Condensed Matter Physics I Final written test academic year 2009/2010 July 12, 2010

(Time: 3 hours)

Exercise 1: Bravais lattices with basis and structure factors

Some superconductors are made by $CuO₂$ layers, that in some cases have a pattern like the one shown in Fig. 1. Let us assume a the minimum distance between two Cu atoms.

- 1. Describe a possible choice for a set of primitive lattice vectors and basis (write the vectors!); draw the primitive unit cell.
- 2. Assuming that the atomic form factors are $f_{Cu} = 2f_O$, calculate the structure factor and find the points of the reciprocal lattice where the structure factor is maximum and where it is vanishing.
- 3. Other compounds are characterized by the fact the the atomic positions of O are not equivalent, but they are slightly displaced in direction perpendicular to the plane by a certain quantity $\pm \delta$, as shown in Fig. 2. Specify and draw the basis vectors, primitive cell, the lattice spacing, the reciprocal lattice basis vectors in this other case.

Exercise 2: Examples of Fermi gases

- 1. Electrons in 3D: Calculate the Fermi energy for electrons in tungsten $(Z=2,$ density 10.3 g cm[−]³). What is the corresponding Fermi temperature (i.e., the Fermi energy expressed in temperature units)?
- 2. Electrons in 1D: Some long-chain organic molecules with mobile electrons given by donors are 1D conductors. Derive expressions for E_F for a 1D conductor with n free electrons per unit length. Evaluate E_F for an atomic spacing of 2.5 Å between donor atoms and 0.5 free electron per donor atom.
- 3. Liquid ${}^{3}He$: Liquid ${}^{3}He$ (it liquifies at about 3 K), the light isotope of helium, has spin $1/2$ and so is a fermion. Making the approximation that ³He as a perfect gas and noting that its density is 0.081 g cm³, calculate the Fermi energy E_F .

Exercise 3: Tight binding model

Consider s-type electrons in a one-dimensional lattice with lattice paramenter a. Make use of a *tight binding* model with *nearest and next-nearest neighbor hopping* and with negligible *overlap*. With reference to the texbook for the definitions of $\gamma(\mathbf{R})$, consider: $\gamma(\mathbf{R}_{NN})=t$ where \mathbf{R}_{NN} is for nearest neighbors, $\gamma(\mathbf{R}_{NNN})=t'$ where \mathbf{R}_{NNN} is for nextnearest neighbors, $\gamma(\mathbf{R})=0$ otherwise.

- 1. Write explicitely the expression for the energy band. (for the sake of simplicity, write $E_s + \beta \equiv E_0$, again with reference to the textbook for the definition of β)
- 2. Consider $t' = -t$ and make a plot of the band in the first Brillouin zone, specifying peculiar points.
- 3. Calculate the effective mass in the points corresponding to the maxima and minima of the band calculated in (2).
- 4. Make the extension to the 2d case, considering a square lattice but with nearest neighbor hopping only and again with negligible overlap. Write explicitely also in this case the expression for the energy band. (again write $E_s + \beta \equiv E_0$).
- 5. What is the Fermi energy in case of half-filling of the band, i.e. in case of one spin- $1/2$ electron per unit cell and at $T=0$?
- 6. For the case considered above (5), draw the Fermi surface ("curve", actually, in 2d) in the (k_x, k_y) plane.

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.