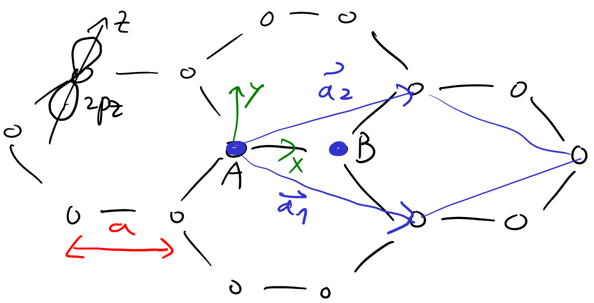
Izračunaj disperzijo el. pasu v grafenu, ki ga tvorijo $2p_z$ orbitale



$o = C$

$C = 1s^2 \underbrace{2s^2 2p^2}$

$\downarrow$

$2sp_2,\ 2p_z$

$\vec{a}_1 = a\left(\frac{3}{2}, -\frac{\sqrt{3}}{2}\right)$

$\vec{a}_2 = a\left(\frac{3}{2}, \frac{\sqrt{3}}{2}\right)$

$\left.\begin{array}{l}\vec{r}_A = 0 \\ \vec{r}_B = a(1,0)\end{array}\right\} \vec{r}_m \quad m \in \{A, B\}$

približek tesne vezi:

$$\cancel{\varepsilon(\vec{k}) = \varepsilon_0 - \frac{\beta + \sum_{\vec{R}=n.s.\phi} \gamma(\vec{R}) e^{i\vec{k}\cdot\vec{R}}}{1 + \sum_{\vec{R}=n.s.\phi} \alpha(\vec{R}) e^{i\vec{k}\cdot\vec{R}}}}\ *$$

ena orbitala na osnovno celico

grafen: $2 \times 2p_z$ orbitala

$$|\psi\rangle = \sum_{\vec{R}m} c_{\vec{R}m} |\vec{R}m\rangle \qquad \langle\vec{r}|\vec{R}m\rangle = \phi_{2p_z}(\vec{r} - \vec{R} - \vec{r}_m)$$

$$H|\psi\rangle = E|\psi\rangle$$

$$\sum_{\vec{R}m} c_{\vec{R}m} (H - E)|\vec{R}m\rangle = 0 \quad / \langle\vec{R}'m'|$$

$$\forall \vec{R}'m': \quad \sum_{\vec{R}m} c_{\vec{R}m}\Big(\langle\vec{R}'m'|\underset{H^{at}_{\vec{R}'m'} + \Delta V_{\vec{R}'m'}}{H}|\vec{R}m\rangle - E\langle\vec{R}'m'|\vec{R}m\rangle\Big) = 0$$

$$H = H^{at}_{\vec{R}'m'} + \Delta V_{\vec{R}'m'} \qquad \Delta V_{\vec{R}'m'} = \sum_{\vec{R}m \neq \vec{R}'m'} V^{at}_{\vec{R}m}$$

$$H^{at}_{\vec{R}'m'} |\vec{R}'m'\rangle = \varepsilon_{m'} |\vec{R}'m'\rangle$$

$$\sum_{\vec{R}m} c_{\vec{R}m}\Big(\varepsilon_{m'}\langle\vec{R}'m'|\vec{R}m\rangle + \langle\vec{R}'m'|\Delta V_{\vec{R}'m'}|\vec{R}m\rangle - E\langle\vec{R}'m'|\vec{R}m\rangle\Big) = 0$$

$$\sum_{\vec{R}m} = \sum_{\vec{R}m = \vec{R}'m'} + \sum_{\vec{R}m \neq \vec{R}'m'}$$

