Tutorial 1 - Graphene

1 Tight binding models

We would like to analyze the general problem of non-interacting electrons in a periodic potential that results from a lattice of ions. We note that the tight binding method is more general than what is presented here. If you would like to learn more, the book by Ashcroft and Mermin has a very good chapter on this subject.

In first quantization, we write the corresponding Schrodinger equation as

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V_{ion}(\vec{r})\right)\psi(\vec{r}) = E\psi(\vec{r}), \tag{1}$$

with $V_{ion}(\vec{r}) = \sum_{\mathbf{R}} V_i(\vec{r} - \vec{R})$. Here, $V_i(\vec{r})$ is the contribution to the potential from a single ion located in the origin, and the set of vectors $\vec{R}$ are the lattice vectors.

We start by approaching the problem from the limit where the ions are extremely far apart. In this limit, the single-particle eigenstates will be those that correspond to the problem of an electron affected by a single ion:

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V_i(\vec{r})\right)\phi_n(\vec{r}) = E_n\phi_n(\vec{r}). \tag{2}$$

The solutions are bound to the corresponding ion, hence the name tight binding.

Once the spatial extent of the single ion wavefunctions becomes comparable to the lattice spacing, this stops being true, and coupling between different sites must be taken into account. However, within the tight binding formalism, we write the corrections to the above ideal picture in terms of the localized wavefunctions ϕ_n.

The coupling between $\phi_n(\vec{r})$ and $\phi_n(\vec{r}-\vec{R})$, which correspond to different ions introduces matrix elements of the form

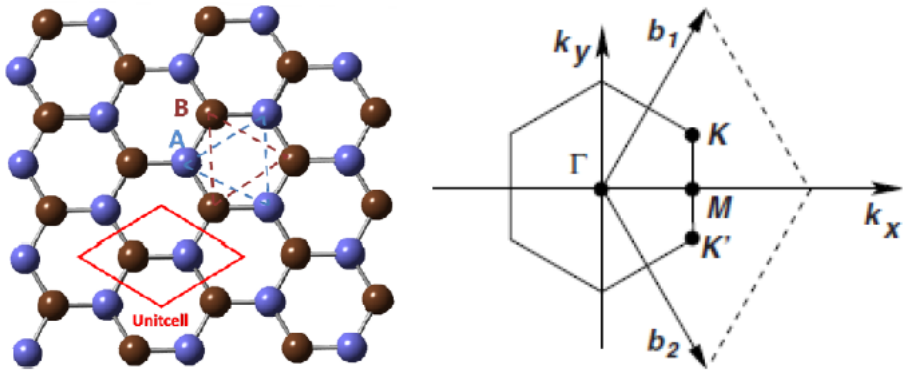
$$\left\langle \phi_n(\vec{r} - \vec{R}) \left| H \right| \phi_n(\vec{r}) \right\rangle \equiv -t_n(\vec{R}). \tag{3}$$

Working in second quantization, we define an operator $c_n^\dagger(\vec{R})$ that creates an electron in the state $\phi_n(\vec{r}-\vec{R})$. In terms of these, we write the Hamiltonian in the quadratic form

$$H = -\sum_{n,\mathbf{R},\mathbf{R}'} t_n(\vec{R} - \vec{R}')c_n^\dagger(\vec{R})c_n(\vec{R}'). \tag{4}$$

2 Graphene

Graphene is a material made of a single atomic layer. This two dimensional system is made of Carbon atoms, arranged in a honeycomb lattice, as depicted in figure 1a.



(a) (b)

Figure 1

Remember that a honeycomb lattice is actually an hexagonal lattice with a basis of two ions in each unit cell. If a is the distance between nearest neighbors, the primitive lattice vectors can be chosen to be

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

and the reciprocal-lattice vectors are spanned by

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

The first Brillouin zone is shown in figure 1b.

In this tutorial we want to calculate the spectrum of non-interacting electrons in this material. We restrict ourselves here to the case of nearest-neighbor tunneling terms only. In the homework, you will extend this to slightly more complicated situations, and you will see that the important features of the spectrum remain the same as long as very large deviations are not included.

