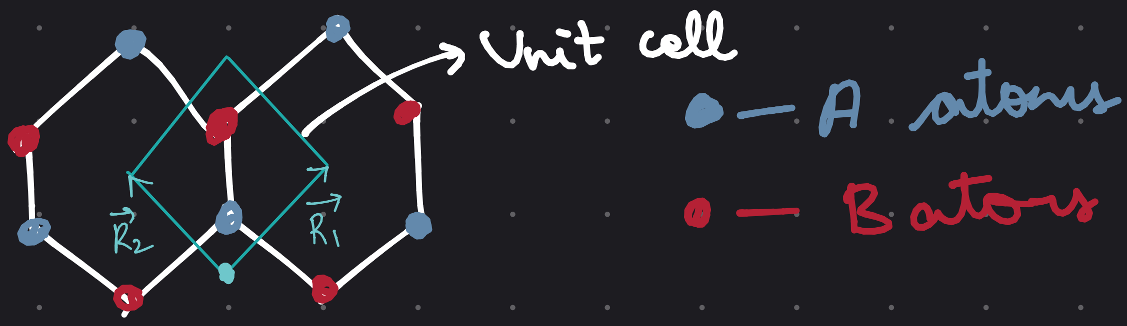
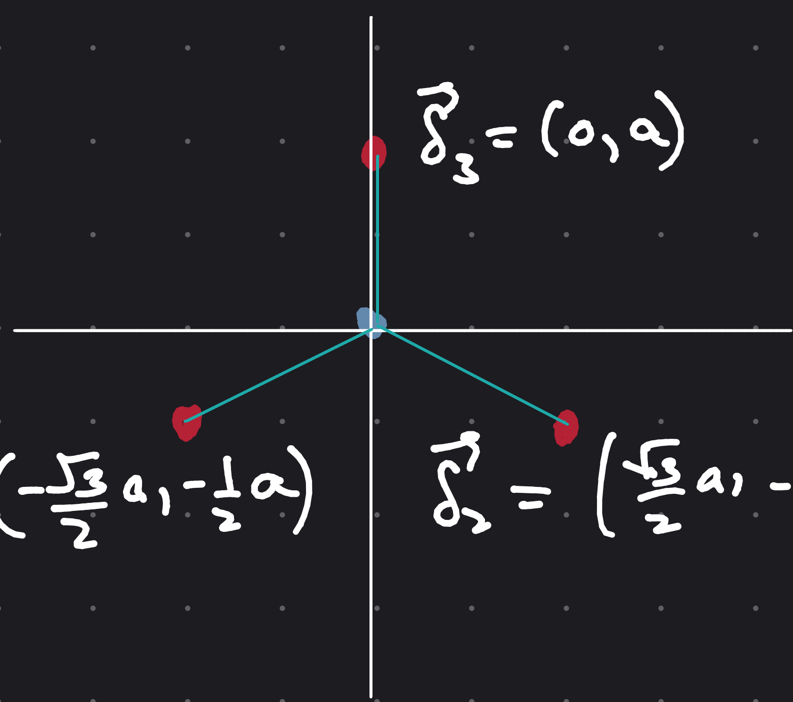
SECTION 1

Graphene Hamiltonian

Graphene hamiltonian



Looking at A atoms, we see that it is coupled to 3 B atoms.



$\vec{\delta}_3 = (0, a)$

$\vec{\delta}_1 = \left(-\frac{\sqrt{3}}{2}a, -\frac{1}{2}a\right)$ $\quad$ $\vec{\delta}_2 = \left(\frac{\sqrt{3}}{2}a, -\frac{1}{2}a\right)$

In case of graphene, $a = 1.42\,\text{Å}$. The primitive lattice vectors are $\vec{a}_{1,2} = \pm\left(\frac{\sqrt{3}}{2}a, \frac{3a}{2}\right)$

