Condensed Matter Physics I
I test - 14 November 2013
(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: *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: *BCC and FCC crystalline structures*

At low and moderate temperature, iron has the BCC crystal structure. As the material is heated above 913^{o}C, its structure changes to FCC. (This property of iron is at the base of the production, processing and properties of steel.)

1. What are the coordinates of the largest interstitial hole in the FCC structure? (Hint: where should we put an extra atom if we were looking for the most room?)

2. Considering that the lattice parameters for the two structures of iron are a(BCC) = 2.910 Å and a(FCC) = 3.647 Å, what is the fractional volume change of iron in the BCC→FCC transformation upon heating?

3. What would be instead the fractional volume change if Fe atoms of fixed radius pack as hard spheres?

4. Explain why X-ray diffraction may be observed in first order from the (110) planes of a crystal with a BCC lattice, but not from the (110) planes of a crystal with a FCC lattice.

5. Derive the general selection rules for which planes are observed in BCC and FCC lattices. Show that these selection rules hold independent of what atoms are in the primitive unit cell, so long as the lattice is BCC or FCC respectively.

6. What are the Miller indices of BCC and FCC (100) planes in their *primitive* unit cells? (pay attention: *not* with reference to the conventional simple cubic structure)