Electrons in crystals – I written test –academic year 2006/2007, November 6, 2006(revised)

(Time: 3 hours)

Solve all the exercises. Each one corresponds to a maximum score of 18 (36 total for both). If the score is between 33 and 36 it is considered equal to 30/30 cum laude, if it is between 30 and 32 it is considered equal to 30/30.

Exercise 1: Free electron model

$First \ part$

Sodium (Na) in normal conditions of temperature and pressure is a metal with BCC structure, with density of about 2.7 g cm⁻³, mass number of about 23 and Fermi energy E_F of about 3 eV.

- 1. Calculate the Fermi temperature T_F .
- 2. Calculate the Fermi velocity v_F and the average kinetic energy at 0 K.
- 3. Which is the variation of the average kinetic energy at room temperature?
- 4. If you would consider the electron gas as a classical gas, which would be the average kinetic energy at 0 K? And at room temperature?
- 5. From the given Fermi energy, calculate the density n of free electrons present in the metal.
- 6. Calculate the numerical density of Na atoms and then the average number of free electrons per atoms. Is it what you expected? Comment.

Second part

- 1. Derive the expression of the density of the electron states for a two-dimensional electron gas.
- 2. Considering the electron density n as a parameter, study the behaviour of E_F as a function of the temperature.
- 3. Discuss the high and low temperature limits.
- 4. Derive the expression of the density of the electron states for a four-dimensional electron gas.

Exercise 2: Diffraction of neutron on Cesium Chloride

Consider Cesium Chloride. Let α and β be the atomic form factor of Cl and Cs respectively. In the following we will not consider the dependence of α and β on the transferred wave vector. This structure is evidently a Bravais lattice with basis.

- 1. Specify which is the Bravais lattice and the basis.
- 2. Write the expression of the intensity of the diffracted wave in terms of the geometrical structure factor $S(\mathbf{k})$.
- 3. Write the expression of $S(\mathbf{k})$ for a generic \mathbf{k} of the reciprocal space.
- 4. Calculate explicitly $S(\mathbf{K})$ for $\alpha = \beta$ for \mathbf{K} of the reciprocal *lattice*.
- 5. As before, but with $\alpha = -\beta$
- 6. What is the relationship between the two lattices found in (d) and (e)?

NOTE:

- 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.
- When required, numerical evaluations should be given exactly with 3 significant figures, if not otherwise indicated.