The tight-binding hamiltonian is given by:

$$H_g = -\gamma_0 \sum_{\vec{R}} \hat{\psi}_A^{\dagger}(\vec{R}) \left[\hat{\psi}_B(\vec{R}+\vec{\delta}_1) + \psi_B(\vec{R}+\vec{\delta}_2)\right] + h.c$$

Fourier transforming

$$\hat{c}_{A,\vec{k}} = \frac{1}{\sqrt{N}} \sum_{\vec{R}} e^{i\vec{k}\cdot\vec{R}} \hat{\psi}_A(\vec{R})$$

$$\hat{c}_{B,\vec{k}} = \frac{1}{\sqrt{N}} \sum_{\vec{R}} e^{i\vec{k}\cdot\vec{R}} \hat{\psi}_A(\vec{R})$$

The hamiltonian becomes:

$$\hat{H}_g = -\frac{\gamma_0}{N}\sum_{\vec{R}} e^{i\vec{k}\cdot\vec{R}}\, \hat{c}^{\dagger}_{A,\vec{k}} \left(e^{-i\vec{k}\cdot(\vec{R}+\vec{\delta}_1)}\hat{c}_{B,\vec{k}} + e^{-i\vec{k}\cdot(\vec{R}+\vec{\delta}_2)}\hat{c}_{B,\vec{k}} + e^{-i\vec{k}\cdot(\vec{R}+\vec{\delta}_3)}\hat{c}_{B,\vec{k}}\right) + h.c.$$

$$= -\gamma_0 \sum_{\vec{k}} \hat{c}^{\dagger}_{A,\vec{k}}\hat{c}_{B,\vec{k}}\left(e^{-i\vec{k}\cdot\vec{\delta}_1} + e^{-i\vec{k}\cdot\vec{\delta}_2} + e^{-i\vec{k}\cdot\vec{\delta}_3}\right) + h.c$$

$$= \sum_{\vec{k}} \hat{\Psi}^{\dagger}_{\vec{k}} \begin{bmatrix} 0 & -\gamma_0\gamma_{\vec{k}} \\ -\gamma_0\gamma^{*}_{\vec{k}} & 0 \end{bmatrix} \hat{\Psi}_{\vec{k}}$$

$$|\vec{\gamma}_k| = \left|2\cos k_x\frac{\sqrt{3}a}{2}\, e^{+ik_y\frac{a}{2}} + e^{-ik_y a}\right|$$

$$= \left|2\cos k_x\frac{\sqrt{3}a}{2}\, e^{ik\frac{3a}{2}} + 1\right|$$

$$= \sqrt{\left(1+2\cos k_x\frac{\sqrt{3}a}{2}\cos k_y\frac{3a}{2}\right)^2 + \left(2\cos k_x\frac{\sqrt{3}a}{2}\sin k_y\frac{3a}{2}\right)^2}$$

$$|\gamma_k| = \sqrt{1 + 4\cos^2 k_x\frac{\sqrt{3}a}{2} + 4\cos k_x\frac{\sqrt{3}a}{2}\cos k_y\frac{3a}{2}}$$

$$\Rightarrow \varepsilon_{\pm}(\vec{k}) = \pm\gamma_0|\gamma_k| = \pm\gamma_0\sqrt{3+2\cos(k_x\sqrt{3}a) + 4\cos\left(\frac{k_x\sqrt{3}a}{2}\right)\cos\left(\frac{3k_y a}{2}\right)}$$

Reciprocal lattice vectors:

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

$$\vec{b}_1 = 2\pi\left(\frac{\vec{a}_2\times\hat{z}}{(\vec{a}_1\times\vec{a}_2)\cdot\hat{z}}\right) = \frac{2\pi}{a}\left[\frac{-\frac{\sqrt{3}}{2}\hat{y} + \frac{3}{2}\hat{x}}{3/2}\right]$$

$$\vec{b}_2 = -2\pi\,\frac{\vec{a}_1\times\hat{z}}{(\vec{a}_1\times\vec{a}_2)\cdot\hat{z}} = \frac{2\pi}{a}\left(\frac{\hat{x}}{\sqrt{3}} + \frac{\hat{y}}{3}\right)$$

