Electrons in crystals - I written test academic year 2007/2008, 29/10/07

(*time 2:30 hours)*

- Solve all the exercises, corresponding to a total maximum score of 36. 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.
- 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.

Exercise 1: *Free electrons model*

1. Given the density of Potassium (Atomic mass number A=39) in the metallic state equal to 0.86 $g \cdot cm^{-3}$, what is its plasma frequency?
2. Calculate the mean electron kinetic energy at 0K, in the free electron approximation.
3. Calculate the electronic contribution to the specific heat at T = 300 K within the Sommerfeld's theory.
4. Justifying the answer, indicate whether the Fermi energy of a metal increases, by decreasing the volume V, as:
   (a) V^{-1}
   (b) $V^{-1/2}$
   (c) $V^{-2/3}$
   (d) in another way.
5. Derive the expression of the electronic density of states in the one-dimensional free electron case.
6. Indicate whether in that case the Sommerfeld's expansion is valid or not, and give the explicit expression of the chemical potential as a function of the temperature T up to the II order in T.

Exercise 2: *Crystalline structures*

1. Iron at room temperature has a BCC structure with lattice parameter $a = 2.86$ Å. At 910^o C it has a phase transition to a FCC structure. Neglecting the volume variation, calculates the percentage of variation of the minimum interatomic distance.

2. Ni and Al form an ordered alloy Ni_3Al, with Ni and Al atoms distributed on the sites of an FCC lattice, occupying alternatively planes of the (001) family. Sketch the unitary cell of this structure, indicate which is the corresponding Bravais lattice and write the coordinates of the basis.

Exercise 3: *Neutron diffraction from Cesium Chloride*

Consider Cesium Chloride and indicate with f_{Cl} and f_{Cs} the atomic form factor of Cl and Cs respectively. In the following we are going to neglect their dependence on the transferred wave vector. Cesium chloride forms a Bravais lattice with basis.

1. Indicate the Bravais lattice and the vectors of the atomic basis $\mathbf{d}_j$.

2. Write the explicit expression of the geometric structure factor on a generic vector of the reciprocal space: $S(\mathbf{k}) = \sum_j f_j e^{i\mathbf{d}_j \cdot \mathbf{k}}$

3. Calculate explicitely $S(\mathbf{k})$ for f_{Cl}=f_{Cs} on the reciprocal lattice vectors $\mathbf{K}$.

4. Considering again f_{Cl}=f_{Cs}, write the condition that must be satisfied by the $\mathbf{K}$ vectors in order to make $S(\mathbf{K})$ non vanishing; which kind of lattice do those $\mathbf{K}$ vectors form?