$$\langle\vec{R}'m'|\vec{R}'m'\rangle = 1$$

$$\beta_{m'} = -\langle\vec{R}'m'|\Delta V_{\vec{R}'m'}|\vec{R}'m'\rangle$$

$$\alpha_{m'm}(\vec{R} - \vec{R}') = \langle\vec{R}'m'|\vec{R}m\rangle$$

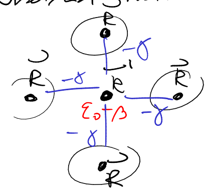
$$\gamma_{m'm}(\vec{R} - \vec{R}') = -\langle\vec{R}'m'|\Delta V_{\vec{R}'m'}|\vec{R}m\rangle$$

$$c_{\vec{R}'m'}(\varepsilon_{m'} - E - \beta_{m'}) + \sum_{\vec{R}m \neq \vec{R}'m'} c_{\vec{R}m}\Big[\cancel{(\varepsilon_{m'} - E)\alpha_{m'm}(\vec{R} - \vec{R}')} - \gamma_{m'm}(\vec{R} - \vec{R}')\Big] = 0$$

$\varepsilon_{m'} = \varepsilon_0$ za $\forall m'$

$$\forall \vec{R}'m': \quad \boxed{(\varepsilon_{m'} - \beta_{m'})c_{\vec{R}'m'} - \sum_{\vec{R}m \neq \vec{R}'m'} \gamma_{m'm}(\vec{R} - \vec{R}')c_{\vec{R}m} = E c_{\vec{R}'m'}}$$

primer: ... kvadratna mreža: $m \in \{1\}$ $\quad \vec{r}_1 = 0$



$\varepsilon_{m'} \to \varepsilon_0$

$\beta_{m'} \to \beta$

$\gamma_{m'm}(\vec{R} - \vec{R}') \to \gamma(\vec{R} - \vec{R}') = \begin{cases} \gamma; & \vec{R} \text{ in } \vec{R}' \text{ n.s.} \\ \phi; & \text{sicer} \end{cases}$

$c_{\vec{R}m} \to c_{\vec{R}}$

skakalni integral

$$(\varepsilon_0 - \beta)c_{\vec{R}'} - \gamma \sum_{\vec{R} = n.s.\vec{R}'} c_{\vec{R}} = E c_{\vec{R}'} \quad / \forall \vec{R}'$$

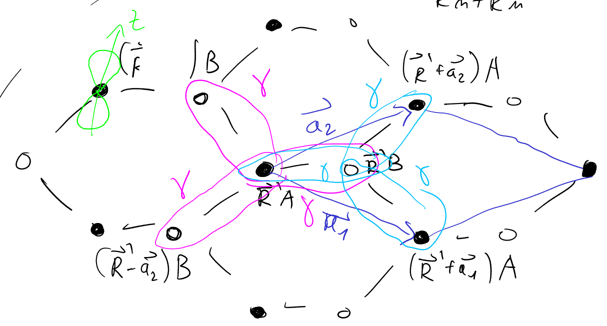
nastavek: $c_{\vec{R}} = c\, e^{i\vec{k}\cdot\vec{R}}$

$$(\varepsilon_0 - \beta)\cancel{c}\, e^{i\vec{k}\cdot\vec{R}'} - \gamma \sum_{\vec{R} = n.s.\vec{R}'} \cancel{c}\, e^{i\vec{k}\cdot\vec{R}} = E\cancel{c}\, e^{i\vec{k}\cdot\vec{R}'} \quad / \cdot e^{-i\vec{k}\cdot\vec{R}'}$$

$$\varepsilon_0 - \beta - \gamma \sum_{\vec{R} = n.s.\vec{R}'} e^{i\vec{k}\cdot(\vec{R} - \vec{R}')} = E$$

$$\to \quad E = \varepsilon_0 - \beta - \gamma \sum_{\vec{R} = n.s.\phi} e^{i\vec{k}\cdot\vec{R}} \quad *$$

$$\forall \vec R'_{m'}: \quad (\varepsilon_{m'} - \beta_{m'})\, c_{\vec R' m'} - \sum_{\vec R m \neq \vec R' m'} \gamma_{m' m}(\vec R - \vec R')\, c_{\vec R m} = E\, c_{\vec R' m'}$$



