CMP Ex1 part 2

May 10, 2021

due:23/05/21

1 Bilayer graphene

In this problem we will discuss the electronic properties of two sheets of graphene stacked one on top of the other. We will consider a particular stacking (which is energetically favored and therefore often found in natural graphite), the so called "Bernal stacking" or AB stacking. In this configuration, an A-atom of layer-2 (A_2), is positioned directly above the B-atom of layer-1(B_1), while $A_1$and B_2 are exactly aligned within an hexagon of the other layer, see Fig1.

(a) Let us consider the tight-binding Hamiltonian of bilayer Graphene. There are three hopping processes we want to account for: (i) the intra-layer hopping (you are already familiar with), with amplitude t; (ii) the strong inter-layer hopping, which couples overlapping A_2 and B_1 atoms, with amplitude γ_1; and finally (iii) the much smaller coupling between neighboring A_1 and B_2 atoms, with amplitude γ_3.

Write down the tight-binding Hamiltonian in terms of creation/annihilation operators on the sites A_1, B_1, A_2, B_2. Transform it to k-space to find the Bloch Hamiltonian, and write it in the form :

$$H = \sum_k \Psi^\dagger\left(\vec{k}\right) h\left(\vec{k}\right) \Psi\left(\vec{k}\right)$$

with $\Psi\left(\vec{k}\right) = \left(\psi_{A_1,\vec{k}}, \psi_{B_1,\vec{k}}, \psi_{A_2,\vec{k}}, \psi_{B_2,\vec{k}}\right)$a spinor of annihilation operators
.

(b) From this point on, we will use the fact that $\gamma_3 \ll \gamma_1$ and set $\gamma_3 = 0$. Diagonalize the Hamiltonian and plot its spectrum as a function of $\vec{k}$ for $\gamma_1 \ll t$, and $\gamma_1 \lesssim t$. Compare your results with the spectrum we obtained for single-layer Graphene. Is the spectrum gapped?

(c) If the spectrum is not gapped, what is the symmetry that protect it? (remember that a symmetry operator mix both sub-lattice and momenta subspaces)

(d) Expand the Bloch Hamiltonian around the K/K' points and find its low-momentum description. How does the spectrum behave at low energies and small momenta?
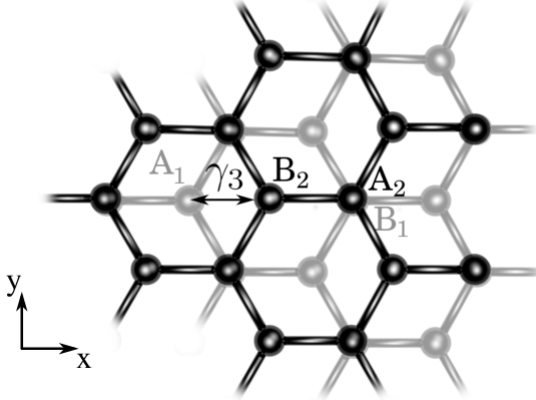
Figure 1: Stacking of two layers of Graphene. Atoms of the bottom layer "1" appear in gray, while in the top layer "2" appear in black. In the stacking depicted, A_2 and B_1 atoms overlap and have a hopping amplitude of γ_1, whereas A_1 atoms are located in the center of layer-2 hexagons, and B_2 atoms are centered with respect to layer-1 hexagons. Nearby A_1 and B_2 atoms are connected by a hopping amplitude γ_3

Using second order perturbation theory in $\frac{v_F |\vec{k}|}{\gamma}$, derive the effective low-energy 2X2 Hamiltonian acting on the spinor $\tilde{\Psi}(k) = (\psi_{A_1,k}, \psi_{B_2,k})$ (you may want to consult the book of Sakurai Chapter 5.2). Can you define (and find) the mass of the electrons from the spectrum?

(e) Add to the 2X2 Bloch Hamiltonian you found a term accounting for a chemical potential bias between the layers. In other words, an energy cost for electrons to be located on layer-1 atoms, and an identical energy gain for being located on layer-2. Such a setup can be experimentally achieved by, e.g., placing the bilayer inside a two-plate capacitor. What is the effect of such a term on the spectrum? Would an insertion of single layer graphene within such two plate capacitor show a similar effect?

2 Topological Insulator

Let us consider a simple spinless tight-binding model for a 2D topological insulator on a square lattice:

$$H = \sum_k \left(\psi_s^+(k), \psi_p^+(k) \right) \hat{h}(k) \begin{pmatrix} \psi_s(k) \\ \psi_p(k) \end{pmatrix}$$

$$\hat{h}(k) = A\left(\sin(k_x)\tau_x + \sin(k_y)\tau_y \right) + \left(m - t\cos(k_x) - t\cos(k_y) \right)\tau_z$$

where the τ's are the pauli matrices acting in the orbital basis.

(a) Find the corresponding real-space representation of the tight-binding Hamiltonian.

(b) Discuss σ_{xy} as a function of m.

remember that σ_{xy} of a full band is the integral of the Berry curvature, or the chern number.

(c) Plot the pseudo spin configuration as a function of $e = m/t$ for different values of e_a, choose them wisely.

(d) Assume that the crystal exist only for $x < 0$, and that for $x > 0$ there is vacuum. write the schrodinger equation for the single particle solutions near the Fermi energy and (assume $m > 0$, and that e is close to the critical value).

     (i) What are the boundary condition at $x = 0$

     (ii) What are the conditions for the existence of a gapless solution on the boundary?

     (iii) What is the decay length of the wave function?

     (iv) What happens to the solution at the critical value of the parameter e?

(e) Now assume that the crystal exist for all x. Consider the situation where for $x < 0$ the parameter e is slightly higher than the critical value, and for $x > 0$ the parameter e is slightly smaller than it. Find the gapless 1D mode residing on the boundary.

(f) Can you generalize the model to one that realizes an arbitrary Chern number?