Electrons in crystals
Final written test
academic year 2010/11
June 9, 2011

(*Time: 3 hours*)

Exercise 1: *Free electrons - Sommerfeld model*

Copper (Cu) in normal temperature and pressure conditions is a metal with FCC structure and mass density of about 8.96 g cm^{-3}. It has an average mass number of 63.55 and Fermi energy of 7.00 eV.

1. From the given Fermi energy, derive the density n of the free electrons.
2. Using the Sommerfeld expansion, calculate the electronic contribution to the specific heat at room temperature.
3. Using now its mass density and its mass number, calculate the *atomic* density n_{at}. Using this result and the result in (1), calculate the average number of free electrons per atom. Is it what you would expect?

Exercise 2: *Diffraction*

1. The lattice parameter of a cubic crystal is a_0=2.62 Å. Determine the Bragg angle correspondent to the reflection from planes (100), (110), (200) and (211) when the wavelength of the incoming beam is λ=1.54 Å.
2. Knowing that, for the same wavelength, the Bragg reflection angle from (110) planes of Iron (BCC structure) is 22°, calculate the lattice parameter of Iron.
3. Calculate the atomic form factor for an atom with Z valence electrons considering them uniformly distributed inside a sphere of radius R.

Exercise 3: *Band structures for free electrons*

Consider the BCC lattice.

1. Plot the contours of the Ist Brillouin zone in the $k_x k_y$ plane, specifying the relevant points.
2. Write explicitly the expression of the first energy band $\mathcal{E}_1(\mathbf{k})$ for free electrons from Γ to N=$\frac{2\pi}{a}(1/2,\, 1/2,\, 0)$ as a function of the modulus of $\mathbf{k}$ and plot it in the reduced zone scheme.
3. Calculate and plot the other three lowest bands, $\mathcal{E}_n(\mathbf{k})$ for $n = 2, 3, 4$.

Exercise 4: *Tight binding model and velocity of Bloch electrons*

1. Consider a 1D crystal and write the expression of the energy in the tight binding model for s band, neglecting the overlap but including the interaction with any order of neighbors.
2. Write explicitly the expression for the velocity of a Bloch electron in this model and show that it vanishes in the center and at the boundaries of the Ist Brillouin zone.
3. Calculate the effective mass in those points; compare and comment the results.

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.