● A

○ B

● = ○ = C

$\varepsilon_A = \varepsilon_B = \varepsilon_{2p_z} = \varepsilon_0$

$\beta_A = \beta_B = \beta \qquad \beta_{m'} = \langle \vec R' m' | \Delta V_{\vec R' m'} | \vec R' m' \rangle$

$2p_z$ osno simetrične glede na os z

trištevna os (rotacija okoli osi z za 120°)

$$\gamma_{BA}(0) = \gamma_{BA}(-\vec a_1) = \gamma_{BA}(-\vec a_2) = \gamma$$
$$\gamma_{AB}(0) = \gamma_{AB}(\vec a_1) = \gamma_{AB}(\vec a_2) = \gamma$$

$$\gamma = -\langle \vec R' B | \Delta V_{\vec R' B} | \vec R' A \rangle \in \mathbb{R}$$

$$\phi_{2p_z}(\vec r) \in \mathbb{R}$$

$$\forall \vec R' A: \quad (\varepsilon_0 - \beta)\, c_{\vec R' A} - \gamma\left(c_{\vec R' B} + c_{(\vec R' - \vec a_1)B} + c_{(\vec R' - \vec a_2)B}\right) = E\, c_{\vec R' A}$$
$$\forall \vec R' B: \quad (\varepsilon_0 - \beta)\, c_{\vec R' B} - \gamma\left(c_{\vec R' A} + c_{(\vec R' + \vec a_1)A} + c_{(\vec R' + \vec a_2)A}\right) = E\, c_{\vec R' B}$$

$$c_{\vec R' A} = c_A e^{i\vec k \cdot \vec R}$$
$$c_{\vec R' B} = c_B e^{i\vec k \cdot \vec R}$$

$$/ e^{i\vec k \cdot \vec R'}$$
$$(\varepsilon_0 - \beta)\, c_A e^{i\vec k \cdot} \quad \gamma\left(e^{i\vec k \cdot} \quad e^{i\vec k\cdot(\vec R' - \vec a_1)} + e^{i\vec k \cdot (\vec R' - \vec a_2)}\right) c_B = E\, c_A e^{i\vec k \cdot \vec R'}$$
$$(\varepsilon_0 - \beta)\, c_B e^{i\vec k \cdot \vec R'} - \gamma\left(e^{i\vec k \cdot \vec R'} + e^{i\vec k \cdot (\vec R' + \vec a_1)} + e^{i\vec k \cdot (\vec R' + \vec a_2)}\right) c_A = E\, c_B e^{i\vec k \cdot \vec R'}$$

$$(\varepsilon_0 - \beta)\, c_A - \gamma\left(1 + e^{-i\vec k \cdot \vec a_1} + e^{-i\vec k \cdot \vec a_2}\right) c_B = E\, c_A$$
$$(\varepsilon_0 - \beta)\, c_B - \gamma\left(1 + e^{i\vec k \cdot \vec a_1} + e^{i\vec k \cdot \vec a_2}\right) c_A = E\, c_B$$

$$\forall \vec k: \quad \begin{bmatrix} \varepsilon_0 - \beta - E, & -\gamma\left(1 + e^{-i\vec k \cdot \vec a_1} + e^{-i\vec k \cdot \vec a_2}\right) \\ -\gamma\left(1 + e^{i\vec k \cdot \vec a_1} + e^{i\vec k \cdot \vec a_2}\right), & \varepsilon_0 - \beta - E \end{bmatrix} \begin{bmatrix} c_A \\ c_B \end{bmatrix} = 0$$

