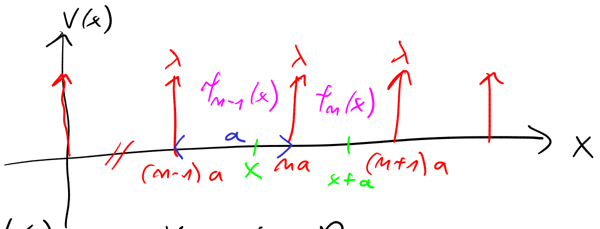
1D $\quad V(x) = \sum_{n=0}^{N-1} \lambda\, \delta(x - na)$



$\lambda > 0$

$$-\frac{\hbar^2}{2m}\psi''(x) + V(x)\psi(x) = E\psi(x)$$

Kronig-Penney

$$\psi_n(x) = A_n e^{ipx} + B_n e^{-ipx} \qquad p = \sqrt{\frac{2mE}{\hbar^2}} \qquad E = \frac{\hbar^2 p^2}{2m}$$

RP. $\quad \psi_{n-1}(na) = \psi_n(na)$

$$\psi_n'(na) - \psi_{n-1}'(na) = \frac{2m\lambda}{\hbar^2}\psi_n(na) = 2Q\,\psi_n(na) \qquad Q = \frac{m\lambda}{\hbar^2}$$

$$A_{n-1}e^{ipna} + B_{n-1}e^{-ipna} = A_n e^{ipna} + B_n e^{-ipna}$$

$$ip\left(A_n e^{ipna} - B_n e^{-ipna}\right) - ip\left(A_{n-1}e^{ipna} - B_{n-1}e^{-ipna}\right) = 2Q\left(A_n e^{ipna} + B_n e^{-ipna}\right)$$

homogen sistem 2N lin. enačb

PRP: $\quad \psi(x + Na) = \psi(x)$

iščemo : $\underbrace{NA,\ NB}_{2N \text{ koeficientov}},\ E$

Blochov teorem

$$T\psi(x) = \psi(x+a)$$

$$[H, T] = 0 \qquad TV(x) = V(x+a) = V(x)$$

lastne funkcije operatorja translacije T

$$T\psi(x) = \lambda\psi(x) = \psi(x+a)$$

$$T^N\psi(x) = \lambda^N\psi(x) = \psi(x+Na) = \psi(x)$$

$\lambda^N = 1$

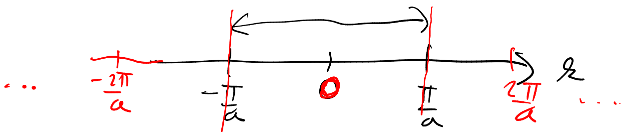
$|\lambda| = 1$

$= e^{ika}$

$ka = \frac{2\pi}{N}m \qquad m \in \mathbb{Z}$

$ka \in [-\pi, \pi)$

1. Brillouinova cona $\qquad K = \frac{2\pi}{a}m \quad m \in \mathbb{Z}$



$ka \qquad e^{ika} = \lambda$

$ka + 2\pi \qquad e^{i(ka+2\pi)} = e^{ika} = \lambda$

Wigner-Seitzova osnovna celica recipročne mreže

$$T\psi(x) = \boxed{\psi(x+a) = e^{ika}\psi(x)} \text{ Blochova stanja}$$

$$\psi_n(x+a) = e^{ika}\psi_{n-1}(x)$$

$$A_n e^{ip(x+a)} + B_n e^{-ip(x+a)} = e^{ika}\left(A_{n-1}e^{ipx} + B_{n-1}e^{-ipx}\right)$$

$\underline{\quad}$: $\quad A_n e^{ipa} = A_{n-1}e^{ika} \rightarrow A_{n-1} = A_n e^{i(p-k)a}$