The dirac points are points at which

$$\varepsilon_+(\vec{k}) = \varepsilon_-(\vec{k}),$$

$$\vec{K}_1 = \frac{2\pi}{a}\left(\frac{\hat{x}}{3\sqrt{3}} + \frac{\hat{y}}{3}\right) \quad \vec{K}_2 = \frac{-2\pi}{a}\frac{2}{3\sqrt{3}}\hat{x} \quad \vec{K}_3 = \frac{2\pi}{a}\left(\frac{\hat{x}}{3\sqrt{3}} - \frac{\hat{y}}{3}\right)$$

$$\vec{K}_1' = \frac{2\pi}{a}\left(\frac{-\hat{x}}{3\sqrt{3}} + \frac{\hat{y}}{3}\right) \quad \vec{K}_2' = \frac{2\pi}{a}\frac{2}{3\sqrt{3}}\hat{x} \quad \vec{K}_3' = \frac{2\pi}{a}\left(\frac{-\hat{x}}{3\sqrt{3}} - \frac{\hat{y}}{3}\right)$$

However, the other dirac point just differ by a reciprocal lattice vector.

The $\gamma_{\vec{k}}$ at the dirac points is given by:

$$\gamma_{\vec{k}} = \sum_j e^{-i\vec{k}\cdot\vec{\delta}_j} = e^{-ik_y\frac{a}{2}} \cdot 2\cos\left(k_x\frac{\sqrt{3}a}{2}\right) + e^{-ik_y a}$$

$$\gamma_{\vec{k}} = 0$$

$$\Rightarrow \quad \cos\left(k_x\frac{\sqrt{3}a}{2}\right) = -\frac{1}{2}e^{-i\frac{3k_y a}{2}}$$

(i) $k_y = 0$ $\qquad k_x = \pm\frac{4\pi}{3\sqrt{3}a}$

(ii) $k_y = \pm\frac{2\pi}{3a}$ $\Rightarrow \cos\left(k_x\frac{\sqrt{3}a}{2}\right) = \frac{1}{2} \Rightarrow k_x = \pm\frac{2\pi}{3\sqrt{3}a}$

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

Linearize around $\vec{K}, \vec{K}'$ dirac points:

$$H = -\gamma_0 \sum_{\vec{k}} \begin{pmatrix} 0 & \gamma_{\vec{k}} \\ \gamma^*_{\vec{k}} & \end{pmatrix}$$

$$\gamma_{\vec k} = \sum_{j=1}^{3} e^{i\vec k\cdot\vec\delta_j}$$

to linearize $\gamma_{\vec k+\vec p} = \sum_{j=1}^{3} e^{i(\vec k+\vec p)\cdot\vec\delta_j}$ around the dirac point, $\vec K, \vec K'$

Choose $\vec k = \vec K_2$.

$$\gamma_{\vec K+\vec p} = \sum_{j=1}^{3} e^{-i(\vec K+\vec p)\cdot\vec\delta_j} = \sum_{j=1}^{3} e^{-i\vec K\cdot\vec\delta_j}\left(1 - i\vec p\cdot\vec\delta_j - i\vec p\cdot\vec\delta_j\right)$$

$$\vec K\cdot\vec\delta_1 = -\frac{2\pi}{3}, \quad \vec K\cdot\vec\delta_2 = \frac{2\pi}{3}, \quad \vec K\cdot\vec\delta_3 = 0$$

$$\gamma_{\vec K\cdot\vec p} = -i\left[e^{-i\vec K\cdot\vec\delta_1}(\vec p\cdot\vec\delta_1) + e^{-i\vec K\cdot\vec\delta_2}(\vec p\cdot\vec\delta_2) + e^{-i\vec K\cdot\vec\delta_3}(\vec p\cdot\vec\delta_3)\right]$$

$$= -p_x\frac{3}{2}a + i p_y\frac{a}{2} + i p_y\frac{a}{2}$$

$$= -\frac{3}{2}a(p_x - ip_y)$$