8.511 Theory of Solids I **Problem Set 4** **Due 8:00pm**
October 13, 2014

1. Honeycomb Lattice

(a) Consider a graphite sheet which forms a honeycomb lattice. The separation between carbon atoms is a.

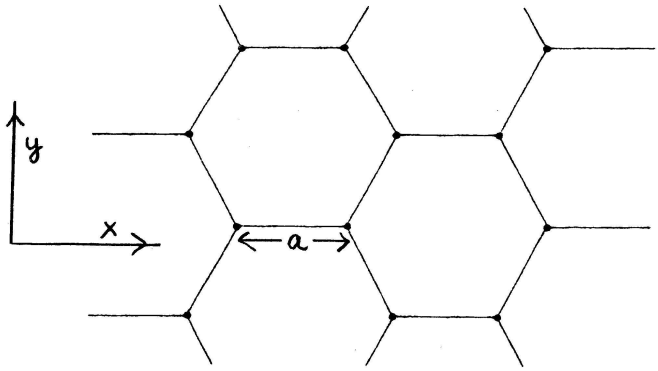

FIG. 1:

Write down the Bravais lattice vectors in terms of the two-dimensional Cartesian coordinates. There are two carbon atoms in the unit cell. Write down the basis vectors $\boldsymbol{\tau}_\alpha$, α = 1,2. Draw the first Brillouin zone which is consistent with the above lattice and label the dimension. (Note that the orientation matters.)

(b) The carbon atom has four valence electrons in the $2s$ and $2p$ orbitals. For the purpose of this problem, we focus on the p_z orbitals which form a π band by their overlap between nearest neighbors. One electron per carbon is assigned to the p_z orbital. In the following we construct the π band structure using a nearest-neighbor tight binding approximation.

Define

$$\chi^\alpha_{\mathbf{k}} = \frac{1}{\sqrt{N}} \sum_i e^{i\mathbf{k}\cdot\mathbf{R}^\alpha_i} \phi(\mathbf{r} - \mathbf{R}^\alpha_i). \tag{1}$$

α labels the basis, N is the number of unit cells, ϕ is the p_z orbital, $\mathbf{R}^\alpha_i = \mathbf{R}_i + \boldsymbol{\tau}_\alpha$ is the position of the carbon atoms in each basis set ($\{\mathbf{R}_i\}$ is the set of Bravais lattices). The tight binding wavefunction is

$$\psi_{\mathbf{k}} = \sum_{\alpha} c_{\alpha} \chi^{\alpha}_{\mathbf{k}} \tag{2}$$

We shall keep only matrix elements of the Hamiltonian between nearest-neighbor carbon atoms. We assume orbitals on neighboring atoms are orthogonal. We set the energy of the orbital to be zero. Show that the Schrodinger equation $H\psi_{\mathbf{k}} = E(\mathbf{k})\psi_{\mathbf{k}}$ reduces to a 2×2 matrix

$$M_{\mathbf{k}} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} \quad = E(\mathbf{k}) \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} \tag{3}$$

where $M_{\mathbf{k},11} = M_{k,22} = 0$

$$M_{\mathbf{k},12} = M^*_{\mathbf{k},21} = t \sum_i e^{i\mathbf{k}\cdot\boldsymbol{\mu}_i} \tag{4}$$

where $\boldsymbol{\mu}_i$ is the set of nearest neighbors to a given atom and $t =< \phi(\mathbf{r})|H|\phi(\mathbf{r} - \boldsymbol{\mu}_i) >$ is the matrix element of the Hamiltonian between nearest neighbors.

(c) Calculate the energy bands $E(\mathbf{k})$ by solving Eq. (3).

2. Carbon Nanotubes

(a) It turns out that the band structure you found in Problem 1 has the following interesting property. $E_{\pm}(\mathbf{k}) = 0$ for $\mathbf{k}$ at the Brillouin zone corners. Furthermore, near the corner with momentum $\mathbf{K}$, they can be expanded as

$$E_{\pm}(\mathbf{k}) = \pm\frac{3ta}{2}|(\mathbf{k} - \mathbf{K})| \tag{5}$$

i.e., the energy bands near the zone corners are cones which touch at $E = 0$. In particle physics this is called the massless Dirac cone. Verify that Eq. (5) is true. We will proceed with the assumption that the low energy eigenvalues are well approximated by these Dirac cones centered at the zone corners.

(b) How many of these Dirac cones are inequivalent? Show that the Fermi energy equals zero. What is the density of states for energy E near the Fermi energy?

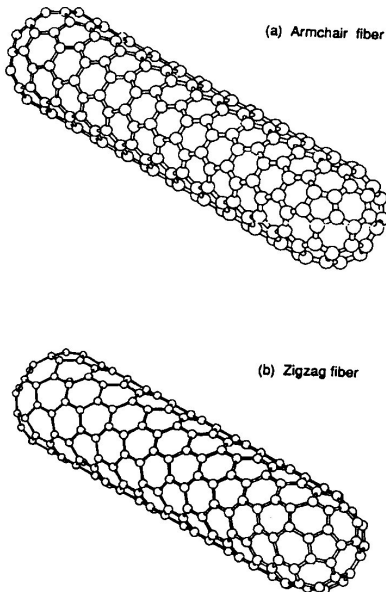

FIG. 2: Atomic arrangements of carbon atoms in the (a) armchair fiber and (b) zigzag fiber. From Saito, Fujita, Dresselhaus and Dresselhaus, Phys. Rev. B **46**, 1804 (1992).

(c) Carbon nanotubes are formed by rolling up strips of graphite sheets. Rolling along the x or y directions produces two inequivalent nanotubes, shown in Fig. 2. We now consider the band structure of these nanotubes.

The periodic boundary condition restricts the allowed $\mathbf{k}$ values to a set of parallel lines in the Brillouin zone. Identify these lines for the armchair tube and the zigzag tube, respectively.

(d) The low energy bands are determined by the lines which come closest to the Dirac cones. For the armchair tube, show that the system is metallic, i.e., there is no energy gap at the Fermi energy. Sketch the energy band near the Fermi energy. Calculate the density of states near $E = 0$.

(e) Find the conditions under which the zigzag tubes may be metallic or semiconducting. Sketch the energy band for the semiconducting case. In the metallic case, how does the density of states near the Fermi energy compare with that of the armchair tube?