$\sim$: $\quad B_n e^{-ipa} = B_{n-1}e^{ika} \rightarrow B_{n-1} = B_n e^{-i(p+k)a}$

$$\underbrace{A_m e^{i(p-k)a}}_{A_{m-1}} e^{ipma} + \underbrace{B_m e^{-i(p+k)a}}_{B_{m-1}} e^{-ipma} = A_m e^{ipma} + B_m e^{-ipma}$$

$$ip\left(A_m e^{ipma} - B_m e^{-ipma}\right) - ip\left(\underbrace{A_m e^{i(p-k)a}}_{A_{m-1}} e^{ipma} - \underbrace{B_m e^{-i(p+k)a}}_{B_{m-1}} e^{-ipma}\right) =$$

$$= 2Q\left(A_m e^{ipma} + B_m e^{-ipma}\right)$$

homogen sistem lin. enačb za neznanki A_m, B_m

$$\tilde{A} = A_m e^{ipma}$$

$$\tilde{B} = B_m e^{-ipma}$$

$$\tilde{A} e^{i(p-k)a} + \tilde{B} e^{-i(p+k)a} = \tilde{A} + \tilde{B}$$

$$ip\left(\tilde{A} - \tilde{B}\right) - ip\left(\tilde{A} e^{i(p-k)a} - \tilde{B} e^{-i(p+k)a}\right) = 2Q\left(\tilde{A} + \tilde{B}\right)$$

$$\begin{bmatrix} 1 - e^{i(p-k)a} \,, & 1 - e^{-i(p+k)a} \\ 2Q - ip + ip e^{i(p-k)a} \,, & 2Q + ip + ip e^{-i(p+k)a} \end{bmatrix} \begin{bmatrix} \tilde{A} \\ \tilde{B} \end{bmatrix} = 0$$

$$\downarrow$$

$$\det\left[\quad\right] = 0$$

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

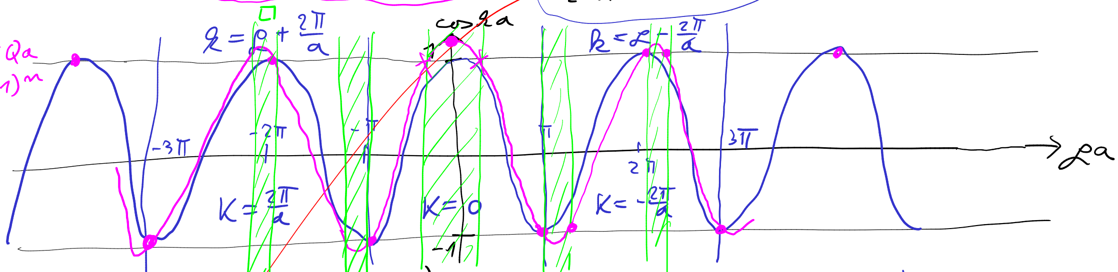
izberemo $k \in \left[-\frac{\pi}{a}, \frac{\pi}{a}\right)$

izračunamo $p \rightarrow E = \frac{\hbar^2 p^2}{2m}$

$$\cos ka = \cos \rho a + Qa \frac{\sin \rho a}{\rho a} \qquad \frac{\hbar^2 \rho^2}{2m} = E = \varepsilon$$

$\rho a = 0: 1 + Qa$

$\rho a = m\pi: (-1)^m$, $m \neq 0$



$\cos ka = 1 \qquad k = 0$ (središče 1BC)

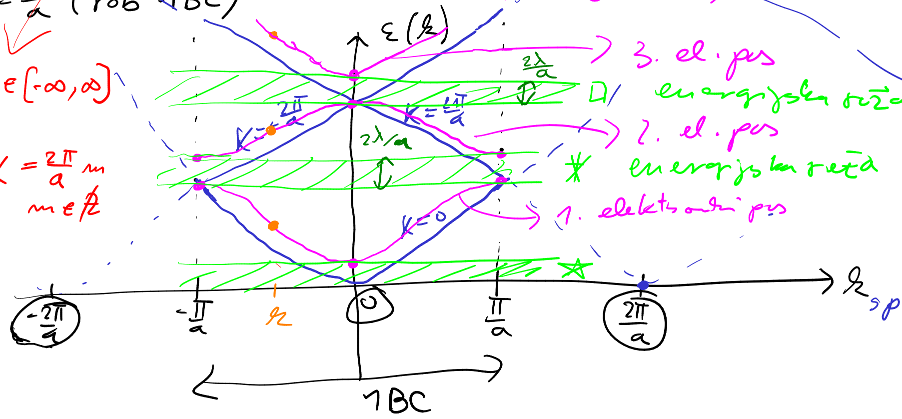
$\cos ka = -1 \qquad k = \pm \frac{\pi}{a}$ (rob 1BC)

