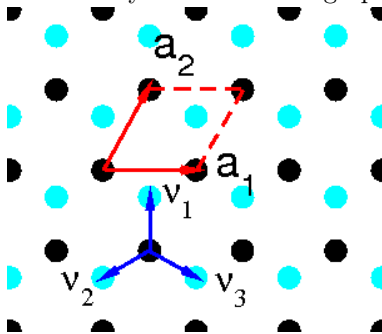Figure 1: Honeycomb lattice of graphene.

1 Continuum approximation to graphene: Dirac-Weyl equation

To see how the Dirac-Weyl equation arises from the particular symmetry and electron number of graphene is not difficult. First consider a simple tight-binding model for graphene

$$H = -\gamma \sum_{i \in A} \sum_{a=1,2,3} \left[(c_{i+a}^B)^\dagger c_i^A + (c_i^A)^\dagger c_{i+a}^B \right] \tag{1}$$

here the sum i is over the sublattice A, while the sum a is over the 3 nearest neighbors to site i. This Hamiltonian just describes the 'hopping' of electrons from sublattice A to B (and back), controlled by the parameter γ. This model is not necessary to derive the effective Dirac-Weyl equation (it can be done more generally) but it makes the derivation very simple, and is a very reasonable model for graphene in any case.

To solve the Hamiltonian in Eq. 1 we introduce the Bloch state wavefunction

$$\left| \Psi_s^\mathbf{k} \right\rangle = \frac{1}{\sqrt{2}} \sum_{i \in s} e^{i\mathbf{k}.\mathbf{r}} (c_i^s)^\dagger \left| 0 \right\rangle \tag{2}$$

We can then consider various overlap elements with these Bloch states and the Hamiltonian in Eq. 1. We have

$$\begin{aligned} \left\langle \Psi_A^\mathbf{k} \right| H \left| \Psi_B^\mathbf{k} \right\rangle &= -\gamma \sum_{a=1,2,3} e^{i\mathbf{k}.\boldsymbol{\nu}_a} \tag{3} \\ &= f(\mathbf{k}) \tag{4} \end{aligned}$$

and its conjugate $\left\langle \Psi_B^\mathbf{k} \right| H \left| \Psi_A^\mathbf{k} \right\rangle = f(\mathbf{k})^*$. In this expression $\{\boldsymbol{\nu}_a\}$ are the nearest neighbor vectors of the honeycomb lattice, see Fig. 1 and Eq. 9 for explicit forms of these vectors. Using these we can then write the Hamiltonian as

$$-\gamma \begin{pmatrix} 0 & f(\mathbf{k}) \\ f(\mathbf{k})^* & 0 \end{pmatrix} \begin{pmatrix} \left| \Psi_A^{\mathbf{k}} \right\rangle \\ \left| \Psi_B^{\mathbf{k}} \right\rangle \end{pmatrix} = E(\mathbf{k}) \begin{pmatrix} \left| \Psi_A^{\mathbf{k}} \right\rangle \\ \left| \Psi_B^{\mathbf{k}} \right\rangle \end{pmatrix} \tag{5}$$

Where we have set $\left\langle \Psi_A^{\mathbf{k}} \right| H \left| \Psi_A^{\mathbf{k}} \right\rangle = \left\langle \Psi_B^{\mathbf{k}} \right| H \left| \Psi_B^{\mathbf{k}} \right\rangle = 0$ (we can do this as these terms just amount to an arbitrary shift). The eigenvalues are obviously given by

$$E(\mathbf{k}) = \pm \gamma |f(\mathbf{k})| \tag{6}$$

Now, to evaluate exactly what this means we have to work out $|f(\mathbf{k})|$ explicitly, for which we need the primitive vectors of the graphene lattice (see Fig. 1),

$$\mathbf{a}_1 = a(1, 0) \tag{7}$$

$$\mathbf{a}_2 = a(\frac{1}{2}, \frac{\sqrt{3}}{2}) \tag{8}$$

as well as the vectors of the nearest neighbors

$$\boldsymbol{\nu}_1 = a(0, \frac{1}{\sqrt{3}}) \tag{9}$$

$$\boldsymbol{\nu}_2 = a(-\frac{1}{2}, -\frac{1}{2\sqrt{3}}) \tag{10}$$

$$\boldsymbol{\nu}_3 = a(\frac{1}{2}, -\frac{1}{2\sqrt{3}}) \tag{11}$$

Using these we then find, after a short calculation,

$$|f(\mathbf{k})| = 3 + 4\cos(\frac{\sqrt{3}k_x}{2})\cos(\frac{k_y}{2}) + 2\cos k_y \tag{12}$$

This function is plotted in Fig 2. What one can see is that the two manifolds corresponding to $\pm\gamma|f(\mathbf{k})|$ touch at several points, which are in fact the vertices of the Brillouin zone. These come in two inequivalent sets of three points, with each set labeled K or K' according to a convention illustrated in the inset of Fig 2.