→ problem lastnih vrednosti

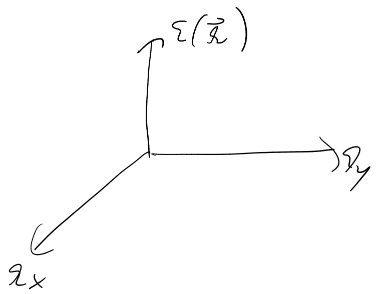
dimenzija = št. orbital v osnovni celici = št. elektronskih pasov

$$\det[\;] = 0$$

$$(\varepsilon_0 - \beta - E)^2 - \gamma^2 \left|1 + e^{i\vec k \cdot \vec a_1} + e^{i\vec k \cdot \vec a_2}\right|^2 = 0$$

→ 2 el. pasova

$$E = \boxed{\varepsilon_0 - \beta \pm \gamma \left|1 + e^{i\vec k \cdot \vec a_1} + e^{i\vec k \cdot \vec a_2}\right| = \varepsilon_\pm(\vec k)}$$

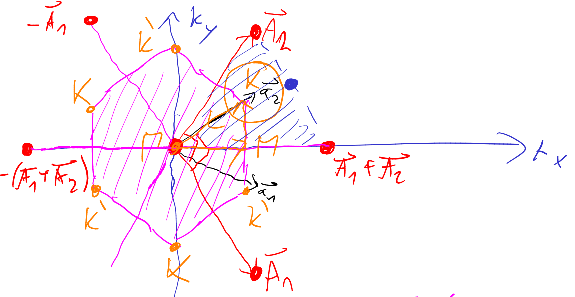


$\vec k = (k_x, k_y) \in 1BC$

$\vec a_1 = a\left(\frac{3}{2}, -\frac{\sqrt 3}{2}\right) \qquad \vec A_i \cdot \vec a_j = 2\pi \delta_{ij}$

$\vec a_2 = a\left(\frac{3}{2}, \frac{\sqrt 3}{2}\right)$

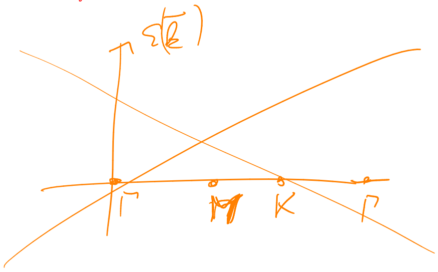
$$\left.\begin{array}{l} |\vec a_1| = |\vec a_2| \\ \sphericalangle\, \vec a_1, \vec a_2 = 60^\circ \end{array}\right\} \text{trikotna Bravaisova mreža}$$



1BC = pravilni šestkotnik

△ enakostranični trikotnik

reciproćna mreža: $\vec K = m_1 \vec A_1 + m_2 \vec A_2$



$\vec k = K + \vec \rho \qquad |\vec \rho| \ll \frac{\pi}{a}$

$$K = \frac{\vec A_2 + (\vec A_1 + \vec A_2)}{2} \cdot \frac{2}{3} = \frac{2}{3}\vec A_2 + \frac{1}{3}\vec A_1$$

$\vec k = K' + \vec \rho \qquad |\vec \rho| \ll \frac{\pi}{a}$

⋮

$$\vec k = \frac{2}{3}\vec A_2 + \frac{1}{3}\vec A_1 + \vec \rho$$

$$\varepsilon(\vec k) = \underline{\varepsilon_0 - \beta} \pm \gamma \left|1 + e^{i\vec k\cdot\vec a_1} + e^{i\vec k\cdot\vec a_2}\right|$$