$\square$ $Qa = 0$ $\qquad \lambda = 0$

$Qa > 0 \qquad \lambda > 0$

1. formulacija: $\rho \in [-\infty, \infty]$

2. formulacija: $k \in [-\frac{\pi}{a}, \frac{\pi}{a}]$ & $K = \frac{2\pi}{a} m$, $m \in \mathbb{Z}$



$\varepsilon(k)$ disperzija

$\lambda = e^{ika}$

$\cos ka = \cos \rho a$

$\rho = k$

$\varepsilon = \frac{\hbar^2 k^2}{2m}$

k splošno; $k = \rho + K$

$\rho = k - K$

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

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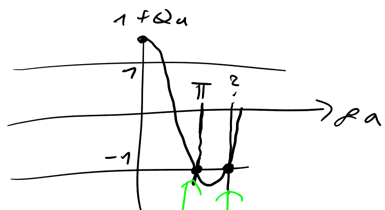
limita šibkega potenciala / limita skoraj prostih elektronov

$Qa \ll 1$

$$\cos ka = \cos \rho a + Qa \frac{\sin \rho a}{\rho a}$$



$\rho a = m\pi \qquad \cos \rho a = (-1)^m$

$m \neq 0 \qquad \frac{\sin \rho a}{\rho a} = 0$

$\rho a = m\pi + \varepsilon \qquad \varepsilon \ll \pi$ (pričakujemo)

$$(-1)^m = \cos(m\pi + \varepsilon) + Qa \frac{\sin(m\pi + \varepsilon)}{m\pi + \varepsilon}$$

$$\cancel{(-1)^m} = \cancel{(-1)^m}\left(1 - \frac{\varepsilon^2}{2}\right) + Qa \frac{(-1)^m \varepsilon}{m\pi} + O(\varepsilon^3, Qa\,\varepsilon^2)$$

$$\cancel{1} = \cancel{1} - \frac{\varepsilon^2}{2} + \frac{Qa}{m\pi}\varepsilon \Rightarrow \varepsilon = 0, \quad \varepsilon = \frac{2Qa}{m\pi} \rightarrow \varepsilon \ll \pi$$

začetek energijske reže: $\rho a = m\pi \longrightarrow E = \frac{\hbar^2 m^2 \pi^2}{2ma^2}$

konec —||—: $\rho a = m\pi + \frac{2Qa}{m\pi} \longrightarrow E = \frac{\hbar^2 m^2 \pi^2}{2ma^2}\left(1 + \frac{2Qa}{m^2\pi^2}\right)^2 =$

$$= \frac{\hbar^2 m^2 \pi^2}{2ma^2} + \cancel{\frac{\hbar^2 m^2 \pi^2}{2ma^2}} \cdot 2 \cdot \frac{2Q\cancel{a}}{\cancel{m^2 \pi^2}} + \dots$$

širina reže:

$$\Delta E = \frac{2\hbar^2 Q}{ma} = \frac{2\hbar^2 \cancel{m}\lambda}{\cancel{m}a\hbar^2} = \frac{2\lambda}{a}$$

približek skoraj prostih elektronov

$$\left(\varepsilon^0_{\vec q-\vec k} - E\right) c_{\vec q-\vec k} + \sum_{\vec k'} V_{\vec k'-\vec k}\, c_{\vec q-\vec k'} = 0$$

$$\boxed{V_{\vec k} = \frac{1}{V_{o.c.}} \int_{\text{po o.c.}} V(\vec r)\, e^{-i\vec k\cdot\vec r}\, d\vec r}$$

Fourierove komponente potenciala $V(\vec r)$

$$\psi_{\vec q}(\vec r) = \sum_{\vec k} \underbrace{c_{\vec q-\vec k}}\, e^{i(\vec q-\vec k)\cdot\vec r}$$

