

Exercise 5.1 Tight-Binding Model of Graphene

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.

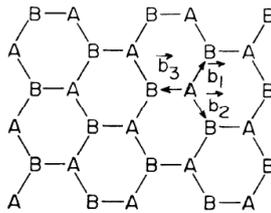


Figure 1:

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 \mathbf{b}_i ($i = 1, 2, 3$) in Fig. 1 for a given site. Use the Fourier transform,

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

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

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

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

Finally, obtain the low-energy structure by expanding the energy to leading order in small deviations \mathbf{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?

Exercise 5.2 Specific Heat of a Semiconductor and a Metal

- a) 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 ($n_h(T)$).

- b) Calculate the specific heat of a metal for small temperatures $k_B T \ll \mu$ by using the Bohr-Sommerfeld expansion

$$\int_{-\infty}^{\infty} d\epsilon \frac{H(\epsilon)}{e^{(\epsilon-\mu)/k_B T} + 1} = \int_{-\infty}^{\mu} d\epsilon H(\epsilon) + \sum_{n=1}^{\infty} a_n (k_B T)^{2n} \left. \frac{d^{2n-1} H(\epsilon)}{d\epsilon^{2n-1}} \right|_{\epsilon=\mu} \quad (3)$$

where $a_1 = \pi^2/6, a_2 = 7\pi^4/360, \dots$

Hint: We use the Jellium model to describe the metal, i.e. we assume free electrons with the dispersion relation

$$\epsilon_{\mathbf{k}} = \frac{\hbar^2 \mathbf{k}^2}{2m} \quad (4)$$

which occupy all states which satisfy $\epsilon_{\mathbf{k}} < E_F$ at $T = 0$. Compute the density of states and calculate the particle density $n(\mu, T)$ and the energy density $u(\mu, T)$ up to second order in T . In order to express u in terms of n and T , determine the chemical potential μ by fixing the particle density.

Office hour:

Monday, March 26th, 2012 (9:00 to 11:00 am)

HIT K 11.3

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