We directly work in second quantization, and define the annihilation operators of an electron at the lowest orbital centered around atoms A and B:

$$A(\vec{R}), B(\vec{R}).$$

These operators satisfy the anti-commutation relations

$$\left\{A(\vec{R}), A^\dagger(\vec{R}')\right\} = \left\{B(\vec{R}), B^\dagger(\vec{R}')\right\} = \delta_{\vec{R},\vec{R}'},$$

$$\left\{A(\vec{R}), A(\vec{R}')\right\} = \left\{B(\vec{R}), B(\vec{R}')\right\} = \left\{A(\vec{R}), B(\vec{R}')\right\} = \left\{A(\vec{R}), B^\dagger(\vec{R}')\right\} = 0.$$

Notice that the nearest neighbor of an ion of type A is always an ion of type B (and vice versa). We therefore write the tight binding Hamiltonian as

$$H = -t \sum_{\langle \vec{R},\vec{R}' \rangle} A^\dagger(\vec{R}) B(\vec{R}') + h.c. = -t \sum_{\vec{R},\tilde{\delta}} A^\dagger(\vec{R}) B(\vec{R}+\tilde{\delta}) + h.c.$$

The vectors $\vec{\delta}$, connecting the A atoms to their nearest neighbors are given by

$$\vec{\delta_1} = \frac{a}{2}\left(1, \sqrt{3}\right), \vec{\delta_2} = \frac{a}{2}\left(1, -\sqrt{3}\right), \vec{\delta_3} = a\left(-1, 0\right).$$

We want to diagonalize the Hamiltonian. Since we have a translation invariant system, it is a good idea to go to Fourier space and write

$$A(\vec{R}) = \frac{1}{\sqrt{N}} \sum_{\vec{k} \in BZ1} A(\vec{k}) e^{i\vec{k}\cdot\vec{R}}, B(\vec{R}) = \frac{1}{\sqrt{N}} \sum_{\vec{k} \in BZ1} B(\vec{k}) e^{i\vec{k}\cdot\vec{R}}.$$

Like the operators in real space, the non-vanishing anti-commutation relations are

$$\left\{A(\vec{k}), A^\dagger(\vec{k}')\right\} = \left\{B(\vec{k}), B^\dagger(\vec{k}')\right\} = \delta_{\vec{k},\vec{k}'},$$

and the rest are zero. Plugging this into the Hamiltonian, we now have

$$H = -t \sum_{\vec{R},\tilde{\delta}} A^\dagger(\vec{R}) B(\vec{R}+\tilde{\delta}) + h.c. = -\frac{t}{N} \sum_{\vec{R},\tilde{\delta}} \sum_{\vec{k},\vec{q}} e^{i\vec{q}\cdot\tilde{\delta}} e^{i\vec{R}\cdot(\vec{q}-\vec{k})} A^\dagger(\vec{k}) B(\vec{q}) + h.c. =$$

$$= -t \sum_{\tilde{\delta}} \sum_{\vec{k},\vec{q}} e^{i\vec{q}\cdot\tilde{\delta}} A^\dagger(\vec{k}) B(\vec{q}) \left(\frac{1}{N} \sum_{\vec{R}} e^{i\vec{R}\cdot(\vec{q}-\vec{k})}\right) + h.c.$$

Using the fact that $\frac{1}{N}\sum_{\vec{R}} e^{i\vec{R}\cdot(\vec{q}-\vec{k})} = \delta_{\vec{q},\vec{k}}$, we get

$$H = -t \sum_{\vec{k},\vec{\delta}} e^{i\vec{k}\cdot\tilde{\delta}} A^\dagger(\vec{k}) B(\vec{k}) + h.c.$$

