naloga