Graphene

Graphene is a 2D sheet of carbon atoms in a honeycomb arrangement. We shall study its band structure using the tight binding model.

Representation

Unfortunately, the honeycomb lattice is not a Bravais lattice. We have to represent it with a Bravais lattice decorated with basis (two atoms per cell).

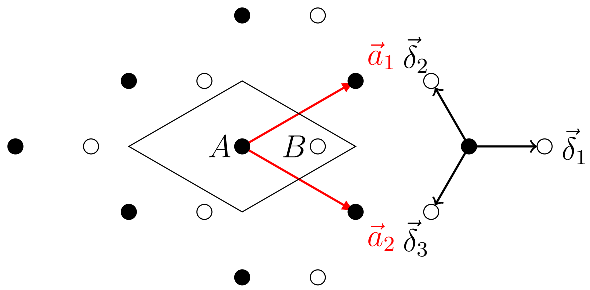

Figure 1: **Bravais lattice** with two atoms (A and B) per unit cell. The Wigner-Seitz cell is shown. The basis are $\vec{0}$ and $\vec{\delta}_1$.

Suppose the distance between neighboring atoms is a, then the basis vectors for the Bravais and Reciprocal lattices are

$$\begin{cases} \vec{a}_1 = \frac{\sqrt{3}a}{2}(\sqrt{3}\hat{x} + 1\hat{y}) \\ \vec{a}_2 = \frac{\sqrt{3}a}{2}(\sqrt{3}\hat{x} - 1\hat{y}) \end{cases} \Rightarrow \begin{cases} \vec{b}_1 = \frac{2\pi}{3a}(\hat{x} + \sqrt{3}\hat{y}) \\ \vec{b}_2 = \frac{2\pi}{3a}(\hat{x} - \sqrt{3}\hat{y}) \end{cases} \tag{1}$$

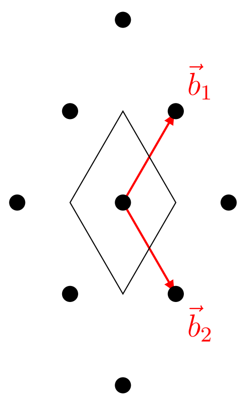

Figure 2: **Reciprocal Lattice** and the first Brillouin zone

Tight Binding

Consider one valance orbital per atom and label the orbital of atom A at $\vec{r}$ as $|\vec{r}, A\rangle$ and the orbital of atom B at $\vec{r}$ as $|\vec{r}, B\rangle$. Suppose electrons can only tunnel between its nearest neighbors with tunneling coefficient t. The tight binding Hamiltonian is then

$$H = -t \sum_{\vec{R}} \left(\left|\vec{R}, A\right\rangle \left\langle \vec{R} + \vec{\delta}_1, B\right| + \left|\vec{R}, A\right\rangle \left\langle \vec{R} + \vec{\delta}_2, B\right| + \left|\vec{R}, A\right\rangle \left\langle \vec{R} + \vec{\delta}_3, B\right| \right) \tag{2}$$

Expanding the orbitals in plane wave basis

$$\begin{cases} |\vec{r}, A\rangle = \frac{1}{\sqrt{N}} \sum\limits_{\vec{k}} e^{-i\vec{k}\cdot\vec{r}} \left|\vec{k}, A\right\rangle \\ |\vec{r}, B\rangle = \frac{1}{\sqrt{N}} \sum\limits_{\vec{k}} e^{-i\vec{k}\cdot\vec{r}} \left|\vec{k}, B\right\rangle \end{cases} \tag{3}$$

And the Hamiltonian becomes (recall $\sum_{\vec{R}} e^{i(\vec{k}-\vec{k}')\cdot\vec{R}} = \delta_{\vec{k},\vec{k}'}$)

$$H = -t \sum_{\vec{k}} \sum_{j=1}^{3} \left(e^{-i\vec{k}\cdot\vec{\delta}_j} \left|\vec{k}, A\right\rangle \left\langle \vec{k}, B\right| + e^{i\vec{k}\cdot\vec{\delta}_j} \left|\vec{k}, B\right\rangle \left\langle \vec{k}, A\right| \right) \tag{4}$$

For a given $\vec{k}$, the Hamiltonian in matrix form

$$H = \begin{pmatrix} 0 & -t \sum\limits_{i=1}^{3} e^{-i\vec{k}\cdot\vec{\delta}_i} \\ -t \sum\limits_{i=1}^{3} e^{i\vec{k}\cdot\vec{\delta}_i} & 0 \end{pmatrix} \tag{5}$$

This becomes a *Bloch Hamiltonian* ($H(\vec{k}+\vec{G}) = H(\vec{k})$) if we make the immaterial change of basis $\left|\vec{k}, B\right\rangle \to e^{i\vec{k}\cdot\vec{\delta}_1} \left|\vec{k}, B\right\rangle$

$$H = \begin{pmatrix} 0 & -t(1 + e^{i\vec{k}\cdot\vec{a}_1} + e^{i\vec{k}\cdot\vec{a}_2}) \\ -t(1 + e^{-i\vec{k}\cdot\vec{a}_1} + e^{-i\vec{k}\cdot\vec{a}_2}) & 0 \end{pmatrix} \tag{6}$$

When $\vec{k}$ is at a *K-point* $\vec{K}_\pm = \frac{2\pi}{3a}(\hat{x} \pm \frac{1}{\sqrt{3}}\hat{y})$

$$H(\vec{K}_\pm) = \begin{pmatrix} 0 & -t(1 + e^{i\frac{2\pi}{3}} + e^{i\frac{4\pi}{3}}) \\ -t(1 + e^{-i\frac{2\pi}{3}} + e^{-i\frac{4\pi}{3}}) & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} \tag{7}$$

Near the K-points $\vec{k} = \vec{K}_\pm + \delta\vec{k}$

$$H(\vec{K}_\pm + \delta\vec{k}) = \frac{3at}{2} \begin{pmatrix} 0 & \delta k_x - i\delta k_y \\ \delta k_x + i\delta k_y & 0 \end{pmatrix} + O(\delta k^2) \tag{8}$$

Dirac Equation

Written in terms of the Pauli matrices

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{9}$$

the tight binding Hamiltonian becomes

$$H = \frac{3at}{2}(\delta k_x \sigma_x + \delta k_y \sigma_y) \tag{10}$$

when compared with the Hamiltonian governing 2D Dirac Fermions with momentum $\delta\vec{k}$ and mass m

$$H_{DF} = \hbar c \delta k_x \sigma_x + \hbar c \delta k_y \sigma_y + mc^2 \sigma_z \tag{11}$$

We see that electrons occupying states near the K-points behave like 2D Dirac Fermions with zero mass and conjugated light speed!

$$v_F = |\frac{1}{\hbar}\frac{\partial E}{\partial \vec{k}}| = \frac{3at}{2\hbar} \tag{12}$$