If we define $\psi(\vec{k}) = \left(A(\vec{k}), B(\vec{k})\right)^T$,we can rewrite this as

$$H = \sum_{\vec{k}} \psi^\dagger(\vec{k}) h(\vec{k}) \psi(\vec{k}),$$

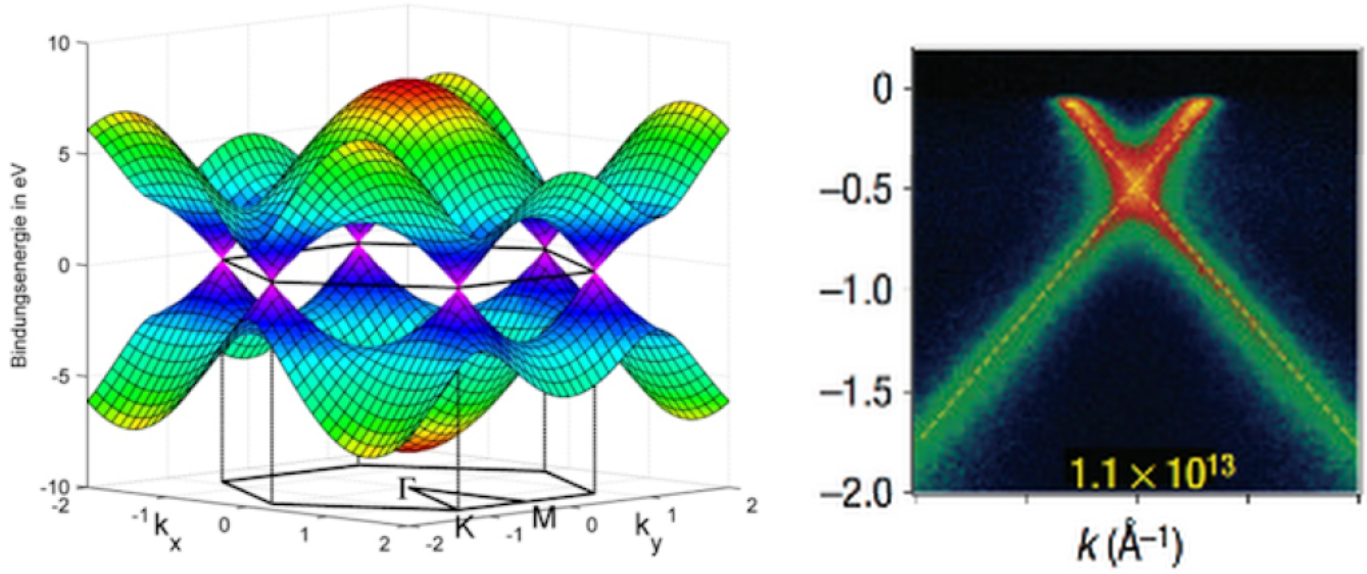
where the matrix h, called the Bloch Hamiltonian, takes the form

$$h = \begin{pmatrix} 0 & f(\vec{k}) \\ f^*(\vec{k}) & 0 \end{pmatrix},$$

with $f(\vec{k}) = -t\sum_\delta e^{i\vec{k}\cdot\vec{\delta}} = -t\left(e^{-ik_x a} + 2e^{ik_x a/2}\cos\left(\frac{k_y a\sqrt{3}}{2}\right)\right)$.

Since h is an Hermitian matrix, it is guaranteed that we can diagonalize it using some unitary matrix U, such that

$$UhU^\dagger = \begin{pmatrix} \varepsilon_+ & 0 \\ 0 & \varepsilon_- \end{pmatrix}.$$



(a) (b)

Figure 2

Defining $U\psi = (c_+, c_-)^T$, we can write

$$H = \sum_{\vec{k}} \varepsilon_+(\vec{k}) c_+^\dagger(\vec{k}) c_+(\vec{k}) + \varepsilon_-(\vec{k}) c_-^\dagger(\vec{k}) c_-(\vec{k}),$$

with the non-vanishing anti-commutation relations

$$\left\{c_+^\dagger(\vec{k}), c_+(\vec{k}')\right\} = \left\{c_-^\dagger(\vec{k}), c_-(\vec{k}')\right\} = \delta_{\vec{k},\vec{k}'}.$$

Notice that we have two bands, one for each element of the unit cell, and the corresponding energy spectra are given by $\varepsilon_\pm(\vec{k})$.

