

**Exercise 1. Tight-Binding Model of Graphene**

In this exercise we will 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. Carbon 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  $\sigma$ -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, and forms weaker  $\pi$ -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.

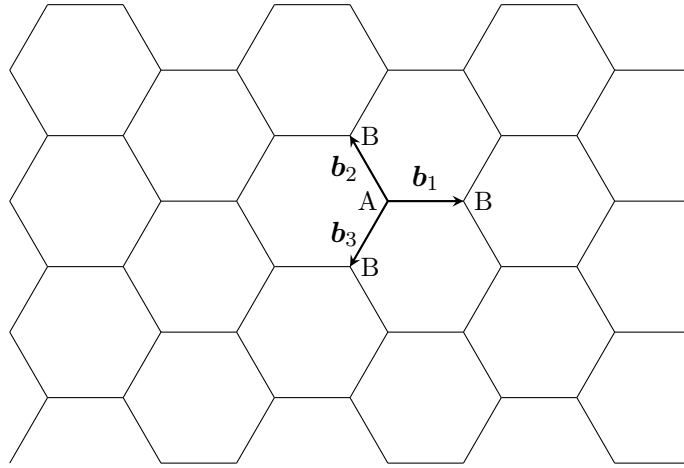


Figure 1: Crystal structure of graphene.

- Find the two lattice vectors  $\mathbf{a}_1$  and  $\mathbf{a}_2$  as well as the reciprocal lattice vectors  $\mathbf{c}_1$  and  $\mathbf{c}_2$ . Write down the vectors  $\mathbf{b}_1$ ,  $\mathbf{b}_2$ , and  $\mathbf{b}_3$  (Fig. 1), which connect nearest neighbors.
- 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

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

- (c) Diagonalize this Hamiltonian and plot the band structure to show that the Fermi “surface” consists of two points by finding the values of  $\mathbf{k}$  for which the energy is zero.
- (d) Calculate 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?
- (e) What happens to the band structure, when you add a staggered chemical potential term of the form

$$\mathcal{V} = \sum_i V(a_i^\dagger a_i - b_i^\dagger b_i) \quad (3)$$

to the Hamiltonian?

- (f) Assume that the lower band is half filled and sketch the particle-hole excitation spectrum along high-symmetry lines in the Brillouin zone for the cases with and without staggered chemical potential.

## Exercise 2. Coulomb Interaction – Excitons

In the following, we consider the half-filled chain with alternating potential from the previous exercise sheet:

$$H_1 = -t \sum_i \left( c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i \right) + V \sum_i (-1)^i c_i^\dagger c_i$$

Electrons are charged particles and therefore they repel. We use a simplified version of the Coulomb potential, namely, we assume that the energy of the system is increased by  $U$  whenever two electrons are on neighboring atoms (note that due to the Pauli principle two spinless fermions can not be on the same site.) In second quantized form the interaction term is written as follows:

$$\hat{U} = U \sum_i n_i n_{i+1} = U \sum_i c_i^\dagger c_{i+1}^\dagger c_{i+1} c_i. \quad (4)$$

We assume that  $U \ll V, t$ . In this case, only the states with momentum in the vicinity of  $\pm\pi/2$  (this is where the Fermi surface is for the half-filled case) are considerably affected by the Coulomb interaction.

- (a) Show that the repulsive interaction between the electrons leads to an attractive interaction between electrons in the conduction band and holes in the valence band:

$$\hat{U} \approx -\frac{4U}{N} \sum_{k, k', q} \cos(k - k') a_{k+q}^\dagger b_k^\dagger b_{k'} a_{k'+q}^\dagger + 4U \sum_k b_k^\dagger b_k. \quad (5)$$

*Hint.* Split the interaction into a sum containing explicitly the number operators of even and odd sites, and Fourier transform those number operators individually. Realize that one can replace all the  $v_k$ 's and  $u_k$ 's by  $v_{-\pi/2}$  ( $= v_{\pi/2}$ ) and  $u_{-\pi/2}$  ( $= u_{\pi/2}$ ). The second term in the above equation is unimportant for the further analysis and may be left out of consideration.

- (b) Let us now calculate the energy of an exciton. We make the following ansatz for the wave function of an exciton with momentum  $q$ :

$$|\psi_q\rangle = \sum_k' A_k^q a_{k+q}^\dagger b_k^\dagger |\Omega\rangle \quad (6)$$

where  $|\Omega\rangle$  is the ground state of the system without interaction (at half filling), and where the sum runs over the reduced Brillouin zone (indicated by the prime). Since we consider a small  $U$  we expect that the electron-hole pair is only weakly bound and that the wave function extends over a large region in real space. On the other hand, in reciprocal space, we expect that the exciton state is strongly localized. Therefore, we replace  $\cos(k - k')$  in Eq. (5) by 1. Show that the energies  $\omega_q$  (we are setting  $\hbar = 1$ ) of the exciton excitations  $|\psi_q\rangle$  are given by the solution of

$$\frac{1}{4U} = \frac{1}{N} \sum_k \frac{1}{E_k + E_{k+q} - \omega_q}. \quad (7)$$

Discuss the solution graphically. How is the excitation spectrum modified by the interaction?

- (c) Show that for small  $q$  the energy of the exciton is

$$\omega_q = 2V - \frac{U^2V}{t^2} + \frac{q^2}{2(2m^*)} \quad (8)$$

where  $m^* = V/(4t^2)$  is the effective mass at the conduction band minimum.

- (d) In the following we will use the continuum limit by expanding  $E_k \approx V + \frac{k^2}{2m^*}$ ,  $k \in \mathbb{R}$ . Show that in the real space expression for the exciton state with  $q = 0$ ,

$$|\psi\rangle = \frac{1}{\Omega} \int dr dr' f(r - r') a(r) b^\dagger(r') |\Omega\rangle, \quad (9)$$

$f(r - r')$  is determined by the Fourier-transform of  $A_k^0$  w.r.t.  $k$ ! As the exciton is a bound state,  $f(r - r')$  is expected to decay exponentially as  $|r - r'| \rightarrow \infty$ , i.e.  $f(r - r') \sim \exp(-|r - r'|/\lambda)$ . Derive an approximate expression for  $\lambda$  (This gives an estimate of the size of the exciton)!