$\hookrightarrow \phi$ (izbira energijske skale)

$$\varepsilon(\vec k) = \pm\gamma\left|1 + e^{i\left(\frac{2}{3}\vec A_2 + \frac{1}{3}\vec A_1 + \vec \rho\right)\cdot\vec a_1} + e^{i\left(\frac{2}{3}\vec A_2 + \frac{1}{3}\vec A_1 + \vec \rho\right)\cdot\vec a_2}\right|$$

$$\varepsilon(\vec k) \pm\gamma\left|1 + e^{i\frac{2\pi}{3}} e^{i\vec\rho\cdot\vec a_1} + e^{i\frac{4\pi}{3}} e^{i\vec\rho\cdot\vec a_2}\right|$$

$$\varepsilon(\vec k) - \gamma\left|1 + e^{i\frac{2\pi}{3}}(1 + i\vec\rho\cdot\vec a_1) + e^{-i\frac{2\pi}{3}}(1 + i\vec\rho\cdot\vec a_2)\right|$$

$$\varepsilon(\vec k) = \pm\gamma\left|\cancel{1 + e^{i\frac{2\pi}{3}} + e^{-i\frac{2\pi}{3}}} + e^{i\frac{2\pi}{3}} i\vec\rho\cdot\vec a_1 + e^{-i\frac{2\pi}{3}} i\vec\rho\cdot\vec a_2\right|$$

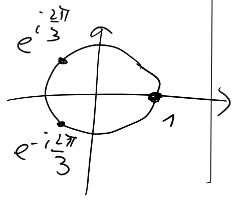
$$\varepsilon(\vec k) = \pm\gamma\left|-\frac{1}{2} i\vec\rho\cdot(\vec a_1 + \vec a_2) + i\frac{\sqrt3}{2} i\vec\rho\cdot(\vec a_1 - \vec a_2)\right|$$

$$\varepsilon(\vec k) = \pm\gamma\left|-\frac{1}{2} i\rho_x \cdot 3a + i\frac{\sqrt3}{2} i\rho_y\cdot(-\sqrt3)a\right| =$$

$$= \pm\gamma\left|-\frac{3}{2} i\rho_x a + \frac{3}{2}\rho_y a\right| =$$

$$= \pm\gamma\frac{3}{2}a\sqrt{\rho_x^2 + \rho_y^2}$$

$\vec a_i \cdot \vec A_j = 2\pi\delta_{ij}$

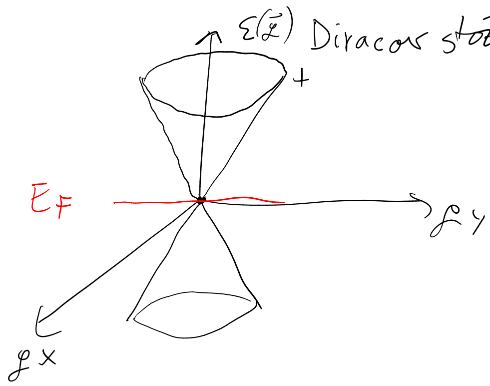


$$e^{\pm i\frac{2\pi}{3}} = \cos\frac{2\pi}{3} \pm i\sin\frac{2\pi}{3} = -\frac{1}{2} \pm i\frac{\sqrt3}{2}$$

$\vec a_1 = a\left(\frac{3}{2}, -\frac{\sqrt3}{2}\right)$

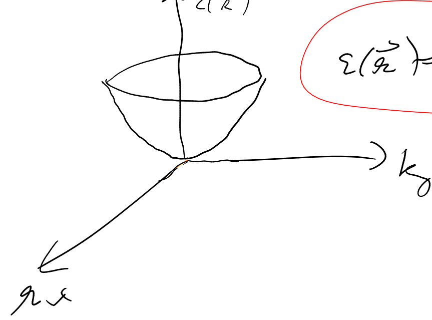
$\vec a_2 = a\left(\frac{3}{2}, \frac{\sqrt3}{2}\right)$

$$\varepsilon(\vec k) = \pm\frac{3}{2}\gamma a|\vec\rho|$$



$\cdot K$

prosti elektroni v 2D



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

brezmasni delci (relativistični)

fotoni: ~~$\omega = ck$~~ ~~$\varepsilon = \hbar c k$~~ bozoni

nevtrini: $m = 0$, spin $= 1/2$ fermioni