Electrons in crystals
Final written test
academic year 2012/13
June 11, 2013

(*Time: 3 hours*)

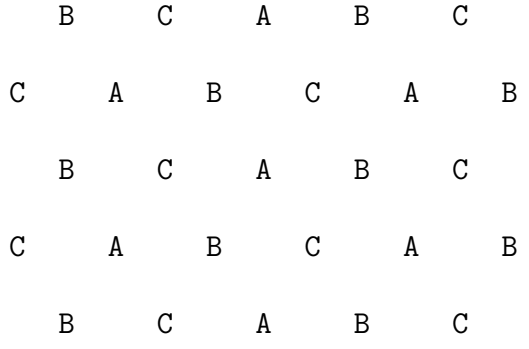
Exercise 1: *Free electrons - Sommerfeld model*

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 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: *Crystal lattices; 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. Consider the 2D lattice in the figure below, made of 3 different atomic species A, B, and C, occupying the sites of a triangular lattice. Let d be the nearest neighbour distance. Write the formula unit ($A_nB_mC_\ell$ with m, n, ℓ=...?), describe the unit cell, sketch it in the figure, giving a possible choice of the primitive translation vectors $\{\mathbf{a}_i\}$ and the basis vectors $\{\mathbf{d}_i\}$ and calculate its area.



Exercise 3: *Electrons in 2d: Fermi surfaces, weak potential*

1. Consider a two-dimensional metal with rectangular Bravais lattice with basis vectors $\mathbf{a_1}$=(a,0) and $\mathbf{a_2}$=(0,b), with a=4Å and a=2b. Give the basis vectors $\mathbf{b_1}$ and $\mathbf{b_2}$ of the reciprocal lattice (using cm^{-1}) and sketch the first Brillouin zone.

2. Consider free electrons, give the general expression of the Fermi "sphere" (or better, "circle", in 2d) as a function of the electron density; then, calculate explicitely the numerical value of its radius in the present case, considering one electron per unit cell.

3. Draw such free-electron Fermi "sphere" in the same (k_x, k_y) plot of the first Brillouin zone, showing and specifying whether it is totally within the first Brillouin zone or not. If not, make a sketch concerning *where* and *how* it would be modified by the presence of a weak periodic potential, and a sketch of a possible second band within the first Brillouin zone.

Exercise 4: *Tight-binding model*

Consider s-type electrons in a 1D lattice with lattice spacing a. Use a *tight binding* model with *first and second neighbor hopping* and no *overlap*. With reference to the definition $\gamma(\mathbf{R})$ in the texbook, consider: $\gamma(\mathbf{R}_{NN})$=t where $\mathbf{R}_{NN}$ is between two nearest beighbors, $\gamma(\mathbf{R}_{NNN})$=t' where $\mathbf{R}_{NNN}$ is between two next- nearest beighbors, otherwise $\gamma(\mathbf{R})$=0.

1. Show that the explicit expression for the energy band (using $E_s - \beta \equiv E_0$ (see again the textbook for the definition of β) is:

$$E(k) = E_0 - 2[t\ cos(ka) + t'\ cos(2ka)]$$

2. Consider $t' = -t$ and make a plot in the first Brillouin zone, identifying and writing the maxima and minima points.

3. Calculate the effective mass in those points.

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.