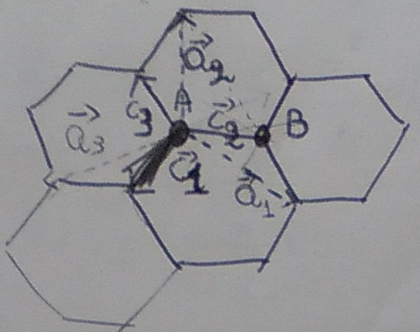
.BAND STRUCTURE

$|\vec{a}_i| = 2.46 \mathring{A} = a$

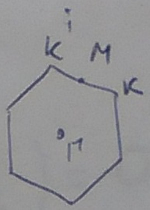
$|\vec{c}_i| = \frac{a}{\sqrt{3}}$

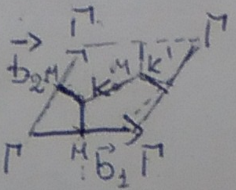


$\vec{b}_i \cdot \vec{a}_j = 2\pi\delta_{ij}$

$|b||a|\frac{\sqrt{3}}{2} = 2\pi$

$|b| = \frac{4}{\sqrt{3}}\frac{\pi}{a}$





$\vec{a}_3 = -(\vec{a}_2 + \vec{a}_1)$

$\underline{K} = \frac{\vec{b}_1}{3} + \frac{\vec{b}_2}{3}$

$\underline{K}' = 2\underline{K}$

$|\underline{K}| = \frac{b}{\sqrt{3}} = \frac{4}{3}\frac{\pi}{a}$

$\underline{K} = \frac{4\pi}{3a^2}(-\vec{a}_3) = (\vec{c}_2 - \vec{c}_1)\frac{4\pi}{3a^2}$

CELL COORDINATES

COORDINATE $R = i_1 a_1 + i_2 a_2$

ATOM COORDINATES $\vec{R} + \vec{\tau}_\alpha \quad \alpha = A, B$

p_z ORBITAL AT $\vec{R} + \vec{\tau}_\alpha$

BLOCH STATE BASIS $|\vec{k}, \alpha\rangle = \sum_{\vec{R}} \frac{1}{\sqrt{N}} e^{i\vec{k}\cdot(\vec{R}+\vec{\tau}_\alpha)} |\vec{R}+\vec{\tau}_\alpha\rangle$

TB HAMILTONIAN $\langle \vec{R}' + \vec{\tau}_{\alpha'} | H | \vec{R} + \vec{\tau}_\alpha \rangle = / \; -t \simeq 3\,eV$ IF $\vec{R} + \vec{\tau}_\alpha$ NN OF $\vec{R}' + \vec{\tau}_{\alpha'}$

$\langle \vec{k}, \alpha | H | \vec{k}', \alpha' \rangle = \delta_{\vec{k},\vec{k}'} H(\vec{k})_{\alpha\alpha'}$

$$H(\vec{k}) = \begin{array}{cc} B & A \\ \end{array} \begin{pmatrix} 0 & f(\vec{k}) \\ f^*(\vec{k}) & 0 \end{pmatrix} \begin{array}{c} B \\ A \end{array} \quad f(\vec{k}) = -t \sum_{i=1}^{3} e^{i\vec{k}\cdot\vec{c}_i}$$

• NOTE THE CONVENTION

$\boxed{H_{\underline{AB}}(\vec{k}) = f(\vec{k})}$

$\mathcal{E}_\pm(\vec{k}) = \pm|f(\vec{k})|$

$a_\pm(\vec{k}) = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ \pm\phi(\vec{k}) \end{pmatrix} \qquad \phi(\vec{k}) = \frac{f^*(\vec{k})}{|f(\vec{k})|}$

$$\|f(\vec{k})\|^2 = t^2\{3 + 2\,\mathrm{Re}[e^{i\vec{k}\cdot\overbrace{(\vec{c}_2 - \vec{c}_3)}^{\vec{a}_1}}] + 2\,\mathrm{Re}[e^{i\vec{k}\cdot\overbrace{(\vec{c}_3 - \vec{c}_1)}^{\vec{a}_2}}] + 2\,\mathrm{Re}[e^{i\vec{k}\cdot\overbrace{(\vec{c}_1 - \vec{c}_2)}^{\vec{a}_3}}]\}$$

$$t^2\{3 + \sum_i 2\,\mathrm{Re}[e^{i\vec{k}\cdot\vec{a}_i}]\} = t^2\{3 + \sum_{i=1}^{3} 2\cos(\vec{k}\cdot\vec{a}_i)\} \qquad \|f(\underline{K})\|^2 = 0$$

