compito 20 dicembre 2019 - ESERCIZIO 2

1) $\vec v = \frac{1}{\hbar}\vec\nabla_{\vec k}\mathcal{E}$; seguendo il suggerimento al punto seguente, calcoliamo $\vec\nabla_{\vec k}\left[\mathcal{E}(\vec k)\left(1+\alpha\mathcal{E}(\vec k)\right)\right] = \vec\nabla_{\vec k}\left(\frac{\hbar^2 k^2}{2m^*}\right)$

che dà: $\vec\nabla_{\vec k}\mathcal{E}\left[1+2\alpha\mathcal{E}\right] = \frac{\hbar^2\vec k}{m^*}$ (eq 2)

Serve dunque esplicitare $\mathcal{E}(\vec k)$ dall'eq. (1):

$$\alpha\mathcal{E}^2+\mathcal{E}-\frac{\hbar^2k^2}{2m^*}=0 \Rightarrow \mathcal{E}_{1,2}(\vec k)=\frac{-1\pm\sqrt{1+2\alpha\frac{\hbar^2k^2}{m^*}}}{2\alpha}$$

Per identificare la soluzione che si riduce alla banda parabolica quando $\alpha\to0$, considero lo sviluppo di Taylor rispetto a α:

$$\mathcal{E}_{1,2}(\vec k)\simeq \frac{-1\pm\left(1+\frac{1}{2}2\alpha\frac{\hbar^2k^2}{m^*}\right)}{2\alpha} = \begin{cases} + & \frac{\hbar^2k^2}{2m^*} \Leftarrow \text{parabola} \\ - & -\frac{1}{\alpha}-\frac{\hbar^2k^2}{2m^*} \ (\text{divergente}) \end{cases}$$

Quindi va considerata la soluz. con "+".

Dall'eq. (2):

$$\boxed{\vec v} = \frac{1}{\hbar}\vec\nabla\mathcal{E} = \frac{\hbar^2\vec k}{\hbar m^*}\frac{1}{1+2\alpha\mathcal{E}_+(\vec k)} = \boxed{\frac{\hbar\vec k}{m^*}\frac{1}{\sqrt{1+2\alpha\frac{\hbar^2k^2}{m^*}}}}$$

2) $$\boxed{g(\mathcal{E})} = 2\oint_{\text{curva a }\mathcal{E}(\vec k)=\text{cost.}=\mathcal{E}}\frac{1}{4\pi^2}\frac{d\vec k}{|\vec\nabla\mathcal{E}|}$$
$d\vec k \to$ elemento di linea su un cerchio (perché $\mathcal{E}(\vec k)=\mathcal{E}(|\vec k|)$, quindi le sup. a energia costante sono cerchi)

$$= 2\oint\frac{1}{4\pi^2}\frac{\cancel{k}\,d\theta}{\underbrace{\frac{\hbar^2\cancel{k}}{m^*}\left[1+2\alpha\mathcal{E}\right]^{-1}}_{\text{dall'eq.(2)}}} = \boxed{\cancel{2}\cdot\cancel{2\pi}\cdot\frac{1}{\cancel{4}\pi^2}\frac{m^*\left[1+2\alpha\mathcal{E}\right]}{\hbar^2\cancel{\left[1+2\alpha\mathcal{E}\right]}}}\ , \ \mathcal{E}\geq0$$

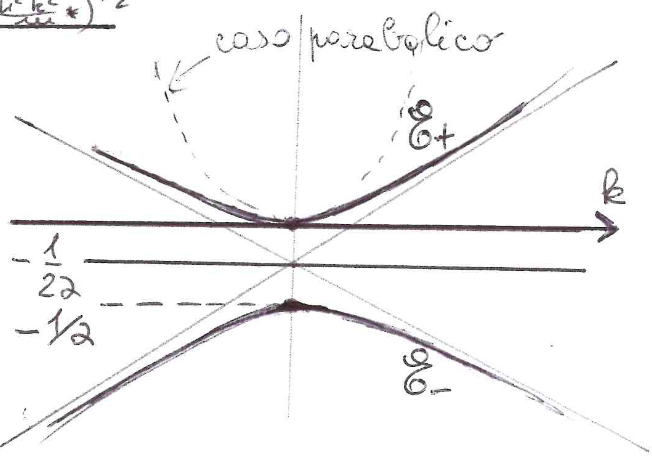
che si riduce a $g(\mathcal{E})=\frac{m^*}{\hbar^2\pi}$ per $\alpha\to0$ ($\mathcal{E}\geq0$)

