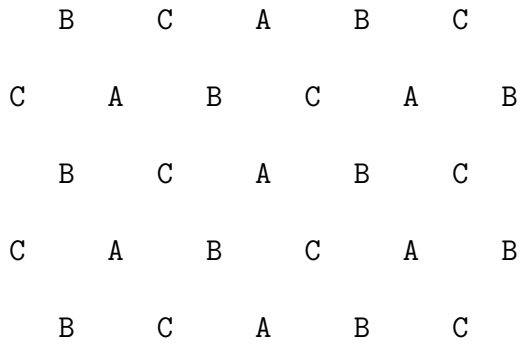
Condensed Matter Physics I
Final written test
academic year 2009/2010
February 18, 2010

(*Time: 3 hours*)

Exercise 1: *Bravais lattices with basis and structure factors*

Consider the 2D lattice in the figure, constituted by 3 different atomic species A, B and C, occupying sites of a triangular lattice. Let d be the AB, BC, AC nearest neighbor distances.



1. Sketch the primitive cell, write the formula unit ($A_nB_mC_\ell$ with m, n, ℓ=...?), a possible choice of the primitive translation vectors $\{\mathbf{a}_i\}$ and the vectors of the basis $\{\mathbf{d}_i\}$ and the area of the unit cell.

2. Write the primitive translation vectors of the reciprocal lattice $\{\mathbf{b}_i\}$ and calculate the area of the reciprocal space unit cell.

3. Suppose that atoms B and C are identical, C=B$\neq$A. Answer again to question (1).

4. Suppose now that A=B=C and answer once again to question (1).

5. Go back to the general case where A, B and C are different. Assuming that the atomic form factors are f_A, f_B and f_C, calculate the geometrical structure factor S($\mathbf{K}$) on the reciprocal lattice vectors.

6. Specify the conditions that need to be satisfied to have interference maxima in case of $f_A = f_B = f_C$ and comment the result.

Exercise 2: *Tight binding*

Consider a square lattice with one atom and one s orbital on each site. Neglect overlap between orbitals on different sites. Neglect also hopping integrals between atoms that are not nearest neighbors (NN) or next nearest neighbors (NNN) and let's indicate with γ_{NN} and γ_{NNN} these two non zero integrals.

1. Write the explicit expression for the dispersion of the energy band E($\mathbf{k}$).
2. Plot E($\mathbf{k}$) in the first Brillouin zone along the line ΓAB, where Γ=(0,0), A=(π/a,0) and B=($\pi/a, \pi/a$) for γ_{NNN}/γ_{NN}=1/4
3. As in (2), but for γ_{NNN}/γ_{NN}=1/2.
4. As in (2), but for γ_{NNN}/γ_{NN}=3/4.
5. Calculate the elements of the inverse mass tensor for γ_{NNN}/γ_{NN}=1/4 at the minimum and at the maximum of the band. Where is the effective mass bigger?
6. Calculate the elements of the inverse mass tensor for γ_{NNN}/γ_{NN}=3/4 at the minimum and at the maximum of the band.

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.