T3 Graphène contraint

(1) $\gamma_k = \beta + e^{-i\vec{k}\vec{a_2}} + e^{-i\vec{k}\vec{a_3}}$

$$\hat{H}_k = \begin{pmatrix} 0 & -t_2\gamma_k^* \\ -t_2\gamma_k & 0 \end{pmatrix}$$

$E_\pm = \pm t_2 |\gamma_k|$

point de contact $\gamma_k = 0 \Rightarrow \begin{cases} \beta + \cos ka_2 + \cos ka_3 = 0 \\ \sin ka_2 + \sin ka_3 = 0 \end{cases}$

$$\boxed{\gamma_k = \beta + 2\cos\frac{\sqrt{3}}{2}k_x a \; e^{i\frac{3}{2}k_y a}}$$

$\gamma_k = 0$: $\sin\frac{3}{2}k_y a = 0$ $\quad \frac{3}{2}k_y a = 0, +\pi, -\pi$

- $k_y = 0$: $\cos\frac{\sqrt{3}}{2}k_x a = -\beta/2$

si $\beta \leq 2$: $k_x = \pm\frac{2}{\sqrt{3}}\frac{1}{a}\mathrm{Arcos}(-\beta/2)$

2 points de contact

si $\beta > 2$: pas de solution

- $k_y = \frac{\pm 2\pi}{3a}$

$\cos\frac{\sqrt{3}}{2}k_x a = +\beta/2$

$$k_x = \pm\frac{2}{\sqrt{3}a}\mathrm{Arcos}(+\beta/2)$$

4 points de contact

$\beta = 2$

$k_x = \pm\frac{2\pi}{\sqrt{3}a}$

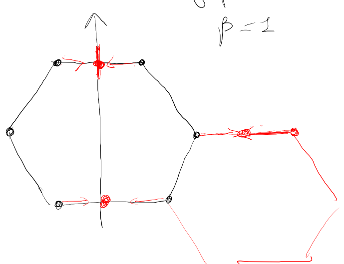
K, K'

distance $\frac{4\pi}{\sqrt{3}a} = 2\vec{a}_1^* + \vec{a}_2^*$

pour $\beta > 2$ pas de solution

Ouverture d'un gap

$\beta = 1$



Regardons la dispersion autour des points de contact pour $\beta = \beta_c$

$$\begin{cases} a_2 = \frac{\sqrt{3}}{2} a \left(u_x + \sqrt{3} u_y\right) \\ a_3 = \frac{\sqrt{3}}{2} a \left(-u_x + \sqrt{3} u_y\right) \end{cases}$$

K_c : $k_x = 0$ $\quad k_y = \frac{2\pi}{3a}$

$$\begin{cases} e^{i\vec{k_c}\vec{a_2}} = e^{i\pi} = -1 \\ e^{i\vec{k_c}\vec{a_3}} = -1 \end{cases}$$

$$\left.\vec{\nabla}_k \gamma_k\right)_{K_c} = -i\left(\vec{a_2} + \vec{a_3}\right) = -3ia\,\vec{u_y}$$

dispersion linéaire suivant (Oy)

Pour (Ox), il faut aller au deuxième ordre

$$\left.\frac{\partial^2 \gamma_{K_c+q}}{\partial q_x^2}\right)_{q=0} = \left(i a_{2x}\right)^2 e^{i(\vec{K}+\vec{q})\vec{a_2}} + \left(i a_{3x}\right)^2 e^{i(K+q)\vec{a_3}}$$

$$= \frac{3}{4} a^2 + \frac{3}{4} a^2 = \frac{3}{2} a^2$$

$$\Rightarrow \boxed{\gamma_{\vec{K_c}+q} = \underbrace{-\frac{3}{2} i a q_y}_{\text{linéaire}} + \underbrace{\frac{3}{4} a^2 q_x^2}_{\text{parabolique}}}$$

$$m^* = \frac{2}{3} \frac{\hbar^2}{a^2}$$

Particules semi-Dirac

$$\hat{H}_k = -t \begin{pmatrix} 0 & \gamma_k^* \\ \gamma_k & 0 \end{pmatrix}$$

$$|u_k\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \frac{\gamma_k}{|\gamma_k|} \end{pmatrix}$$

