Condensed Matter Physics I
23 June 2014
(3 hours)

- Solve all the exercises.
- Give all the steps necessary to understand in detail the solution procedure. Answers with the final result only or with insufficient details will not be considered valid.

Exercise 1: *Electronic bands in 1D and 2D and density of states*

Consider a 1D lattice with lattice constant a with a dispersion relation for the electronic band given by:

$$E(k) = E_0 + 4\gamma sin^2\left(\frac{ka}{2}\right)$$

in a tight-binding model, with γ being a (positive) constant.

1. Calculate the effective electron mass m^* in the extrema of the band, specifying if it is electron-like or hole-like.
2. Calculate (write explicitly the expression) the electronic density of states $g(E)$.
3. What is the Fermi energy in case of a half filled band (one electron per unit cell)?
4. Show that it is symmetric with respect to a proper energy value (and write which one). Calculate its minimum and make a sketch of $g(E)$.
5. Consider now a 2D square crystal with lattice parameter a. Considering s band, no overlap, nearest neighbour hopping integrals, write the expression of the energy band.
6. Sketch the first Brillouin zone and draw the Fermi surface (curve, since we are in 2D) in the (k_x, k_y) plane.

Exercise 2: *Crystal structures*

Boron nitride is a chemical compound with chemical formula BN, consisting of equal numbers of boron and nitrogen atoms. It exists in a stable *hexagonal close-packed* crystal structure corresponding to graphite. The Figure shows the in-plane atomic arrangement, with the in-plane lattice constant is 2.5 Å. We consider the 2D problem, since the bonding between adjacent layers is very weak.

1. Which is the 2D Bravais lattice? Sketch and describe a set of primitive vectors $\vec{a}_i$ and (if existing) of the basis $\vec{d}_j$.

2. Specifying its primitive vectors $\vec{b_j}$, sketch the reciprocal lattice, the first and the second Brillouin zone.

3. Treating the atoms as identical scatterers, calculate explicitly the geometrical structure factor for a generic reciprocal lattice vector $\vec{K} = n_1\vec{b_1} + n_2\vec{b_2}$ as a function of n_1, n_2 and discuss for which $\vec{K}$ the intensity of the Bragg peaks is maximum.

4. Show that for a particular choice of the origin of the direct space, the structure factor is real.

5. Indicating with f_B and f_N the scattering amplitudes of B and N, assume that they are both real. Which is the condition on the relative form factors that causes the intensities of some of the Bragg peaks to vanish?

6. You could now afford the full 3D problem, knowing that the periodicity along the c-axis is 6.66 Å. Give the lattice structure, specifying the atoms in the unit cell (give the set of primitive vectors $\vec{a}_i$ and of the basis $\vec{d}_j$).