MASSACHUSETTS INSTITUTE OF TECHNOLOGY

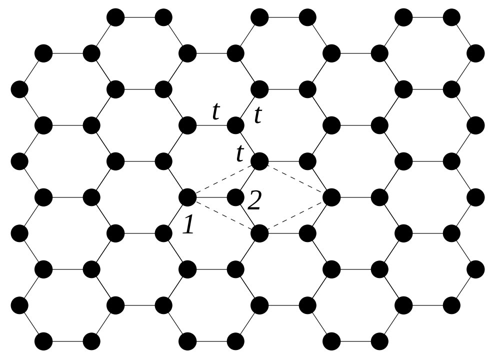
Physics Department

8.231, Physics of Solids I — Due on Wed., Nov. 22.

Problem set #9

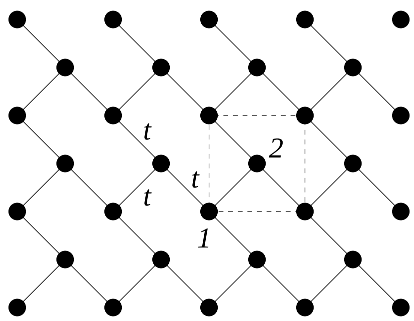
1. **Band structure for graphene – tight binding model**:

   Carbon atoms in graphene form a 2D hexagonal lattice.



Note that there are two atoms per unit cell. We assume that electrons can only hop to the nearest neighbor atoms. The hopping amplitude is t.

To find the band structure of graphene as described by the tight binding model, let us deform the hexagonal lattice to a square lattice



For the square lattice, we can use $|\boldsymbol{i},1\rangle$ and $|\boldsymbol{i},2\rangle$ to represent the states on the Carbon atoms, where

$$\boldsymbol{i} = n_1\boldsymbol{x} + n_2\boldsymbol{y}, \qquad n_1, n_2 = \text{integers}.$$

The hoping Hamiltonian for a single electron can now be written as

$$H = t\sum_{\boldsymbol{i}}(|\boldsymbol{i},1\rangle\langle\boldsymbol{i},2| + |\boldsymbol{i},2\rangle\langle\boldsymbol{i},1|) + t\sum_{\boldsymbol{i}}(|\boldsymbol{i}+\boldsymbol{x},1\rangle\langle\boldsymbol{i},2| + |\boldsymbol{i},2\rangle\langle\boldsymbol{i}+\boldsymbol{x},1|)$$
$$+ t\sum_{\boldsymbol{i}}(|\boldsymbol{i}+\boldsymbol{y},1\rangle\langle\boldsymbol{i},2| + |\boldsymbol{i},2\rangle\langle\boldsymbol{i}+\boldsymbol{y},1|)$$

The three terms represent the the hopping through the three different types of links.

(a) Write the hopping Hamiltonian in the form

$$H = \sum_{\boldsymbol{i},a,b} |\boldsymbol{i}, b\rangle M^0_{ba} \langle \boldsymbol{i}, a| + \sum_{\boldsymbol{i},a,b} \left(|\boldsymbol{i}+\boldsymbol{x}, b\rangle M^1_{ba} \langle \boldsymbol{i}, a| + h.c.\right) + \sum_{\boldsymbol{i},a,b} \left(|\boldsymbol{i}+\boldsymbol{y}, b\rangle M^2_{ba} \langle \boldsymbol{i}, a| + h.c.\right)$$

and find the 2 by 2 matrices M^0, M^1 and M^2. (Hint: note that $(\hat{O} + h.c.) \equiv \hat{O} + \hat{O}^\dagger$.)

