Concepts in Condensed Matter: Exercise 1b

May 2, 2024

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 ($A2$), is positioned directly above the B-atom of layer-1($B1$), while $A1$ and $B2$ are exactly aligned within an hexagon of the other layer.

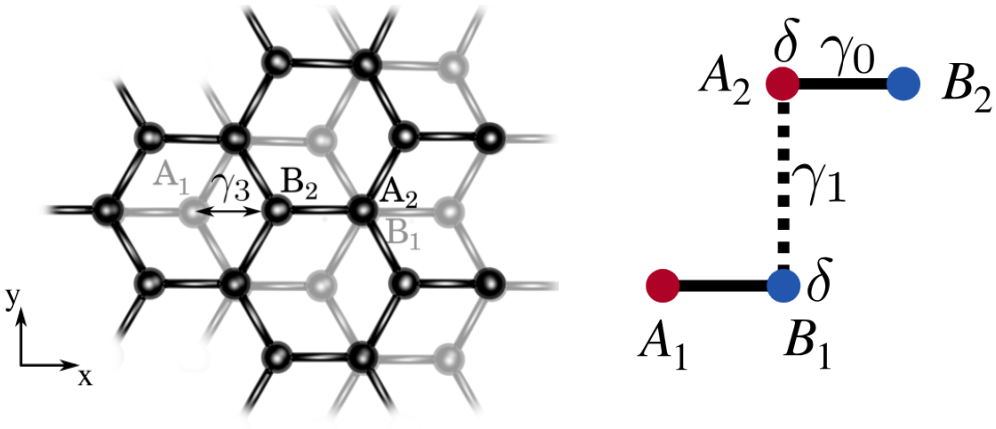

Figure 1: Bernal stacked graphene

(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 γ_0 (ii) the strong inter-layer hopping, which couples overlapping $A2$ and $B1$ atoms, with amplitude γ_1 (iii) the much smaller coupling between neighboring $A1$ and $B2$ atoms, with amplitude γ_3.
Write down the tight-binding Hamiltonian in terms of creation/annihilation operators on the sites $(A1, B1, A2, B2)$. Transform it to k-space and write it in the form

$$\mathcal{H}_{AB} = \sum_{\mathbf{k}} \Psi^{\dagger}_{\mathbf{k}} h\left(\mathbf{k}\right) \Psi_{\mathbf{k}}, \tag{1}$$

where $\Psi_{\mathbf{k}} = (c_{A1,\mathbf{k}}, c_{B1,\mathbf{k}}, c_{A2,\mathbf{k}}, c_{B2,\mathbf{k}})^T$ is a vector of annihilation operators in sublattice space.

(b) From this point on, assume $\gamma_3 = 0$. Diagonalize the Hamiltonian and plot its spectrum, assuming (i) $\gamma_1 \ll \gamma_0$ and (ii) $\gamma_1 \lesssim \gamma_0$.
Compare the results with the results you obtained for mono-layer graphene. What are the similarities? What are the differences?

(c) Is the spectrum gapped? If not, is it protected by a symmetry? (Specify the protecting symmetry).

(d) What are the eigenstates and eigenvectors at the K and K' points?
(Hint: you should be able to write it without making any derivation, using your knowledge about mono-graphene)

(e) Based on your answer to (d), write an effective 2×2 Hamiltonian around the K and K' points, acting on $\tilde{\Psi}_{\mathbf{k}} = (c_{A1,\mathbf{k}}, c_{B2,\mathbf{k}})^T$. perform second-order perturbation theory in tunneling to the two excluded sublattices $(A2, B1)$, assuming $\frac{v_F|k|}{\gamma_1}$ to be a small parameter, in order to derive the effective Hamiltonian. (you may want to consult the book of Sakurai Chapter 5.2)

(f) Assume an electric field is applied perpendicular to the graphene plane, and include the appropriate term in the effective Hamiltonian. What is the effect of this term on the spectrum? does it open a gap? Would it have a similar effect on a single layer of graphene? (Think of the protecting symmetries)

(g) Bonus: Show that for n layers stacked in a similar way (A of layer $l+1$ on top of B of layer l) the dispersion around the K and K' points goes like $|k|^n$

2. **Topological insulator**
Consider the following model on a square lattice

$$\mathcal{H} = \sum_{\mathbf{k}} \left(c^\dagger_{s,\mathbf{k}}, c^\dagger_{p,\mathbf{k}}\right) \begin{pmatrix} m - t\left(\cos k_x + \cos k_y\right) & A\left(\sin k_x + i \sin k_y\right) \\ A\left(\sin k_x - i \sin k_y\right) & t\left(\cos k_x + \cos k_y\right) - m \end{pmatrix} \left(c_{s,\mathbf{k}}, c_{p,\mathbf{k}}\right)^T . \tag{2}$$

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

(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 a few different values of e.

(d) Assume that the crystal exist only for $x < 0$, and that for $x > 0$ there is vacuum. write the Schrödinger equation for the single particle solutions near the Fermi energy (assume $m > 0$, and e 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) Can you generalize the model to one that realizes an arbitrary Chern number?