We understand that in order to get the spectrum, we need to diagonalize the Bloch Hamiltonian h.

The corresponding eigenvalues are given by

$$\varepsilon_\pm = \pm\left|f(\vec{k})\right| = \pm t\sqrt{3 + 2\cos\left(\sqrt{3}k_y a\right) + 4\cos\left(\sqrt{3}k_y a/2\right)\cos\left(3k_x a/2\right)}.$$

The spectrum is shown in Fig. 2a

3 Emergent Dirac physics

Notice that the two bands touch at some points in the first Brillouin zone. Since Graphene has one accessible electron per atom, we get by taking spin into account that the lower band is exactly filled. This means that

if we would like to discuss small excitations above the ground state, the excitations that will contribute are those near the crossing points.

To write the low energy theory, we would therefore like to identify these points. We get them from the condition $f(\vec{k}) = 0$. The two real equations that result from this requirement are

$$\cos(k_x a) + 2\cos(k_x a/2)\cos\left(\frac{k_y a\sqrt{3}}{2}\right) = 0 \quad (5)$$

$$-\sin(k_x a) + 2\sin(k_x a/2)\cos\left(\frac{k_y a\sqrt{3}}{2}\right) = 0. \quad (6)$$

We can manipulate equation 6 such that it takes the form

$$\sin(k_x a/2)\left(-\cos\left(\frac{k_x a}{2}\right) + \cos\left(\frac{k_y a\sqrt{3}}{2}\right)\right) = 0.$$

So we have two options: either $\sin(k_x a/2) = 0$ (which means that $\cos(k_x a/2) = \pm 1$), or $\cos\left(\frac{k_x a}{2}\right) = \cos\left(\frac{k_y a\sqrt{3}}{2}\right)$.

The first option gives us the points $\left(0, \pm\frac{4\pi}{3\sqrt{3}a}\right)$ plus any reciprocal lattice vector. The second option gives us $\pm\frac{2\pi}{3a}\left(1, \frac{1}{\sqrt{3}}\right)$, and $\pm\frac{2\pi}{3a}\left(1, -\frac{1}{\sqrt{3}}\right)$ (again, up to reciprocal lattice vectors).

Actually, all the points listed above sit in the corners of the first Brillouin zone. A simple inspection shows that the above set of k-space vectors is not independent: the set of vectors $\left(0, \frac{4\pi}{3\sqrt{3}a}\right), \frac{2\pi}{3a}\left(1, -\frac{1}{\sqrt{3}}\right), \frac{2\pi}{3a}\left(-1, -\frac{1}{\sqrt{3}}\right)$ can be connected by a reciprocal lattice vector. This is correct for the set $\left(0, -\frac{4\pi}{3\sqrt{3}a}\right), \frac{2\pi}{3a}\left(-1, \frac{1}{\sqrt{3}}\right), \frac{2\pi}{3a}\left(1, \frac{1}{\sqrt{3}}\right)$ as well. To see this, we write

$$\left(0, \frac{4\pi}{3\sqrt{3}a}\right) + \vec{b}_2 = \frac{2\pi}{3a}\left(1, -\frac{1}{\sqrt{3}}\right) \quad (7)$$

$$\left(0, \frac{4\pi}{3\sqrt{3}a}\right) - \vec{b}_1 = \frac{2\pi}{3a}\left(-1, -\frac{1}{\sqrt{3}}\right). \quad (8)$$

The other equivalence relations result from taking linear combinations of the above equations. We choose one representative vector from each set. These are conventionally called K and K':

$$\vec{K} = \frac{2\pi}{3a}\left(1, \frac{1}{\sqrt{3}}\right), \vec{K}' = \frac{2\pi}{3a}\left(1, -\frac{1}{\sqrt{3}}\right).$$

Remember that the energy bands cross at these points, and the gap closes. Because of that, there are two branches of low energy excitations - one of excitations with a given momentum close to K and another close to K'.