3) grafico di $\mathcal{E}(\vec k)$: $\mathcal{E}(\vec k)=\frac{-1\pm\left(1+2\alpha\frac{\hbar^2k^2}{m^*}\right)^{1/2}}{2\alpha}$

Identifichiamo gli asintoti:

$$\mathcal{E}(|\vec k|)\underset{|\vec k|\to+\infty}{\sim}\underbrace{\frac{-1\pm\sqrt{2\alpha\hbar^2/m^*}\,k}{2\alpha}}_{\text{chiamo }\mathcal{E}_0(k)}$$

Ho: $\mathcal{E}_0(k=0)=-\frac{1}{2\alpha}$



Per $\alpha\to0$ la curva $\mathcal{E}(\vec k)$ da iperbole diventa parabola $\Rightarrow g(\mathcal{E})$ è diversa

$a = |\vec a_1| = |\vec a_2|$

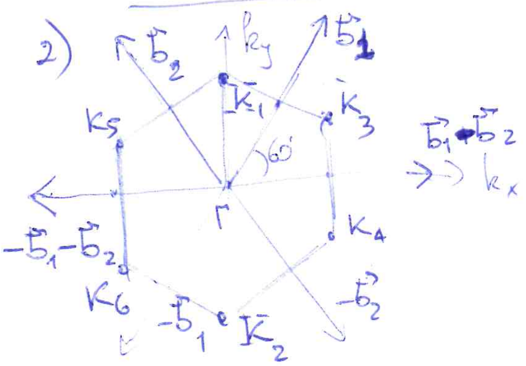
1) $\vec a_{1,2} = \left(\pm a\frac{\sqrt3}{2}, \frac{a}{2}\right)$ $\Rightarrow$

- $\vec b_1 \perp \vec a_2 \Rightarrow$ $\vec b_1$ inclinato di 60°: $\vec b_1 = b\left(\frac12, \frac{\sqrt3}{2}\right)$
- $\vec b_2 \perp \vec a_1 \Rightarrow$ $\vec b_2$ inclinato di 120°: $\vec b_2 = b\left(-\frac12, \frac{\sqrt3}{2}\right)$

$\vec b_1 \cdot \vec a_1 = 2\pi \Rightarrow a\frac{\sqrt3}{2} b \frac12 + \frac{a}{2}\frac{\sqrt3}{2} b = 2\pi \Rightarrow ab\frac{\sqrt3}{2} = 2\pi \Rightarrow b = \frac{4\pi}{\sqrt3}\frac1a$

$\Rightarrow \vec b_{1,2} = \left(\pm \frac{2\pi}{\sqrt3}\frac1a, \frac{2\pi}{a}\right)$ $\rightarrow b = |\vec b_{1,2}| = \frac{2\pi}{a}\left(\frac13 + 1\right)^{\frac12} = \frac{4\pi}{\sqrt3}\frac1a$

2)



$K_{1,2} = \left(0, \pm\frac{4\pi}{3}\frac1a\right)$

$K_{3,4,5,6} = \left(\frac{\vec b_1 - \vec b_2}{2}\right) = \left(\frac{b}{2}, \frac{\cancel{K} k_y}{2}\right) = \left(\frac{b}{2}, \frac{k_y}{2}\right)$

$= \left(\frac{2\pi}{\sqrt3 a}, \frac{2\pi}{3a}\right)$ $\pm, \pm$ tutte le 4 combinaz