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

širina energijske reže v $q=\frac{\pi}{a}$

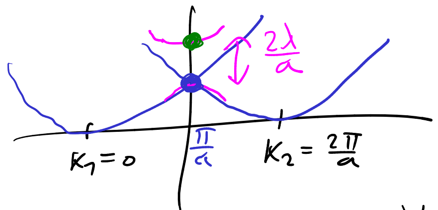
$\underline{Q_1=0}$ → degeneracija

$K_1=0$

$K_2=\frac{2\pi}{a}$

$$\varepsilon^0_{q-k_1} = \frac{\hbar^2}{2m}\left(\frac{\pi}{a}\right)^2 = \varepsilon^0$$

$$\varepsilon^0_{q-k_2} = \frac{\hbar^2}{2m}\left(\frac{\pi}{a}-\frac{2\pi}{a}\right)^2 = \frac{\hbar^2}{2m}\left(\frac{\pi}{a}\right)^2 = \varepsilon^0$$



$$\det\begin{bmatrix} \varepsilon^0 + V_{K_1-K_1} - E, & V_{K_2-K_1} \\ V_{K_1-K_2}, & \varepsilon^0 + V_{K_2-K_2} - E \end{bmatrix} = 0$$

$$V_K = \frac{1}{a}\int_{o.c.} V(x)\, e^{-iKx}\, dx = \frac{1}{a}\int_0^a \lambda\,\delta(x)\, e^{-ikx}\, dx = \frac{\lambda}{a}$$

$$\begin{vmatrix} \varepsilon^0 + \frac{\lambda}{a} - E, & \frac{\lambda}{a} \\ \frac{\lambda}{a}, & \varepsilon^0 + \frac{\lambda}{a} - E \end{vmatrix} = 0$$

$$\left(\varepsilon^0 + \frac{\lambda}{a} - E\right)^2 - \left(\frac{\lambda}{a}\right)^2 = 0$$

$$\varepsilon^0 + \frac{\lambda}{a} - E = \pm\frac{\lambda}{a}$$

$$E = \varepsilon^0 + \frac{\lambda}{a} \pm \frac{\lambda}{a} = \begin{cases} \varepsilon^0 \\ \varepsilon^0 + \underline{\frac{2\lambda}{a}} \end{cases}$$

$$\begin{bmatrix} \varepsilon^0 + V_{K_1-K_1} - E, & V_{K_2-K_1} \\ V_{K_1-K_2}, & \varepsilon^0 + V_{K_2-K_2} - E \end{bmatrix}\begin{bmatrix} c_{q-K_1} \\ c_{q-K_2} \end{bmatrix} = 0$$

$K_1=0;\ K_2=\frac{2\pi}{a}$

$\underline{E=\varepsilon^0}$

$$\begin{bmatrix} \frac{\lambda}{a}, & \frac{\lambda}{a} \\ \frac{\lambda}{a}, & \frac{\lambda}{a} \end{bmatrix}\begin{bmatrix} c_{q-k_1} \\ c_{q-k_2} \end{bmatrix} = 0 \quad \longrightarrow \quad \begin{bmatrix} 1 \\ -1 \end{bmatrix}$$

$$\psi(x) \propto 1\cdot e^{i(q-k_1)x} - 1\, e^{i(q-k_2)x} \propto e^{iqx} - e^{i(q-\frac{2\pi}{a})x}$$

$\underline{E=\varepsilon^0+\frac{2\lambda}{a}}$

$$\begin{bmatrix} -\frac{\lambda}{a}, & \frac{\lambda}{a} \\ \frac{\lambda}{a}, & -\frac{\lambda}{a} \end{bmatrix}\begin{bmatrix} c_{q-k_1} \\ c_{q-k_2} \end{bmatrix} = 0 \quad \longrightarrow \quad \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

$$\psi(x) \propto 1\, e^{i(q-k_1)x} + 1\, e^{i(q-k_2)x} \propto e^{iqx} + e^{i(q-\frac{2\pi}{a})x}$$

$$\rho(x) = |\psi(x)|^2 \propto \sin^2\frac{\pi x}{a}$$

$$\rho(x) = |\psi(x)|^2 \propto \cos^2\frac{\pi x}{a}$$