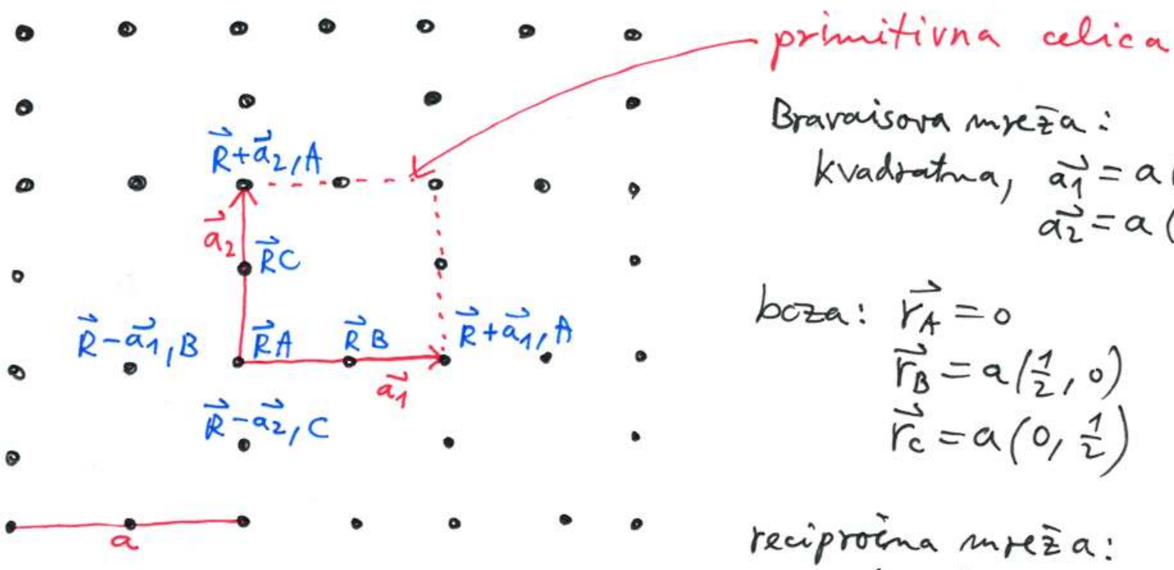
1 a)



Bravaisova mreža:

kvadratna, $\vec{a}_1 = a(1,0)$

$\vec{a}_2 = a(0,1)$

baza: $\vec{r}_A = 0$

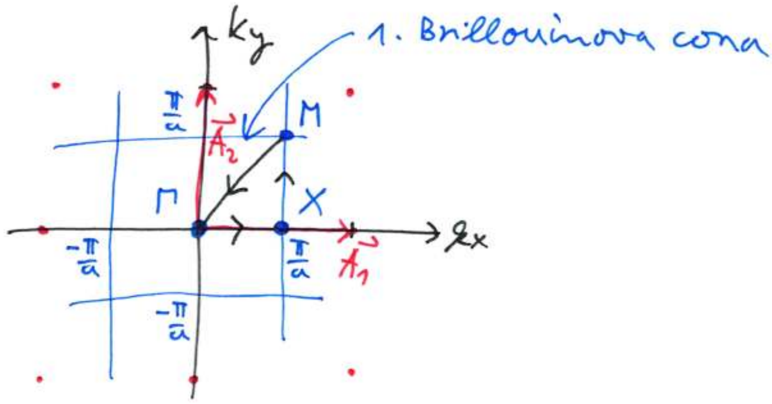
$\vec{r}_B = a(\frac{1}{2}, 0)$

$\vec{r}_C = a(0, \frac{1}{2})$

recipročna mreža:

