8.231 Physics of Solids I — Fall 2017
Problem Set 5

Posted: Tuesday, Oct 10, 2017
Due: **Tuesday, Oct 17, 2017**

Readings (Optional)

- Simon, Steven H. *The Oxford Solid State Basics*, Chapter 12-14.

Note: Bonus problems are more challenging. It is fine you do not solve them. By solving them you can earn extra credits.

Problem 1

Some 3D Crystal Structures

The crystal structure can be fully specified by (i) the lattice (smallest repeating unit, i.e., the unit cell) and (ii) the basis (locations of atoms within the unit cell). Write down (i) the primitive lattice vectors and (ii) the basis for the following crystal structures.

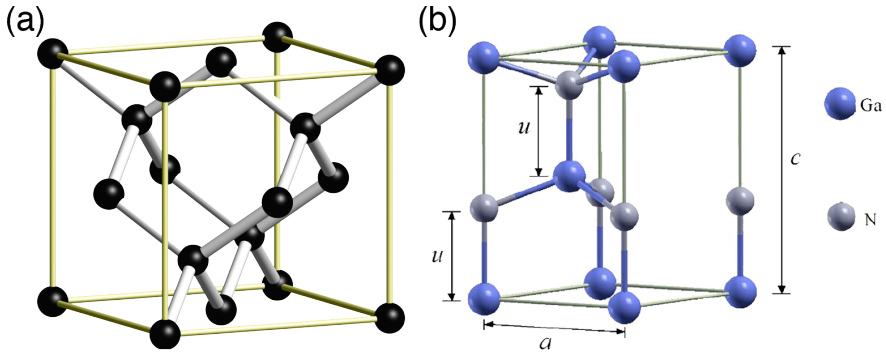

Figure 1: Crystal structures for diamond (left) and GaN (right).

(a) Diamond, shown in Figure 1(a). The lattice constant is a.
(Hint: There are two atoms per primitive cell.)

(b) Isamu Akasaki, Hiroshi Amano and Shuji Nakamura are awarded Nobel Prize in Physics in 2014 "for the invention of efficient blue light-emitting diodes (LED) which has enabled bright and energy-saving white light sources". GaN is a wide-gap semiconductor used for blue LED, which crystalizes in wurtzite structure as shown in Figure 1(b).
(Hint: There are four atoms per primitive cell.)

Problem 2

Reciprocal Lattice

(a) Consider three dimensional lattices. Denote the volume of the unit cell of the direct lattice as Ω, and that of the reciprocal lattice (i.e., first Brillouin zone) as Ω^*. Prove $\Omega\Omega^* = (2\pi)^3$.

(Hint: The volume of a parallelepiped spanned by $\mathbf{x}$, $\mathbf{y}$ and $\mathbf{z}$ is $\mathbf{x} \cdot (\mathbf{y} \times \mathbf{z})$.)

(b) Prove the reciprocal lattice of fcc (face-centered cubic) lattice is bcc (body-centered cubic) lattice.

Problem 3

Emergent Dirac Fermion in Graphene

Andre Geim and Konstantin Novoselov are awarded Nobel Prize in Physics in 2010 "for groundbreaking experiments regarding the two-dimensional material graphene".

Part I: Crystal Structure The crystal structure of graphene is shown in Figure 2. You may assume the spacing between carbon atoms is a.

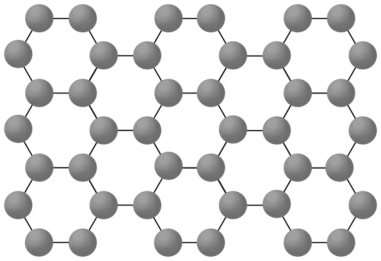

Figure 2: Crystal structure of graphene.

(a) What are the primitive lattice vectors $\mathbf{a}_1$ and $\mathbf{a}_2$? Draw the primitive unit cell.

(b) What are the reciprocal lattice vectors $\mathbf{b}_1$ and $\mathbf{b}_2$? Draw the first Brillouin zone (BZ), which should be a hexagon.

(c) Two points are equivalent in the BZ if they differ by the translation of a reciprocal lattice vector. Show that there are only two inequivalent vertices in the first BZ, although the hexagon has six vertices. These two points are denoted K and K' in the literature. Write down their coordinates.