$$\underline{K} = \frac{4}{3}\frac{\pi}{a^2}\left(\vec{c}_2 - \vec{c}_1\right)$$

$$\underline{K}\cdot\vec{c}_1 = \frac{4}{3}\frac{\pi}{a^2}\frac{a^2}{3}\cdot\left(-\frac{1}{2}-1\right) = -\frac{2}{3}\pi$$

$$\underline{K}\cdot\vec{c}_2 = +\frac{2\pi}{3}$$

$$\underline{K}\cdot\vec{c}_3 = \frac{4}{3}\frac{\pi}{a^2}\frac{a^2}{3}\left(-\frac{1}{2}+\frac{1}{2}\right) = 0$$

$$f(\underline{K}) = 0$$

$$f(\underline{K}+\vec{q}) \simeq 0 + \vec{q}\,\nabla_K f(\underline{K}) = -t\,\vec{q}\cdot\left(\vec{c}_1 e^{-i\frac{2\pi}{3}} + \vec{c}_2 e^{+\frac{2}{3}\pi} + \vec{c}_3\right)$$

$$= -t\vec{q}\left[\vec{c}_1\left(-\frac{1}{2}-\frac{\sqrt{3}}{2}i\right) + \vec{c}_2\left(-\frac{1}{2}+\frac{\sqrt{3}}{2}i\right) + \vec{c}_3\right]$$

$$= -t\vec{q}\Big[\underbrace{\vec{c}_3 - \frac{\vec{c}_1}{2} - \frac{\vec{c}_2}{2}}_{\frac{3}{2}\vec{c}_3}\Big] - ti\vec{q}\left[\frac{\sqrt{3}}{2}\underbrace{(c_2 - c_1)}_{-a_3}\right]$$

$$= -t\vec{q}\cdot\left(\frac{3}{2}\vec{c}_3 - i\frac{\sqrt{3}}{2}\vec{a}_3\right) \qquad -\vec{c}_3 = \frac{a}{\sqrt{3}}\hat{x}$$

$$-\vec{a}_3 = a\hat{y}$$

$$= +\frac{\sqrt{3}}{2}at(q_x - iq_y) = +\hbar v_F(q_x - iq_y)$$

$$\hbar v_F = \frac{\sqrt{3}}{2}\,2.46\,\text{Å}\;3\,\text{eV} = 6.4\,\text{eVÅ} \qquad v_F = 10^6\,\text{m/s}$$

$$H(\vec{q}) = \hbar v_F \begin{pmatrix} 0 & q_x - iq_y \\ q_x + iq_y & 0 \end{pmatrix} = v_F \vec{\sigma} \cdot \vec{p}$$

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad \vec{p} = \hbar \vec{q}$$

AT K' $H(\vec{q}) = -v_F \vec{\sigma}^* \cdot \vec{p}$

DIRAC HAMILTONIAN FOR RELATIVISTIC PARTICLES

4×4 MATRIX $\mathbb{1} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$

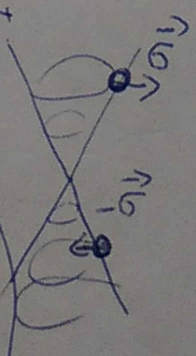
$$H_D = \begin{pmatrix} mc^2 \mathbb{1} & c\vec{\sigma} \cdot \vec{p} \\ c\vec{\sigma} \cdot \vec{p} & -mc^2 \mathbb{1} \end{pmatrix} \qquad c = 300\ 10^6 m/s$$

$m = 0$ BY A BASE ROTATION

$$H_D' = \begin{pmatrix} c\vec{\sigma} \cdot \vec{p} & 0 \\ 0 & -c\vec{\sigma} \cdot \vec{p} \end{pmatrix} \rightarrow \text{LIKE GRAPHENE AT } \vec{K} \text{ AND } \underline{K}'$$

$$\varepsilon_{\vec{q}\pm} = \pm \hbar v_F |\vec{q}|$$

$$a_\pm(\vec{q}) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \pm \frac{q_x + iq_y}{\sqrt{q_x^2 + q_y^2}} \end{pmatrix}$$



Electron AT $\vec{q}$
EIGENVECTOR OF
$\vec{\sigma} \cdot \vec{q}$
SPEUDOSPIN IN THE
DIRECTION OF $\vec{q}$