$\vec{A}_1 = \frac{2\pi}{a}(1,0)$

$\vec{A}_2 = \frac{2\pi}{a}(0,1)$



b)

$$E c_{\vec{R}A} = -\gamma c_{\vec{R}B} - \gamma c_{\vec{R}-\vec{a}_1, B} - \gamma c_{\vec{R}C} - \gamma c_{\vec{R}-\vec{a}_2, C}$$

$$E c_{\vec{R}B} = -\gamma c_{\vec{R}A} - \gamma c_{\vec{R}+\vec{a}_1, A}$$

$\gamma \in \mathbb{R}$, saj so orbitale realne

$$E c_{\vec{R}C} = -\gamma c_{\vec{R}A} - \gamma c_{\vec{R}+\vec{a}_2, A}$$

nastavek: $c_{\vec{R}m} = c_m e^{i\vec{k}\cdot\vec{R}}$ $\quad m \in \{A, B, C\}$

$$E c_A = -\gamma(1+e^{-i\vec{k}\cdot\vec{a}_1}) c_B - \gamma(1+e^{-i\vec{k}\cdot\vec{a}_2}) c_C$$

$$E c_B = -\gamma(1+e^{i\vec{k}\cdot\vec{a}_1}) c_A$$

$$E c_C = -\gamma(1+e^{i\vec{k}\cdot\vec{a}_2}) c_A$$

$$\det\begin{bmatrix} -E, & -\gamma(1+e^{-i\vec{k}\cdot\vec{a}_1}), & -\gamma(1+e^{-i\vec{k}\cdot\vec{a}_2}) \\ -\gamma(1+e^{i\vec{k}\cdot\vec{a}_1}), & -E, & 0 \\ -\gamma(1+e^{i\vec{k}\cdot\vec{a}_2}), & 0, & -E \end{bmatrix} = 0$$

$$-E^3 + E\gamma^2\left(|1+e^{i\vec{k}\cdot\vec{a}_1}|^2 + |1+e^{i\vec{k}\cdot\vec{a}_2}|^2\right) = 0$$

$$E_1 = 0$$

$$E_{2,3} = \pm 2\gamma\sqrt{\cos^2\frac{k_x a}{2} + \cos^2\frac{k_y a}{2}}$$

b) ... $\Gamma \to X$ $\quad k_y = 0$, $k_x \in [0, \frac{\pi}{a}]$

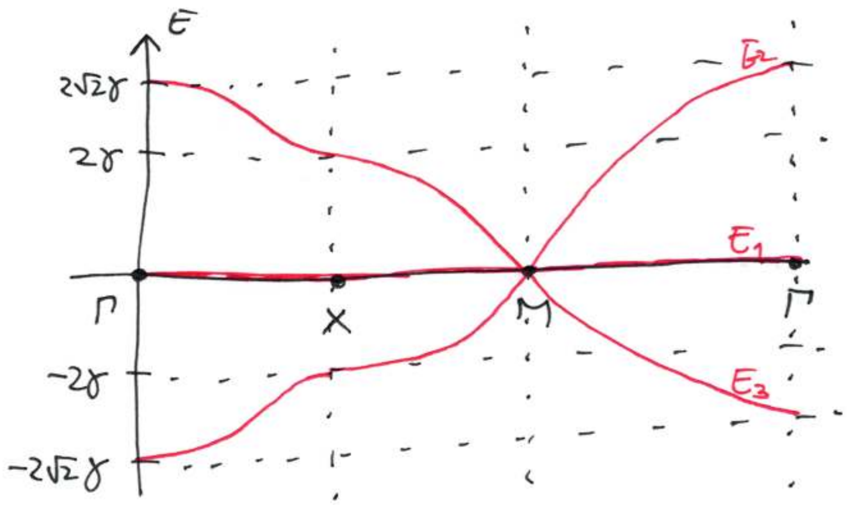
$$E_1 = 0$$
$$E_{2,3} = \pm 2\gamma\sqrt{\cos^2\frac{k_x a}{2} + 1}$$

$X \to M$ $\quad k_x = \frac{\pi}{a}$, $k_y \in [0, \frac{\pi}{a}]$

$$E_1 = 0$$
$$E_{2,3} = \pm 2\gamma \cos\frac{k_y a}{2}$$

$M \to \Gamma$ $\quad q \equiv k_x = k_y \in [\frac{\pi}{a}, 0)$

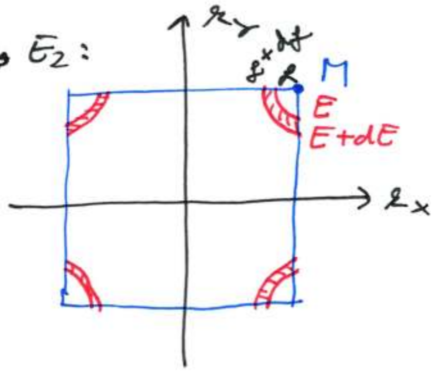
$$E_1 = 0$$
$$E_{2,3} = \pm 2\sqrt{2}\gamma \cos\frac{q a}{2}$$



c) K gostoti stanj pri energijah $|E| \ll \gamma$ prispeva pas E_1 in stanja v bližini točke M iz pasov $E_{2,3}$.

