Condensed Matter Physics I
Final written test
academic year 2011/12
July 11, 2012

(*Time: 3 hours*)

Exercise 1: *Free electrons - Sommerfeld model*

The Sommerfeld model is very accurate in describing the properties of the elemental solid Na. The structure is BCC with lattice parameter a_0=4.23 Å.

1. The Fermi sphere is fully contained in the first Brillouin zone or not? Justify numerically the answer.
2. What about all the other elemental solids made of the atoms of the I column of the periodic table? Justify numerically the answer.
3. These solids are metallic or not? Justify the answer.

Exercise 2: *Bravais lattices with basis*

The copper-oxide high-Tc superconductors contain CuO_2 planes (sketch in Fig. (1)).

1. Write a possible choice of basis vectors, descrive and sketch the primitive cell.
2. Assuming that the atomic form factors are such that $f_{Cu} = 2f_O$, calculate the geometrical structure factor S(**K**) on the reciprocal lattice vectors, and specify for which **K** it is maximum and for which ones it vanishes.
3. There are other compounds having a similar structure, but with non equivalent atoms in the oxigen positions, as indicated in Figure (2). Specify in this case which is the primitive cell, the lattice parameter and the basis vectors of the reciprocal space.

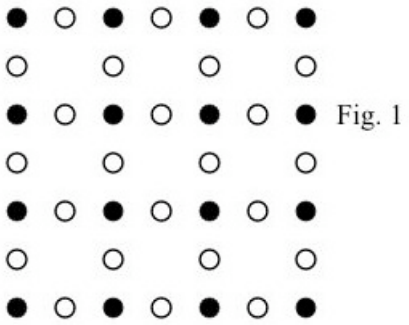

Fig. 1

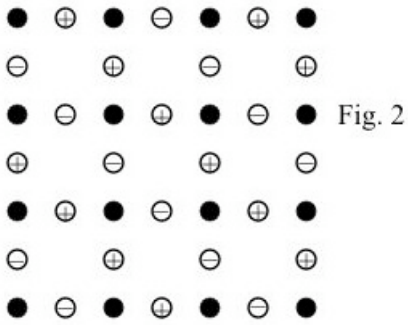

Fig. 2

Exercise 3: *Band structures for free electrons*

Consider the BCC lattice.

1. Plot the contours of the I Brillouin zone in the $k_x k_y$ plane, specifying the relevant point.
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*

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. 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 larger?

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.