$\frac{b_1}{2} = \frac{\sqrt3}{2}\overline{\Gamma K_1}$

3) $E(\vec K_{1,2}) = \pm\gamma\sqrt{1 + 4\underbrace{\cos\left(\frac{\sqrt3 a\cdot 0}{2}\right)}_{=1}\cos\left(\frac{4\pi}{3}\frac{a}{a}\frac12\right) + 4\cos^2\left(\frac{4\pi}{3a}\frac{a}{2}\right)}$

$= \pm\gamma\left(1 + 2\cos\left(\frac{2\pi \cancel{a}}{3\cancel{a}}\right)\right) = \pm\gamma\left(1 + 2\cdot\left(-\frac12\right)\right) = \boxed{0}$

$E(\vec K_{3,4,5,6}) = \pm\gamma\sqrt{1 + 4\underbrace{\cos\left(\frac{\sqrt3 \cancel{a}}{\cancel{2}}\frac{\cancel{2}\pi}{\cancel{\sqrt3 a}}\right)}_{=-1}\cos\left(\frac{2\pi \cancel{a}}{3\cancel{a}\cancel{2}}\right) + 4\cos^2\left(\frac{\pi}{3}\right)}$

$= \pm\gamma\sqrt{1 - 4\cos\frac{\pi}{3} + 4\cos^2\frac{\pi}{3}}$

$= \pm\gamma\left(1 - 2\cos\frac{\pi}{3}\right) = \pm\gamma\left(1 - \frac{2}{2}\right) = \boxed{0}$

$\mathcal{E}(\vec K_i) = 0$ e ~~l'energia è~~ simmetriche rispetto a $E=0$ (le bande sono

4) Per le simmetrie $\Rightarrow$ 1 e^- per atomo $\Rightarrow \boxed{E_F = 0}$

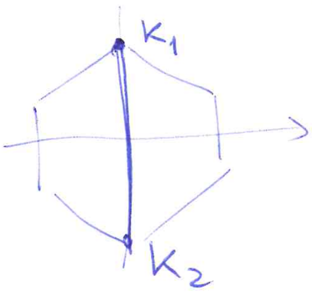
5) $k_x = 0 \Rightarrow$

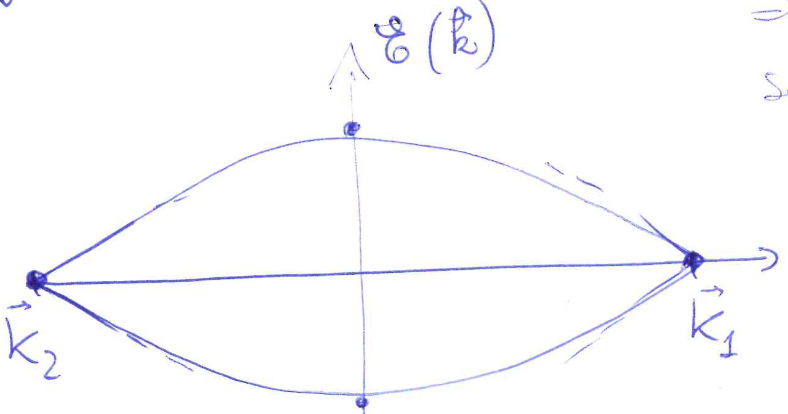
$$\mathcal{E}(0,k_y) = \pm\gamma\sqrt{1+4\cos\left(\frac{k_y a}{2}\right)+4\cos^2\left(\frac{k_y a}{2}\right)}$$

$$= \pm\gamma\left|1+2\cos\left(\frac{k_y a}{2}\right)\right| \longrightarrow \text{periodo } \frac{k_y a}{2} = 2\pi$$