$$\vec{k} = M + \vec{q} \quad \to \quad E_{2,3} \doteq \pm \gamma a q \; ; \; q \equiv |\vec{q}|$$

pas E_2:



$$g_2(E) = \overset{\text{spin}}{2} \cdot \frac{2\pi q\, dq}{\left(\frac{2\pi}{a}\right)^2 S\, dE} = \frac{1}{\pi} \frac{\overset{E/\gamma a}{q}\, \overset{dE/\gamma a}{dq}}{dE} = \frac{E}{\pi\gamma^2 a^2} \quad \text{za } E>0$$

$$g_1(E) = \overset{\text{spin}}{2} \cdot \frac{1}{a^2}\delta(E)$$

$$g(E) = g_1(E) + g_2(E) + g_3(E) = \frac{2}{a^2}\delta(E) + \frac{1}{\pi\gamma^2 a^2}|E|$$

② a) 3 akustične in 3 optične veje ⇒ 2 atoma na primitivno celico

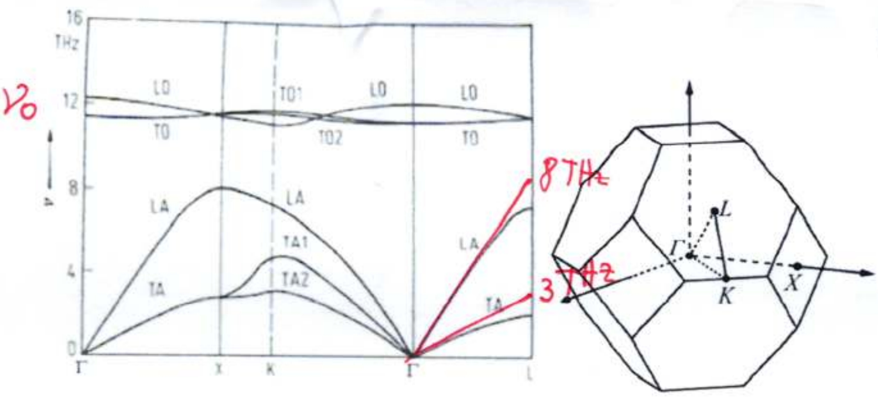
b) V smeri telesne diagonale kubične osnovne celice:

$$\vec{q} \parallel \overline{\Gamma L}$$

$$c = \frac{d\omega}{dq}\Big|_{\vec{q}\to\Gamma} \text{ vzdolž daljice } \Gamma L$$

veja LA: $$C_L \doteq \frac{2\pi \cdot 8\,THz}{\overline{\Gamma L}} = \frac{2\pi \cdot 8\,THz}{\frac{\sqrt{3}\pi}{2Å}} = 1800\,m/s$$

veja TA: $$C_T \doteq \frac{2\pi \cdot 3\,THz}{\overline{\Gamma L}} = \frac{2\pi \cdot 3\,THz}{\frac{\sqrt{3}\pi}{2Å}} = 700\,m/s$$



recipročna mreža: BCC z mrežno razdaljo $\frac{4\pi}{a}$

$$L = \frac{\pi}{a}(1,1,1)$$

$$\overline{\Gamma L} = \frac{\sqrt{3}\pi}{a}$$

c) $$\overline{N} = \frac{1}{e^{\beta\hbar\omega_0} - 1}$$

$$k_B T \doteq \frac{1}{40}\,eV$$

$$\hbar\omega_0 = \hbar\, 2\pi \nu_0 \qquad \nu_0 \doteq 12\,THz$$

$$\overline{N} \doteq 0.2$$