The Dirac Hamiltonian

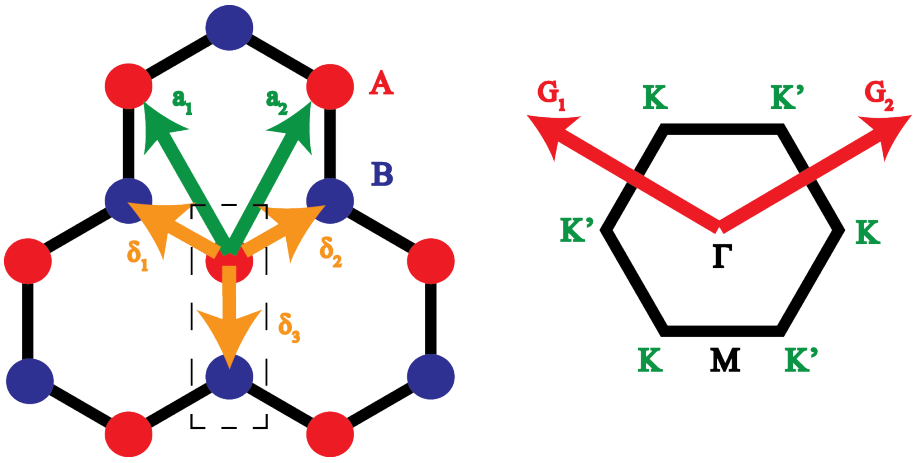

Figure 1: Honeycomb Lattice and Brillouin Zone

I now present the low energy effective theory of electrons on a honeycomb lattice. Suppose we had a honeycomb made of two interpenetrating triangular sublattices, hereby denoted as the A and B sublattices (see Fig. 1). Each triangular sublattice can be constructed by the primitive lattice vectors

$$\mathbf{a}_1 = a\left(-\frac{\sqrt{3}}{2}, \frac{3}{2}\right), \ \mathbf{a}_2 = a\left(\frac{\sqrt{3}}{2}, \frac{3}{2}\right) \tag{1}$$

where a is the distance between a point on the A sublattice (call it the origin) and its nearest neighbors on the B sublattice. The nearest neighbors are

$$\boldsymbol{\delta}_1 = a\left(-\frac{\sqrt{3}}{2}, \frac{1}{2}\right), \ \boldsymbol{\delta}_2 = a\left(\frac{\sqrt{3}}{2}, \frac{1}{2}\right), \ \boldsymbol{\delta}_3 = a\,(0, -1) \tag{2}$$

I define a unit cell to encompass a point on A and its nearest neighbor on B at $\boldsymbol{\delta}_3$.
The reciprocal lattice vectors are

$$\mathbf{G}_1 = \frac{2\pi}{a}\left(-\frac{1}{\sqrt{3}}, \frac{1}{3}\right), \ \mathbf{G}_2 = \frac{2\pi}{a}\left(\frac{1}{\sqrt{3}}, \frac{1}{3}\right) \tag{3}$$

The Brillouin Zone for a triangular lattice is a hexagon with high symmetry points K and K' on its corners:

$$\mathbf{K} = \frac{2\pi}{a}\left(\frac{2}{3\sqrt{3}}, 0\right), \ \mathbf{K}' = \frac{2\pi}{a}\left(-\frac{2}{3\sqrt{3}}, 0\right) \tag{4}$$

Lets now consider a tight binding model with nearest neighbor hopping amplitude t

$$H = U\sum_i a_i^\dagger a_i - U\sum_j b_j^\dagger b_j - t\sum_{\langle i,j\rangle}\left(a_i^\dagger b_j + \text{h.c.}\right) \tag{5}$$

where $a_i^\dagger$ and a_i are the creation and annihilation operators for site i on sublattice A (and similarly, $b_j^\dagger$ and b_j are for B). U is half the energy difference between an electron sitting on sublattice B as opposed to A. I've neglected spin and hopping further than nearest neighbor. I've also assumed points on the A and B sublattice have no internal structure. Applying this Hamiltonian to the state $|A, \mathbf{r}\rangle$ in which a single electron inhabits a point on sublattice A in the unit cell at $\mathbf{r}$:

$$H|A, \mathbf{r}\rangle = U|A, \mathbf{r}\rangle - t\left(|B, \mathbf{r} + \mathbf{a}_1\rangle + |B, \mathbf{r} + \mathbf{a}_2\rangle + |B, \mathbf{r}\rangle\right) \tag{6}$$