$$\hat{H}_k |u_k\rangle_- = -t |\gamma_k| \, |u_k\rangle_-$$

de m̂ $|u_k\rangle_+ = \frac{1}{\sqrt{2}} \begin{pmatrix} +1 \\ -\frac{\gamma_k}{|\gamma_k|} \end{pmatrix}$

$$\vec{\mathcal{A}}_k = i \langle u_k |_{\mp} \vec{\nabla}_k | u_k \rangle_{\mp}$$

$$= \frac{i}{2} \left(1 , \pm \frac{\gamma_k^*}{|\gamma_k|}\right) \begin{pmatrix} 0 \\ \pm \vec{\nabla}_k \frac{\gamma_k}{|\gamma_k|} \end{pmatrix}$$

$$\boxed{\vec{\mathcal{A}}_{\vec{k}} = \frac{i}{2} \frac{\gamma_k^*}{|\gamma_k|} \times \vec{\nabla} \frac{\gamma_k}{|\gamma_k|}}$$

$$\frac{\gamma_k}{|\gamma_k|} = e^{i\varphi_k} \qquad \vec{\nabla}_k \frac{\gamma_k}{|\gamma_k|} = i \vec{\nabla}_k \varphi_k \, e^{i\varphi_k}$$

$$\boxed{\vec{\mathcal{A}}_{\vec{k}} = -\frac{1}{2} \vec{\nabla}_k \varphi_k}$$

$$\oint \mathcal{A}_{\vec{k}} = -\frac{1}{2} 2\pi \underset{\text{winding}}{w} = -\pi w$$

Au voisinage d'un cône

$$\begin{cases} k_x = \frac{4\pi}{3\sqrt{3}\,a} \\ k_y = 0 \end{cases}$$

$$\vec{\nabla}_k \gamma_{\vec{K}+k}\Big|_{\vec{K}} = i\left(\vec{a_2} e^{i\vec{K}\vec{a_2}} + \vec{a_3} e^{i\vec{K}\vec{a_3}}\right)$$

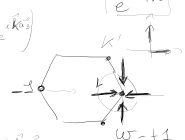
$$= \frac{3a}{2} \begin{bmatrix} -1 \\ -i \end{bmatrix}$$

$$\boxed{\gamma_{\vec{K}+\vec{k}} = -\frac{3a}{2} k_x - i \frac{3a}{2} k_y}$$

$$e^{i\vec{k}\vec{a_1}} \quad \mathcal{I} \quad i e^{i\vec{k}\vec{a_1}} \quad e^{i\vec{k}\vec{a_1}}$$

$$\vec{\nabla} \begin{vmatrix} \frac{\partial}{\partial k_x} (\ ) \\ \frac{\partial}{\partial k_y} (\ ) \end{vmatrix} = \begin{matrix} e^{i\vec{k}\vec{a_1}} \, i a_{1x} \, \cancel{e^{i\vec{k}\vec{a_1}}} \\ e^{i\vec{k}\vec{a_1}} \, i a_{1y} \end{matrix}$$

$$\boxed{e^{i\varphi_k}}$$



On écrit $\dfrac{\gamma_k}{|\gamma_k|} = e^{i\varphi_k}$

$$\vec{\nabla}_k \frac{\gamma_k}{|\gamma_k|} = i\,\vec{\nabla}_k \varphi_k \quad e^{i\varphi_k}$$

$$\frac{\gamma_k^*}{|\gamma_k|} = e^{-i\varphi_k} \Longrightarrow \boxed{\vec{A}^+(k) = -\frac{1}{2}\vec{\nabla}_k \varphi_k}$$

$$\oint \vec{A}^+ \, \vec{dk} = -\frac{2\pi}{2} \times \omega$$

$\llcorner$ winding

Calculons $\vec{\nabla}_k \gamma_k$ au voisinage du cône de Dirac $\left| \begin{array}{l} k_x = \dfrac{4\pi}{3\sqrt{3}\,a} \\ k_y = 0 \end{array} \right.$

