

Exercise 5.1 Tight-Binding Model of Graphene

- a) Compute the low-energy band structure of graphene within a tight-binding description taking only nearest-neighbor hopping into account!

To get started, consider the electronic configuration of C. C has four valence electrons which occupy $2s^2$ and $2p^2$ orbitals. The hexagonal structure of the lattice suggests that three of these valence electrons occupy hybrid sp^2 -orbitals to form covalent σ -bonds with their nearest neighbors (bonding angle $2\pi/3$). Due to the large binding energy, there are no low-energy excitations involving these electrons. The remaining electron occupies the p_z orbital that sticks out of the planar lattice forms weaker π -bonds with the neighboring atoms. Based on these considerations, it seems reasonable to focus solely on the electrons in the p_z -orbitals, so that the problem reduces to one electron and one orbital per atom.

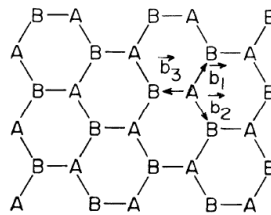


Figure 1:

Hint: Before embarking into the calculation, you may wish to refresh your memory about the unit cell and Brillouin zone for a hexagonal lattice.

To write down the hopping Hamiltonian, divide the lattice into two sublattices A and B as shown in Fig. 1 and introduce fermionic field operators a_i and b_i (i labels the site) on these sublattices. Then argue that the hopping matrix element is the same for all \vec{b}_i ($i = 1, 2, 3$) in Fig. 1 for a given site. Use the Fourier transform,

$$\begin{aligned} a_i &= \frac{1}{\sqrt{N}} \sum_{\vec{k} \in \text{BZ}} \tilde{a}_{\vec{k}} e^{i\vec{k} \cdot \vec{R}_{a,i}} \\ b_i &= \frac{1}{\sqrt{N}} \sum_{\vec{k} \in \text{BZ}} \tilde{b}_{\vec{k}} e^{i\vec{k} \cdot \vec{R}_{b,i}}, \end{aligned} \quad (1)$$

where N is the number of unit cells and $\vec{R}_{a,i}$ ($\vec{R}_{b,i}$) is the position of the i -th site on sublattice A (B) to obtain a Hamiltonian of the form

$$\mathcal{H} = \sum_{\vec{k} \in \text{BZ}} \begin{pmatrix} \tilde{a}_{\vec{k}}^\dagger & \tilde{b}_{\vec{k}}^\dagger \end{pmatrix} \begin{pmatrix} h_{aa}(\vec{k}) & h_{ab}(\vec{k}) \\ h_{ba}(\vec{k}) & h_{bb}(\vec{k}) \end{pmatrix} \begin{pmatrix} \tilde{a}_{\vec{k}} \\ \tilde{b}_{\vec{k}} \end{pmatrix}. \quad (2)$$

Plot the band structure and show that the Fermi “surface” consists of two points by finding the values of \vec{k} for which the energy is zero.

Finally, obtain the low-energy structure by expanding the energy to leading order in small deviations \vec{k} around the Fermi points. The low-energy Hamiltonian can be shown to be equivalent to the celebrated Dirac Hamiltonian for relativistic fermions (in a $(2 + 1)$ -dimensional space-time). Can you see what is ‘relativistic’ about the dispersion relation?

- b) Now, assume we have a small perturbation in our system and let us investigate the effects on its band structure. The simplest non-trivial perturbation would be an energy splitting between the two sublattices A and B . Take a perturbation of the form

$$V = \begin{pmatrix} v & 0 \\ 0 & -v \end{pmatrix} \quad (3)$$

into account and derive the dispersion. What happens to the “Fermi-surface”?

Exercise 5.2 Specific Heat of a Semiconductor

Calculate the specific heat of a semiconductor under the assumption $k_B T \ll E_g$, where E_g is the band gap. Show that it is given by an ideal gas-like part $(3/2)n(T)k_B$ plus a correction, where $n(T)$ is the number of excitations. Is this correction small or large?

Hint: First, approximate the dispersion of both the conduction and the valence band parabolically, with the two effective masses m_v and m_c . Then, calculate the chemical potential μ from the condition, that the number of electrons in the conduction band ($n_e(T)$) must be equal to the number of holes in the valence band ($n_h(T)$).

Office hour:

Monday, March 28th, 2011 (9:00 to 11:00 am)

HIT K 11.3

Daniel Müller