Therefore, if we would like to focus on the low energy physics, we expand the Hamiltonian around each of these points. Expanding around K', for example, we get

$$f(\vec{K}' + \vec{q}) \approx -\frac{3ta}{2}e^{-\frac{2\pi i}{3}}(q_y + iq_x).$$

This means that the Hamiltonian can be approximated as

$$h(K'+\mathbf{q}) = -\frac{3ta}{2}\begin{pmatrix} 0 & e^{-\frac{2\pi i}{3}}(q_y+iq_x) \\ e^{\frac{2\pi i}{3}}(q_y-iq_x) & 0 \end{pmatrix}.$$

Upon changing the phases of A and B, which physically means changing the phases of the basis wavefunctions ϕ_n, this matrix can be brought to the form

$$h(\vec{K}'+\vec{q}) = \hbar v_F \vec{q}\cdot\vec{\sigma}, \tag{9}$$

where σ is the vector of Pauli-matrices. This is just the 2D massless Dirac Hamiltonian, which describes free relativistic electrons, where the speed of light has been replaced by $v_F = \frac{3ta}{2\hbar}$.

Remember that the Dirac Hamiltonian takes the form $H_{Dirac} = c\sum_i \alpha_i p_i + \beta mc^2$, where the matrices α and β satisfy the relations

$$\beta^2 = 1$$
$$\{\alpha_i, \beta\} = 0$$
$$\{\alpha_i, \alpha_j\} = 2\delta_{ij}.$$

The effective Hamiltonian in equation 9 takes exactly this form in 2D, if we identify $\alpha_i = \sigma_i$, and $m = 0$.

The eigenvalues and eigenfunctions of this equation are

$$E = \pm\hbar v_F |\vec{q}|, \psi_\pm = \frac{1}{\sqrt{2}}(\ e^{i\theta_\mathbf{q}/2} \quad , \pm e^{-i\theta_\mathbf{q}/2}\ )^T.$$

Here, $\theta_\mathbf{q}$ is the angle of the planar vector $\vec{q}$ with respect to the x-axis.

Note that the phase of the wavefunction changes by π as $\mathbf{q}$ winds around the origin, and completes a full winding as we wind twice around the origin. The phase after a full cycle does not depend on the trajectory. We can view this phase as a vortex, and the corresponding winding number as an integer which characterizes this Dirac cone. This is an example of a topological property, as it is insensitive to small deviations.

You will see in the homework how this topological property, together with the symmetries of the problem, makes it difficult to get rid of the Dirac cones. This means that the effective Dirac theory in our system is not an artifact of our nearest neighbor approximation, and can actually be expected to be observed in experiments. Indeed, the Dirac spectrum has been successfully measured (see Fig. 2b).

Note that a similar derivation would give us, $h(\vec{K}+\vec{q}) = h^*(\vec{K}'+\vec{q})$, and we get the same spectrum around K.

If we want to describe the full low energy theory, we have two independent Dirac modes, one around K and another around K'. It's therefore useful to work in a basis $\Psi = \left(A_{\vec{K}+\vec{q}}, B_{\vec{K}+\vec{q}}, A_{\vec{K}'+\vec{q}}, B_{\vec{K}'+\vec{q}}\right)$, in terms of which the full low energy Hamiltonian takes the form

$$h = v_F\begin{pmatrix} (\vec{q}\cdot\sigma)^* & 0 \\ 0 & \vec{q}\cdot\sigma \end{pmatrix}.$$

We have found emergent Dirac physics. The physical picture we have at large length scales (that is, small q's) is completely different from the physics at the microscopic level. We started from a problem of non-relativistic electrons, and got that the low energy physics of the problem corresponds to that of relativistic fermions.

This is very exciting because now can use this fact to directly measure relativistic effects, and even some which have never tested in any particle physics experiment. As an example of such a property, the Klein paradox, where a relativistic electron, obeying the Dirac equation, is fully transmitted after hitting a very strong potential barrier, has been measured in Graphene.