Condensed Matter Physics I
Final written test
academic year 2011/2012
February 24, 2012

(*Time: 3 hours*)

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.

Exercise 1: *Sommerfeld model*

Considered free and non-interacting electrons in the Sommerfeld model.

1. Show in general that the density of states at the Fermi energy for a free electron gas in d-dimension can be written with respect to the electron density n and the Fermi energy E_F as:
$$g^{dD}(E_F) = \frac{d}{2}\frac{n}{E_F}$$

2. Consider a triangular lattice with lattice parameter a=5Å in two dimensions, with 6 electrons per site: calculate the radius of the Fermi sphere (circle).

3. Make a sketch of the reciprocal lattice and, in scale, of the Fermi sphere for (2.).

4. Calculate the density of states at the Fermi energy for (2.) (*give a number with units of measure!)*

5. Consider now a 3D electron gas of an elemental metal made of atoms of valence Z. Starting from the expression of the specific heat as a function of the temperature and Fermi energy,
$$c_v = \frac{\pi^2}{2}\left(\frac{k_B T}{E_F}\right) n k_B,$$
give an expression of c_v as a function of the valence Z and Fermi energy E_F only (with fundamental constants and numerical coefficients, of course).

6. The experimental heat capacity of potassium metal at low temperatures has the form: c_v = (2.08 T + 2.6 T^3)mJ mol^{-1} K^{-1} where T is in Kelvin. Consider which is the electronic term in this expression and, using only this datum and the valence Z of K, make an estimate of the Fermi energy (in eV) for potassium metal using the Sommerfeld model.

Exercise 2: *Crystal Structures, lattice planes, diffraction*

1. We have shown in class that the spacing d between the planes with Miller indices $(hk\ell)$ in a *cubic* crystal with lattice parameter a is

$$d = \frac{a}{\sqrt{h^2 + k^2 + \ell^2}}$$

   What is the generalization of this formula for an *orthorhombic* crystal?

2. For an orthorhombic lattice, show that $|b_j| = 2\pi/|a_j|$. Hence, show explicitly that the length of the reciprocal lattice vector $\mathbf{G} = h\mathbf{b_1} + k\mathbf{b_2} + \ell\mathbf{b_3}$ is equal to $2\pi/d$, where d is the spacing of the $(hk\ell)$ planes (see above).

3. $BaTiO_3$ has a primitive cubic lattice and a basis with atoms having fractional coordinates (in units of a):
   Ba (0,0,0) ; Ti (1/2, 1/2, 1/2) O: (1/2, 1/2, 0), (1/2, 0, 1/2), (0, 1/2, 1/2).
   Sketch the unit cell.

4. Indicating with f_{Ba} the atomic form factor for Ba, etc. ... (neglect their dependence on the scattering vector), write the general expression of the (crystal) structure factor $S_{hk\ell}$, where $hk\ell$ are the coefficients of a reciprocal lattice vector $\mathbf{K}_{hk\ell}$ written on the conventional reciprocal lattice basis set.

5. Show that the structure factor for the (00ℓ) Bragg reflections is given by $S_{00\ell} = f_{Ba} + (-1)^\ell f_{Ti} + [1 + 2(-1)^\ell] f_O$.

6. Calculate the ratio I_{002}/I_{001}, where $I_{hk\ell}$ is the intensity of the X-ray diffraction from the $(hk\ell)$ planes. You may assume that the atomic form factor is proportional to atomic number (Z) [Z(Ba) = 56, Z(Ti) = 22, Z(O) = 8]