Condensed Matter Physics I final written test academic year 2013/2014 February 17, 2014

(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: Crystalline structures

(You may solve this first exercise directly on this sheet of paper) The figure below shows a 2D periodic array of atoms of two different types.

- 1. Identify the type of Bravais lattice, write the primitive basis vectors $\{\mathbf{a}_i\}$, sketch them in the figure, together with the corresponding primitive unit cell.
- 2. Is this a *simple* Bravais lattice or is it a *lattice with a basis*? If it is a *lattice with a basis*: (i) how many points are in the basis? (ii) sketch them in the figure and write the corresponding vectors.
- 3. Write the primitive vectors $\{\mathbf{b}_i\}$ of the reciprocal lattice.
- 4. Write the geometrical structure factors $S(\mathbf{K})$ on a generic reciprocal lattice vector \mathbf{K} .
- 5. Specify the expression of $S(\mathbf{K})$ if all the atoms have the same atomic form factor.
- 6. Show that in the latter case there are some reciprocal lattice vectors \mathbf{K} where $S(\mathbf{K})$ vanishes. Show that the removal of these vectors of zero structure factor from the reciprocal lattice reduces it to a new lattice. Specify which one and why.



Exercise 2: Free electrons, Sommerfeld model

- 1. The mass density of copper is 8.96 g/cm³, and its atomic weight is 63.5 g/mole at 0K. Calculate its electron density and its Fermi energy E_F in the Sommerfeld model. (Copper can be considered monovalent)
- 2. Calculate (in atmospheres) the pressure exerted by the copper electrons gas according to the Sommerfeld model. If the volume expands, the total energy will increase or decrease? Why can we explain that the electron gas in a metal does not expand? (What are we neglecting?)

Exercise 3: Energy bands, Tight-binding and Effective Mass

- 1. Consider electrons on a 2D "empty" square lattice (free electrons).
- 2. Now draw the Fermi-surface for (a) one electron per site and (b) two electrons per site. In either case is this a metal or an insulator?
- 3. Consider now (for the electrons in the same 2D lattice) the tight-binding approximation, with only nearest neighbours hopping and no overlap. Calculate the energy dispersion. Sketch a few constant energy lines in the (k_x, k_y) plane.
- 4. Consider now a tight-binding model for a simple cubic 3D crystal, again, with only nearest neighbours hopping and no overlap, and the energy dispersion. Calculate the effective mass tensor (M_{ij}) for electrons at the center $\mathbf{k} = \frac{\pi}{a}(0,0,0)$, at the face center $\mathbf{k} = \frac{\pi}{a}(0,0,1)$) and at the corner $\mathbf{k} = \frac{\pi}{a}(1,1,1)$ of the Brillouin zone. Discuss the usefulness of the effective mass concept at $\mathbf{k} = \frac{\pi}{a}(0,0,1)$.
- 5. Consider now that the lattice is compressed in the z direction, so that we can consider a stronger hopping in z. How does the effective mass tensor change?