Part II: Tight-binding Model The carbon atom has four valence electrons. Three of them form σ bonding (sp^2 hybridization) connecting carbon atoms with each other. The remaining π bonding (p_z orbital) is responsible for the electronic properties of graphene, which we will consider below using a tight-binding model.

Assume only there is nearest neighbour hopping between carbon atoms, whose strength is t, and the on-site energy for p_z orbital is $\mathcal{E}$.

(a) Show that the band dispersion is obtained by solving the eigenvalue of the following matrix:

$$H(\mathbf{k}) = \begin{pmatrix} \mathcal{E} & -t\sum_{i=1}^{3} e^{-i\mathbf{k}\cdot\mathbf{d}_i} \\ -t\sum_{i=1}^{3} e^{i\mathbf{k}\cdot\mathbf{d}_i} & \mathcal{E} \end{pmatrix}. \tag{1}$$

This matrix is called the Bloch Hamiltonian. Find out what $\mathbf{d}_i$, $i = 1, 2, 3$ are by yourself.

(Hint: The ansatz for the tight-binding model on a *simple* two-dimensional square lattice is of the form $|\psi(\mathbf{k})\rangle \sim \sum_i e^{i\mathbf{k}\cdot\mathbf{R}_i} |i\rangle$, where $\mathbf{R}_i$ is the position of the atom i.)

(b) Solve the band dispersion $E(\mathbf{k})$. Your result should look like Figure 3:

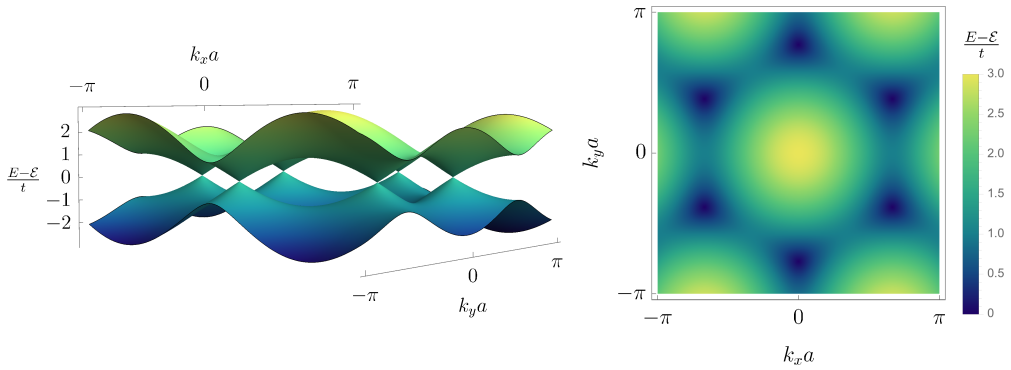

Figure 3: Band dispersion of graphene. Left: Both bands; Right: Upper band.

(c) Expand the Bloch Hamiltonian $H(\mathbf{k})$ near K and K' to the leading order of $\mathbf{k}$. You shall find the Hamiltonian is of the same form of Dirac equation in two dimensions:

$$H_{\text{Dirac}} = c\boldsymbol{\sigma} \cdot \mathbf{p} + mc^2\sigma_z. \tag{2}$$

Here $\boldsymbol{\sigma} \equiv (\sigma_x, \sigma_y)$ are Pauli matrices. Dirac equation governs the motion of relativistic fermions. Identify "speed of light" c and fermion "mass" m of the "emergent Dirac fermion" in graphene. What is the difference between the Dirac fermion at K and K'?

(Hint: You may need to rotate the coordinate of frame in order to reproduce Dirac equation.)

(d) Is graphene an insulator or a metal? What is the density of state at Fermi energy? You may want to recall the Problem 1 in Pset 2.

(e) (Bonus) The crystal structure of boron nitride (BN) is similar to graphene (Figure 4), except that the p_z atomic energy is different boron and nitrogen. This energy difference is denoted as Δ. What is the band structure of BN? What is the "velocity of light" and fermion "mass" in BN? Is BN an insulator or a metal?

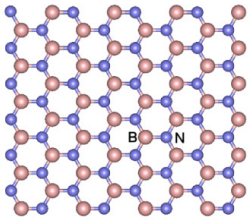

Figure 4: Crystal structure of boron nitride.