$$\vec{\nabla}_k \gamma_{\vec{K}+k}\Big|_{k=0} = i\left(\vec{a}_2 e^{i\vec{K}\vec{a}_2} + \vec{a}_3 e^{i\vec{K}\vec{a}_3}\right)$$

$$= i \left| \begin{array}{l} \frac{\sqrt{3}}{2} a \, 2i \sin 2\pi/3 \\ 3/2 \, a \, 2 \cos 2\pi/3 \end{array} \right.$$

$$= \frac{3a}{2}\begin{bmatrix} -1 \\ -i \end{bmatrix}$$

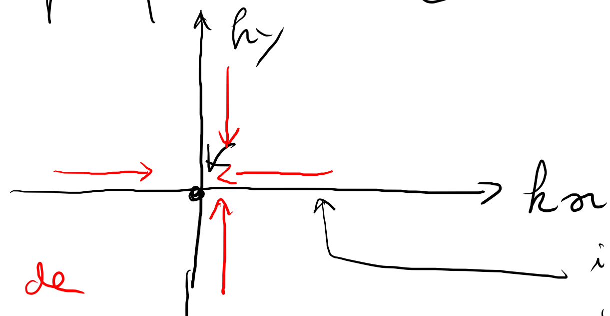
$$\Longrightarrow \boxed{\gamma_{\vec{K}+\vec{k}} = -3/a \, a \, k_x - i \frac{3a}{2} k_y}$$

$$\boxed{\gamma_{\vec{K}+\vec{h}} = -\frac{3}{a}\, a\, h_x - i\,\frac{3a}{2}\, h_y}$$

$$\frac{\gamma_{\vec{K}+\vec{h}}}{\left|\gamma_{\vec{K}+\vec{h}}\right|} = e^{i\varphi_k} = \cos\varphi_k + i\sin\varphi_k$$

On peut le représenter comme un vecteur

Représentons graphiquement $e^{i\varphi_k}$ autour du point K :

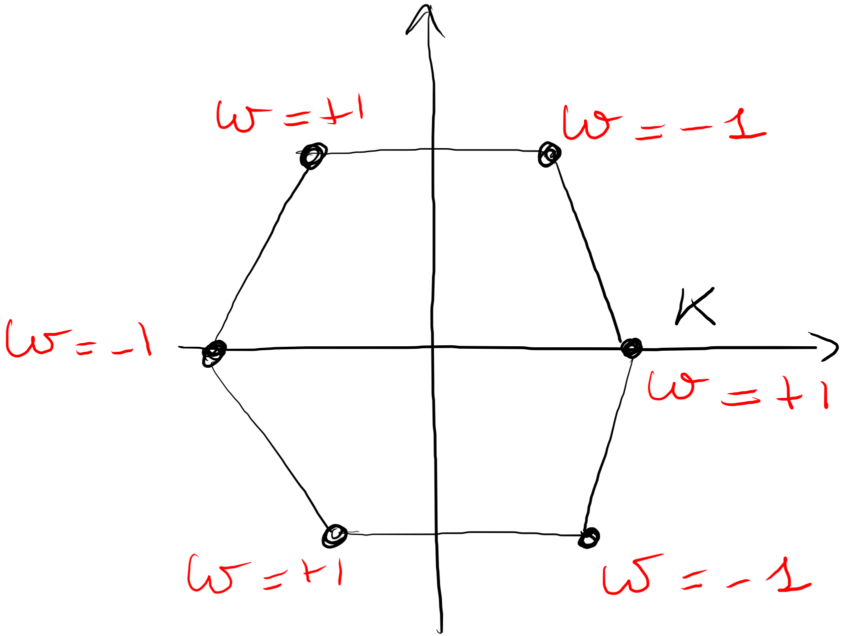


ici $h_y = 0$, $h_x > 0$

On trouve le résultat avec la formule de $\gamma_{\vec{K}+\vec{h}}$

Le vecteur tourne de $+2\pi$ autour de K

$\Longrightarrow w = +1$



Voir les planches du cours