Condensed Matter Physics I
I test - 20 November 2015
(2 hours 30')

Exercise 1: *Free electrons - Sommerfeld model*

The Fermi energy for copper at T = 0 K is E_F=7.0 eV. Consider valid the Sommerfeld model (free and independent electrons obeying the Fermi-Dirac distribution function).

1. Assume that the chemical potential does not vary with the temperature and calculate the probability of an energy level at 7.15 eV being occupied by an electron at: 0 K, 300 K, 1000 K.

2. Calculate now the chemical potential at 300 K and at 1000 K and discuss the assumption used in (1).

3. Estimate the fraction of electrons excited above the Fermi level at room temperature for Cu.

4. Consider Fermi and Boltzmann distributions. Above which energies measured from the Fermi-level E_F (i.e. $\Delta E = E - E_F$) the Fermi distribution can be approximated by a Boltzmann distribution with an error of less than 10% and 1%, respectively, at temperatures T = 300 K and T= 1000 K ?

5. Calculate the valence electron density from E_F.

6. Knowing that the mass density of copper is 8.96 g/cm^3 and its atomic mass is 63.546 amu, use these data to calculate the valence electron density in an alternative way. How does this results compare with that in (5)?

Exercise 2: *Crystalline structures*

Heusler alloys (showing half-metallicity at room temperature, i.e., a metallic character in one spin channel and semiconducting in the other) are categorized into two distinct groups according to their crystalline structure: half Heusler alloys and full Heusler alloys, schematically drawn in Figs. (a) and (b), respectively.

1. Describe structure (a) indicating the chemical formula ($X_n Y_m Z_\ell$) and the Bravais lattice, writing a set of primitive vectors and those of the *basis*.
2. Same as 1. for structure (b).
3. Calculate the structure factor S($\mathbf{K}$) for the structure (b) for $\mathbf{K}=\frac{4\pi}{a}(100)$ and $\mathbf{K}=\frac{4\pi}{a}(110)$.
4. Do the same when the atomic form factors of atoms Y and Z are equal. The diffraction pattern in this case would resemble that of ... ? *(justify conceptually and analitically your answer!)*
5. Same as 4., when the atomic form factors of atoms X, Y and Z are equal.