Condensed Matter Physics I Final written test academic year 2012/13 February 15, 2013

(Time: 3 hours)

Exercise 1: Crystal lattices and structure factors

Consider the 2D lattice here sketched, made of three different atomic species A, B, C, placed on the sites of a triangular lattice. For the sake of definiteness, consider the origin in one of the atoms A; let d be the AB distance.

- 1. Choose and write a set of primitive vectors and a basis, sketch the unit cell and calculate its area.
- 2. Write and sketch the basis of the reciprocal lattice.
- 3. Calculate the structure factor $S(\mathbf{k})$ in the general case, when the atomic form factors f_A , f_B and f_C are different.
- 4. Calculate the structure factor in case of $f_A = f_B = f_C$. Specify on which reciprocal lattice vectors it is not vanishing. Comment the result.

	В		С		А		В		С	
С		A		В		С		A		В
	В		С		A		В		С	
С		A		В		С		A		В
	В		С		А		В		С	

Exercise 2: Band structures for free electrons

Consider the BCC lattice.

- 1. Plot the contours of the First Brillouin Zone in the (k_x, k_y) plane, specifying the coordinates of the relevant points.
- 2. Write explicitly the expression of the first three energy bands $\mathcal{E}_n(\mathbf{k})$ for n = 1, 2, 3 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 make a plot in the reduced zone scheme.

Exercise 2: Semiclassical model of electron dynamics

Consider the electron orbits in a 3D solid with band dispersion

$$E(\mathbf{k}) = E_0 - 2t[\cos(k_x a) + \cos(k_y a) + \cos(k_z a)]$$

with lattice parameter a, under a uniform static magnetic field $\mathbf{H} = H\hat{y}; t > 0$.

- 1. Describe and write the equation of an orbit in **k** space for $k_y = \frac{\pi}{2a}$ and energy $E(\mathbf{k}) = constant = E_0 4t$.
- 2. Write the Bloch electron velocity in direct space corresponding to the orbit in (1). Describe the orbit in real space.
- 3. Describe and write the equation of an orbit in **k** space for $k_y = \frac{\pi}{2a}$ and energy $E(\mathbf{k}) = constant = E_0$.
- 4. Describe and write the equation of an orbit in **k** space for $k_y = \frac{\pi}{2a}$ and energy $E(\mathbf{k}) = constant = E_0 + 4t t\delta^2$ and $\delta \ll 1$.
- 5. Write explicitly the period of that orbit. What should be t in order to have the same period as for free electrons?
- 6. Indicate the direction of the motion along the orbit.

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.