$\Rightarrow k_y = \frac{4\pi}{a}$

Se vado da $-\frac{4\pi}{3a}$ a $+\frac{4\pi}{3a}$ NON FACCIO TUTTO IL PERIODO





$$\mathcal{E}\left(0,\pm\frac{4\pi}{3}\frac{1}{a}\right) = \pm\gamma\left|1+2\cos\frac{\cancel{4}^{2}\pi}{3}\frac{1}{\cancel{a}}\frac{\cancel{a}}{\cancel{2}}\right| = \pm\gamma\left(1+2\underbrace{\cos\frac{2\pi}{3}}_{=-\frac{1}{2}}\right) = 0$$

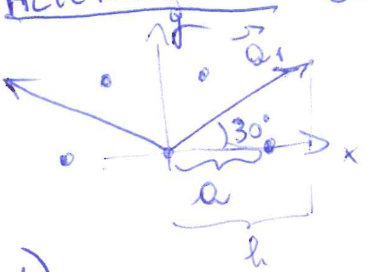
$$\mathcal{E}(0,0) = \pm\gamma\left|1+2\right| = \pm 3\gamma \quad \text{max! min}$$

$$\frac{\partial}{\partial k_y}\mathcal{E}(0,k_y) = \pm\gamma\, 2(-1)\frac{a}{\cancel{2}}\sin\frac{k_y a}{2} = \mp a\gamma\sin\frac{k_y a}{2}$$

$$\lim_{k_y\to\pm\frac{4\pi}{3}\frac{1}{a}}\frac{\partial}{\partial k_y}\mathcal{E}(0,k_y) = \mp a\gamma\sin\frac{\cancel{4}^{2}\pi}{3}\frac{1}{\cancel{a}}\frac{\cancel{a}}{\cancel{2}_{1}} = \mp a\gamma\frac{\sqrt{3}}{2} \neq 0$$

$\Rightarrow$ derivata $\neq 0 \Rightarrow$ comportam. lineare

ALTERNATIVA: chiamo "a" la dist NN



$$\begin{cases} \frac{3}{2} a = h \\ h = a_1 \frac{\sqrt{3}}{2} \end{cases} \Rightarrow \boxed{a_{1,2} = \frac{\cancel{2}}{\sqrt{3}} \frac{3}{\cancel{2}} a = \sqrt{3}\, a}$$

$$\boxed{\vec{a}_{1,2} = \left(\pm \frac{3}{2} a, \frac{\sqrt{3}}{2} a \right)}$$

1)

$$\vec{b}_{1,2} = b\left(\pm\frac{1}{2}, \frac{\sqrt{3}}{2}\right); \quad \vec{b}_1 \cdot \vec{a}_1 = 2\pi \Rightarrow \frac{3}{4} ab + \frac{3}{4} ab = 2\pi \Rightarrow ab = 2\pi \frac{2}{3} = \frac{4\pi}{3},$$

$$\Rightarrow b = \frac{4\pi}{3a} \Rightarrow \boxed{\vec{b}_{1,2} = \frac{2\pi}{3a}\left(\pm 1, \sqrt{3}\right)}$$

$$\vec{b}_1 \cdot \vec{a}_1 = \frac{\cancel{3}}{\cancel{2}} \cancel{a} \cdot \frac{\cancel{2}\pi}{\cancel{3a}} + \frac{\cancel{\sqrt{3}}}{\cancel{2}} \cancel{a} \frac{2\pi}{\cancel{3}} \frac{\cancel{\sqrt{3}}}{\cancel{a}} = 2\pi = \vec{b}_2 \cdot \vec{a}_2$$

$$\vec{b}_1 \cdot \vec{a}_2 = \vec{b}_2 \cdot \vec{a}_1 = 0$$

2) "vecchio a" $\rightarrow \overset{\text{più}}{\sqrt{3}\, a}$

quindi $K_{1,2} = \left(0, \pm \frac{4\pi}{3\sqrt{3}\, a}\right)$

$$k_{3,4,5,6} = \left(\pm\frac{2\pi}{3a}, \pm\frac{2\pi}{3\sqrt{3}\, a}\right)$$

Altri punti di conseguenze ...