(b) Assume that the square lattice has a size $L \times L$ (the lattice constant is assumed to be $a = 1$) and has a periodic boundary condition in both x- and y-directions. Let

$$|\boldsymbol{k}, a\rangle = L^{-1} \sum_{\boldsymbol{i}} e^{i\boldsymbol{k}\cdot\boldsymbol{i}} |\boldsymbol{i}, a\rangle$$

be the plane-wave states that satisfy the periodic boundary condition. Find the quantization condition on $\boldsymbol{k}$. Find the range of $\boldsymbol{k}$ so that different $\boldsymbol{k}$'s in that range will correspond to different states. Show that in terms of the plane-wave states, the hopping Hamiltonian can be rewritten as

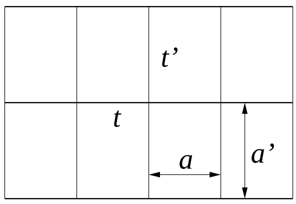
$$H = \sum_{\boldsymbol{k},a,b} |\boldsymbol{k}, b\rangle M_{ba}(\boldsymbol{k}) \langle \boldsymbol{k}, a|$$

Find the 2 by 2 matrix $M(\boldsymbol{k})$.

(c) From the 2 by 2 matrix $M(\boldsymbol{k})$, calculate the dispersions of the two bands $\epsilon_1(\boldsymbol{k})$ and $\epsilon_2(\boldsymbol{k})$. Plot the dispersions. Find the locations in the Brillouin zone where the two band touches, ie $\epsilon_1(\boldsymbol{k}) = \epsilon_2(\boldsymbol{k})$.

2. **Conductivity of a semiconductor with rectangular lattice**

Atoms in a semiconductor form a rectangular lattice. We assume that electrons can only hop to the nearest neighbor atoms. The hopping amplitude is t in the x-direction and t' in the y-direction. The lattice constant is a in the x-direction and a' in the y-direction.



(a) Find the dispersion $\epsilon(\boldsymbol{k})$ of the tight binding band.

(b) Find the mass matrix $(m^{-1})_{ij}$ that describes the mass of an electron near the bottom of the band. (Hint: Near the bottom of band located at $\boldsymbol{k}_0$, $\epsilon(\boldsymbol{k}_0 + \boldsymbol{k})$ has a form

$$\epsilon(\boldsymbol{k}_0 + \boldsymbol{k}) = \frac{1}{2} \sum_{ij} (m^{-1})_{ij} k_i k_j + \text{const.}$$

for small $\boldsymbol{k}$.)

(c) Use the Drude model to calculated the conductivity tensor σ_{ij}. Here we assume that the band is occupied by a dilute gas of electrons (ie the electron density $n \ll 1/aa'$) and the relaxation time is τ. Note that at low temperatures the electrons are near the bottom of the band. (Hint: the equation of motion is given by

$$\frac{dv_i}{dt} = \sum_j (m^{-1})_{ij} F_j - \frac{1}{\tau} v_i$$

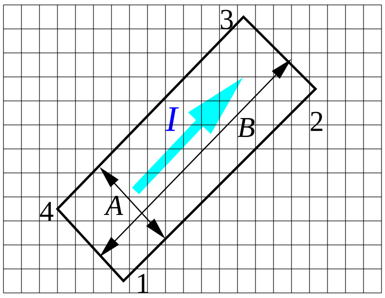
where $\boldsymbol{v}$ is the velocity of the electrons and $\boldsymbol{F}$ is the force that acts on an electron. The conductivity tensor σ_{ij} is defined through

$$J_i = \sum_j \sigma_{ij} E_j$$

where $\boldsymbol{J}$ is the electric current density induced by an electric field $\boldsymbol{E}$.)

(d) Find the resistivity tensor defined through $E_i = \sum_j \rho_{ij} J_j$.

(e) A rectangular stripe of the 2D crystal is cut as shown in the figure below.



The angle between the edge of the stripe and x-direction is 45°. The size of the stripe is $A \times B$. If we pass a current I through the stripe, what is the voltage drop between the corner 1 and the corner 2? What is the voltage drop between the corner 1 and the corner 4?

3. Prob. 2 on page 218 of Kittle.