A crucial point is that the Fermi level of graphene is *exactly* at the meeting point of these bands. Therefore, refering to the enlarged portion of the band structure at one of these points, shown as an inset in Fig 2, we see that *the spectrum for low energy excitations is linear.* This is already very interesting: we know that for free electrons the spectrum should be quadratic in momentum. Recalling that the index $\mathbf{k}$ in a band structure is equivalent to a crystal momentum we see that the low energy excitations (i.e., electron and hole excitations) will behave very differently from free electrons.

To make this statement more precise we can derive an *effective low energy Hamiltonian* that is valid around the K and K' points in the Brillouin zone (but not elsewhere). To do this we must therefore expand the function $f(\mathbf{k})$ in Eq. 5

2

Figure 2: Band structure of graphene; a plot of the function $E(\mathbf{k}) = \pm\gamma|f(\mathbf{k})|$. ($|f(\mathbf{k})|$ is defined in Eq. 12.)
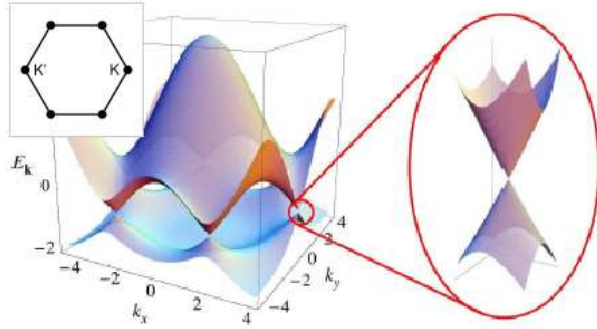
about the K and K' points, for which we need explicit forms of these vectors. The reciprocal space vectors are found to be

$$\mathbf{b}_1 = \frac{2\pi}{a}\frac{2}{\sqrt{3}}(\frac{\sqrt{3}}{2},\frac{1}{2}) \tag{13}$$

$$\mathbf{b}_2 = \frac{2\pi}{a}\frac{2}{\sqrt{3}}(0,1), \tag{14}$$

which then yields for the K and K' points the following vectors

$$\mathbf{K} = (\frac{4\pi}{3a},0) \tag{15}$$

$$\mathbf{K}' = (-\frac{4\pi}{3a},0) \tag{16}$$

$$\tag{17}$$

We can now approximate $f(\mathbf{k})$ by the first two terms of Taylor series

$$f(\mathbf{K}+\mathbf{k}) = f(\mathbf{K}) + \nabla_{\mathbf{k}}f(\mathbf{k}')|_{\mathbf{k}'=\mathbf{K}+\mathbf{k}} \tag{18}$$

and using the formula for $f(\mathbf{K})$, $\mathbf{K}$, and the nearest neighbour vectors $\{\boldsymbol{\nu}_i\}$ we finally find

$$H_0^K = \frac{3\gamma a_{cc}}{2}\begin{pmatrix} 0 & k_x - ik_y \\ k_x + ik_y & 0 \end{pmatrix} \tag{19}$$

3

Now, if we substitue for $k_x = -i\hbar\partial_x$ and similar for k_y we see, after a short calculation that this equation can be written as

$$H_0^K = v_F \boldsymbol{\sigma}.\mathbf{p} \tag{20}$$

where $\boldsymbol{\sigma} = (\sigma_x, \sigma_y)$. This is exactly the Dirac-Weyl equation, so the low energy excitations about the K point in graphene are described not by the Schrödinger equation, but instead by this equation which would normally be used to describe e.g. neutrinos. (The Dirac-Weyl results from the Dirac equation by setting the rest mass of the particle to zero. This results in fact in two equations describing particles of opposite chilarity. The equation above is the right-handed Dirac-Weyl equation.) In a similar way we can expand around the K' point and find the following equation:

$$H_0^{K'} = v_F \boldsymbol{\sigma}'.\mathbf{p} \tag{21}$$

where now $\boldsymbol{\sigma}' = (-\sigma_x, \sigma_y)$. Note that this is not exactly the same as the left-handed Dirac-Weyl equation that results from the Dirac equation.

