Condensed Matter Physics I
final written test
academic year 2016/2017
January 30, 2017

(*Time: 3 hours)*

Exercise 1: *Crystalline structure*

Consider a three-dimensional crystalline lattice formed of Cu and Zn atoms. The Cu atoms form a simple cubic lattice with the lattice constant a. The Zn atoms are at the center of the cube.

1. What is the Bravais lattice and what are the primitive Bravais lattice vectors $\{\mathbf{a}_i\}$, and the primitive vectors $\{\mathbf{b}_i\}$ of the reciprocal lattice? If there is a basis, what are the basis vectors?

2. Write the structure factor $S(\mathbf{K})$ associated with the reciprocal lattice vector $\mathbf{K} = \nu_1\mathbf{b}_1 + \nu_2\mathbf{b}_2 + \nu_3\mathbf{b}_3$ in terms of the atomic form factors f_{Cu} and f_{Zn}.

3. If Cu and Zn atoms randomly occupy the lattice sites, the form factor associated with every lattice site can be assumed to be the same and equal to the average of the two form factors. In this case, there are some $\mathbf{K}$ vectors where $S(\mathbf{K})$ vanishes. Which ones? Which Bravais lattice is described by those $\mathbf{K}$ vectors where $S(\mathbf{K})$ does not vanish? Justify analytically the result.

Exercise 2: *Free electron gas*

Consider a free electron gas in two dimensions in the Sommerfeld model.

1. Find the Fermi energy (in terms of the electron density n).

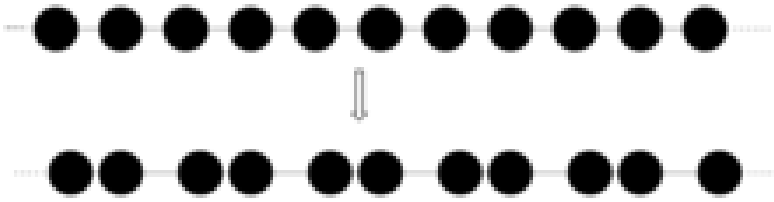
2. Show that the average energy for each electron is $\mathrm{E}_F/2$.

3. Show that the chemical potential μ can be written as:

$$\mu = k_B T\, ln(e^{E_F/k_B T} - 1) \qquad \text{and in particular} \quad \mu \approx \begin{cases} E_F & \text{if} \quad k_B T << E_F \\ kT\, ln(E_F/k_B T) & \text{if} \quad k_B T >> E_F \end{cases}$$

Exercise 3: *One dimensional tight-binding model*

Consider a 1D chain of *monovalent* atoms equispaced by a distance a, like in the top panel of the figure below.



1. Indicate with γ the hopping integral between nearest neighbours (consider an attractive crystalline potential), with E_0 the energy of the atomic level; neglect the on-site (β) and the higher order hopping integrals, and all the overlaps integrals. Write the expression of the tight-binding (TB) lowest energy band $E^{TB}(k)$.

2. Consider also the free electron (FE) energy band, $E^{FE}(k)$, when the crystalline potential vanish. $E^{TB}(k)$ and $E^{FE}(k)$ are different if considered over all the Brillouin zone (Bz), but they can be similar in the low energy region. Determine the parameters of the tight-binding model, E_0 and γ, in terms of physical constants and lattice parameter a, so that the low energy behavior of the tight-binding band matches the free electron result.

3. Calculate explicitly $E^{TB}(k)$ (with the parameters previously determined) and $E^{FE}(k)$ at the borders of the 1st Bz. Plot $E^{FE}(k)$ and $E^{TB}(k)$ over the full 1st Bz. Calculate the Fermi energy E_F for both models (TB and FE) and sketch it in your plot. Is this material an insulator or metal?

4. Now consider that the atoms move off the symmetric sites by alternating small amounts, $\pm\delta$, so that they are alternatively separated by $a - 2\delta$ and $a + 2\delta$, with hopping integrals γ_- and γ_+. Which is the periodicity of the system in this case? Which is the 1st Bz? Plot qualitatively the first two bands $E_n^{TB}(k)$ (n=1, 2) in the new 1st Bz, considering γ_- and γ_+ very similar. What happens at the zone boundaries? Is the distorted material a metal or an insulator?

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.