And similarly for $|B, \mathbf{r}\rangle$ in which a single electron inhabits the point on sublattice B in the unit cell at $\mathbf{r}$:

$$H|B, \mathbf{r}\rangle = -U|B, \mathbf{r}\rangle - t\left(|A, \mathbf{r} - \mathbf{a}_1\rangle + |A, \mathbf{r} - \mathbf{a}_2\rangle + |A, \mathbf{r}\rangle\right) \tag{7}$$

Define Bloch states

$$|A, \mathbf{k}\rangle = \sum_{\mathbf{r}} e^{i\mathbf{k}\cdot\mathbf{r}}|A, \mathbf{r}\rangle \tag{8}$$

$$|B, \mathbf{k}\rangle = \sum_{\mathbf{r}} e^{i\mathbf{k}\cdot\mathbf{r}}|B, \mathbf{r}\rangle \tag{9}$$

where the sum is taken over unit cells indexed by their positions $\mathbf{r}$. Applying the Hamiltonian on these Bloch states,

$$\begin{aligned} H|A, \mathbf{k}\rangle &= U|A, \mathbf{k}\rangle - t\sum_{\mathbf{r}} e^{i\mathbf{k}\cdot\mathbf{r}}\left(|B, \mathbf{r} + \mathbf{a}_1\rangle + |B, \mathbf{r} + \mathbf{a}_2\rangle + |B, \mathbf{r}\rangle\right) \\ &= U|A, \mathbf{k}\rangle - t\left(e^{-i\mathbf{k}\cdot\mathbf{a}_1} + e^{-i\mathbf{k}\cdot\mathbf{a}_2} + 1\right)|B, \mathbf{k}\rangle \qquad (10) \\ H|B, \mathbf{k}\rangle &= -U|B, \mathbf{k}\rangle - t\left(e^{i\mathbf{k}\cdot\mathbf{a}_1} + e^{i\mathbf{k}\cdot\mathbf{a}_2} + 1\right)|A, \mathbf{k}\rangle \qquad (11) \end{aligned}$$

Clearly, the Hamiltonian for each $\mathbf{k}$ subspace can be represented by the matrix

$$H(\mathbf{k}) = -t\begin{pmatrix} U & e^{-i\mathbf{k}\cdot\mathbf{a}_1} + e^{-i\mathbf{k}\cdot\mathbf{a}_2} + 1 \\ e^{i\mathbf{k}\cdot\mathbf{a}_1} + e^{i\mathbf{k}\cdot\mathbf{a}_2} + 1 & -U \end{pmatrix} \tag{12}$$

We can rewrite the Hamiltonian in terms of the Pauli matrices σ_x, σ_y, and σ_z if I define

$$\begin{aligned} X(\mathbf{k}) &= -t\left[1 + \cos\left(\frac{\sqrt{3}}{2}k_x a - \frac{3}{2}k_y a\right) + \cos\left(-\frac{\sqrt{3}}{2}k_x a - \frac{3}{2}k_y a\right)\right] \qquad (13) \\ Y(\mathbf{k}) &= t\left[\sin\left(\frac{\sqrt{3}}{2}k_x a - \frac{3}{2}k_y a\right) + \sin\left(-\frac{\sqrt{3}}{2}k_x a - \frac{3}{2}k_y a\right)\right] \qquad (14) \end{aligned}$$

so that $H(\mathbf{k}) = X(\mathbf{k})\sigma_x + Y(\mathbf{k})\sigma_y + U\sigma_z$. At this point, we can calculate the energy $E(\mathbf{k}) = \sqrt{X(\mathbf{k})^2 + Y(\mathbf{k})^2 + U^2}$ for all $\mathbf{k}$ in the Brillouin Zone. However, for reasons that

