Condensed Matter Physics I
final written test
academic year 2014/2015
January 23, 2015

(*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 and Miller indices*

If a conventional cubic unit cell is used to describe a BCC crystal:

1. What are the allowed values for the indices (n_1, n_2, n_3) and (m_1, m_2, m_3) of the real and reciprocal lattice vectors, respectively?
2. Consider the (001) plane in the conventional notation. How would it be indexed using the primitive vectors?
3. Consider the [001] direction in the conventional notation. How would it be indexed using the primitive vectors?

Exercise 2: *Almost free electrons in 2D and semiclassical model of dynamics*

Consider a triangular lattice of atoms with valence Z and spacing a, with weak electron-ion interactions.

1. Draw the first Brillouin zone and give the area.
2. Completely neglecting from now on the interaction with the ionic cores ("empty" lattice approximation), calculate the Fermi energy in case of Z=2 and draw the Fermi circle, accurately specifying how it compares with the first Brillouin zone.
3. Which is the minimum valence Z such that the Fermi sphere is not fully contained in the first Brillouin zone? Consider from now on this situation. How are the first two bands (fully occupied, partially occupied...)?
4. Consider a magnetic field $\mathbf{H}$ pointing out of the page: which direction does a Fermi surface electron move on the surface, in the lowest band and in the second band? Justify your answers.

Exercise 3: *Tight binding in 2D*

Consider the 2D crystal made of one atomic plane out of the {100} family of planes of the rocksalt structure of a binary compound AB with lattice parameter a^{3D}.

1. Draw the resulting 2D structure, and indicate the primitive unit cell. Which 2D Bravais lattice is it?

2. Using a convenient choice for the axes and indicating with a the lattice constant of the 2D structure, write a set of primitive vectors and those of the basis.

3. Consider a single s-orbital on each atom (atomic energies E_A, E_B) and nearest neighbor hopping integrals between pairs of each of the atomic types (AA, BB, AB). Neglect overlap. Write the system of equations that one should solve in the tight-binding approximation, in terms of the hopping integrals $\gamma_{AA}, \gamma_{BB}, \gamma_{AB}$ and a (you are not requested to solve it, but to write explicitly the system).
   [Hint: pay attention to the Bravais lattice vectors entering in the sums in order to consider correctly only nearest neighbor interactions]

4. Specify the system of equations when $\gamma_{AB} = 0$. Show that in this case the system reduces to two separate equations whose solutions $E_{A,B}(\mathbf{k})$ have the standard tight-binding form of a square lattice, and write them explicitly. Plot them along the high symmetry direction from the Γ to the corner of the Brillouin zone. In general, are these bands crossing somewhere or not?

5. Keeping $\gamma_{AB} = 0$, which is the condition on the given energy parameters (E_A, E_B, γ_{AA}, γ_{BB}) for having the bands totally separated (in terms of density of states)?