A number of interesting observations can me made about the low energy excitations in graphene at this point. Clearly, the fact that they are governed by the Dirac-Weyl equation means that they have an (effective) internal degree of freedom that mimics the spin degree of freedom in the true Dirac-Weyl equation. This is known as *pseudospin*. Although it behaves very much like the true spin degree of freedom, it *represents* something very simple: each component is just the projection of the particle wavefunction onto sublattice A (spin up) or B (spin down). This is an example of the mix of solid state physics with Dirac-Weyl physics that one often encounters in graphene.

We can write Eq. 19 in the form

$$H_0^K = \hbar v_F |\mathbf{k}| \begin{pmatrix} 0 & e^{-i\theta_{\mathbf{k}}} \\ e^{i\theta_{\mathbf{k}}} & 0 \end{pmatrix} \tag{22}$$

which makes it easy to see that the eigenspectrum is

$$E = \pm\hbar v_F |\mathbf{k}| \tag{23}$$

linear as expected, and with *positive and negative energy solutions*. The associated eigenvectors for positive energies (electron) are

$$\Psi_{\mathbf{k}}^K(\mathbf{r}) = \frac{1}{\sqrt{2}} e^{i\mathbf{k}.\mathbf{r}} \begin{pmatrix} e^{-i\theta_{\mathbf{k}}/2} \\ e^{i\theta_{\mathbf{k}}/2} \end{pmatrix} \tag{24}$$

for negative energies (holes) are

$$\Psi_{\mathbf{k}}^K(\mathbf{r}) = \frac{1}{\sqrt{2}} e^{i\mathbf{k}.\mathbf{r}} \begin{pmatrix} e^{-i\theta_{\mathbf{k}}/2} \\ -e^{i\theta_{\mathbf{k}}/2} \end{pmatrix} \tag{25}$$

At this stage we can note another property of the Dirac-Weyl equation that will be found in graphene physics: *chirality* is a good quantum number. The

chirality in this case can be defined to be the projection of the momentum on the direction of pseudospin: $\boldsymbol{\sigma}.\mathbf{p}/|p|$. Clearly electrons will have positive chirality and holes negative chirality.

2   Some consequences for graphene physics

The fact that the low energy excitations are governed by such a strange equation is clearly going to make the physics of graphene very different from that of e.g. copper. There are two main consequences that will be described here. Firstly, there is an absence of back scattering for long range impurities. This can be seen easily: using the formalism of the previous section we can simply show that the matrix element of the back-scattering process is zero

$$
\begin{aligned}
\langle -\mathbf{k}| H_{imp} |\mathbf{k}\rangle &= \frac{1}{2S} \int d\mathbf{r} e^{i2\mathbf{k}.\mathbf{r}} \left(e^{i\theta_{-\mathbf{k}}/2}\ e^{-i\theta_{-\mathbf{k}}/2} \right) \begin{pmatrix} V(\mathbf{r}) & 0 \\ 0 & V(\mathbf{r}) \end{pmatrix} \begin{pmatrix} e^{-i\theta_{\mathbf{k}}/2} \\ e^{i\theta_{\mathbf{k}}/2} \end{pmatrix} \\
&= 0
\end{aligned}
\tag{26}
$$

(here S is the unit cell area of the graphene lattice). This is rather dramatic since all real materials have impurities, and it is normally these which determine the transport properties of the material. However, in the case of graphene the impurities don't scatter, i.e. they are effectively not there, and hence one has the possibility of *coherent transport* in graphene.

The second consequence can be derived rather easily, but is not done here, and is that if a particle governed by the Dirac-Weyl equation impinges upon a potential barrier with $V > E$ then one doesn't have an exponential tunneling as in the Schrödinger equation, but instead for certain angles of incidence of the particle the tunneling probability approaches *unity* as $V \to \infty$. The reason for this behavior is essentially the fact that one has a chiral degree of freedom, as well as positive and negative energy states. The practical consequence is that it is very hard to localize electrons in graphene with purely a scalar external potential.