will become clear, lets expand $X(\mathbf{k})$ and $Y(\mathbf{k})$ around the K point (i.e., let $\mathbf{k} = \mathbf{K} + \mathbf{q}$):

$$\begin{aligned} X(\mathbf{k}) &= -t\left[1 + \cos\left(\frac{2\pi}{3} + \frac{\sqrt{3}}{2}q_x a - \frac{3}{2}q_y a\right) + \cos\left(-\frac{2\pi}{3} - \frac{\sqrt{3}}{2}q_x a - \frac{3}{2}q_y a\right)\right] \\ &\approx -t\left[-\frac{\sqrt{3}}{2}\left(\frac{\sqrt{3}}{2}q_x a - \frac{3}{2}q_y a\right) + \frac{\sqrt{3}}{2}\left(-\frac{\sqrt{3}}{2}q_x a - \frac{3}{2}q_y a\right)\right] \approx \frac{3at}{2}q_x \qquad (15) \\ Y(\mathbf{k}) &= t\left[\sin\left(\frac{2\pi}{3} + \frac{\sqrt{3}}{2}q_x a - \frac{3}{2}q_y a\right) + \sin\left(-\frac{2\pi}{3} - \frac{\sqrt{3}}{2}q_x a - \frac{3}{2}q_y a\right)\right] \\ &\approx t\left[-\frac{1}{2}\left(\frac{\sqrt{3}}{2}q_x a - \frac{3}{2}q_y a\right) - \frac{1}{2}\left(-\frac{\sqrt{3}}{2}q_x a - \frac{3}{2}q_y a\right)\right] \approx \frac{3at}{2}q_y \qquad (16) \end{aligned}$$

Thus,

$$H(\mathbf{q}) = \hbar v_F \left(q_x \sigma_x + q_y \sigma_y\right) + U\sigma_z \qquad (17)$$

where $v_F = \frac{3at}{2\hbar}$. This is a form of the two-dimensional Dirac Equation with mass U and the speed of light replaced by v_F. A similar expansion can be performed near K'.
Graphene is similar to this tight binding model in that the electrons in graphene hop between the out-of-plane p orbitals. For graphene, there is no energy difference between A and B, so $U = 0$:

$$H(\mathbf{p}) = v_F \mathbf{p} \cdot \boldsymbol{\sigma} \qquad (18)$$

where $\mathbf{p} = \hbar\mathbf{q}$ and $\boldsymbol{\sigma} = (\sigma_x, \sigma_y)$. This leads to the energy-momentum dispersion $E = \pm\hbar v_F q$. Note that there are two symmetric conical bands that meet at $E = 0$, the so-called "Dirac Point." I will use terminology such as "electron-like band," "top band," or π^* band to describe the positive energy states. Likewise, I will refer to the negative energy states as being in the "hole-like band," "bottom band," or π band.
Lets define ϕ such that $\mathbf{q} = (q_x, q_y) = q(\cos(\phi), \sin(\phi))$. Then the graphene Hamiltonian can be rewritten as

$$H(\mathbf{q}) = \hbar v_F q \begin{pmatrix} 0 & e^{-i\phi} \\ e^{i\phi} & 0 \end{pmatrix} \qquad (19)$$

which has eigenvectors

$$\Psi_{\mathbf{K},\pi^*}(\mathbf{q}) = \frac{1}{\sqrt{2}}\begin{pmatrix} e^{-i\phi/2} \\ e^{i\phi/2} \end{pmatrix}, \ \Psi_{\mathbf{K},\pi}(\mathbf{q}) = \frac{1}{\sqrt{2}}\begin{pmatrix} e^{-i\phi/2} \\ -e^{i\phi/2} \end{pmatrix} \qquad (20)$$

Note the similarity to a spin pointing in the ϕ direction. For this reason, the sublattice degree of freedom is referred to as "pseudospin." However, unlike the real spin for a massive particle, pseudospin is locked parallel or antiparallel to $\mathbf{q}$. Thus, while there is spin degeneracy, there is no pseudospin degeneracy. On the other hand, graphene does have a "valley" degeneracy arising from the symmetry between K and K'.