Condensed Matter Physics I
final written test
academic year 2014/2015
February 16, 2015

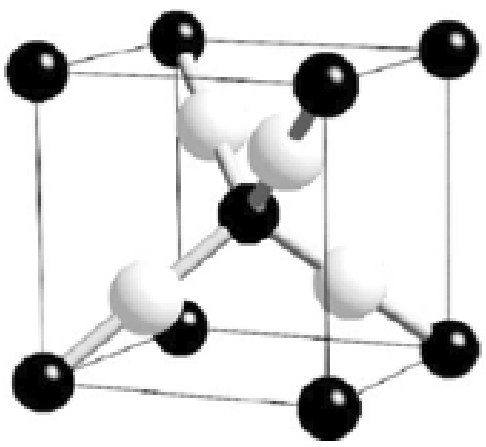
(*Time: 3 hours*)

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: *Cuprite structure*

The cuprite, a copper oxide, has the structure shown in the figure, where oxygen and copper atoms are indicated by the small dark and larger gray circles, respectively.

1. Which is the chemical formula of the compound?
2. Which is the crystalline lattice formed by the oxygen atoms? and the one formed by the copper atoms? Which is the Bravais lattice of the compound?
3. Is the cubic cell shown in the figure the primitive one? How many atoms are in the primitive cell? Write the primitive vectors and the basis.
4. What are the coordinates of the largest interstitial hole in this structure? (Hint: where should we put an extra atom if we were looking for the most room?) How many of these sites are there per unit cell?
5. Sketch in the cubic unit cell the planes (111) and (210).
6. How many different [110]-type directions lie in the (111) plane? Write out the indices for each such direction.
7. Is it possible to choose the origin such that the structure factor is real? In case of positive answer, make this choice. In any case, write the structure factor.



Exercise 2: *Electrons in crystals*

Consider an electron in a periodic lattice, where the energy dependence on the crystalline momentum in the first Brillouin zone is

$$E = \frac{\hbar^2 k^2}{5m_e}$$

where m_e is the free-electron mass.

1. Using the effective mass (and specifying it), write explicitly the time-independent Schrödinger's equation for one electron in the first Brillouin zone, ignoring all interactions except between the electron and the lattice.

Exercise 3: *1D chain of hydrogen atoms*

Consider a one-dimensional chain of hydrogen atoms with lattice spacing a. Using a single $1s$ orbital per atom, construct the tight binding band. You may keep only the nearest-neighbor hopping integrals $\gamma(a) =< \phi(r)|\Delta U|\phi(r+a) >$, and ignore the overlap $< \phi(r)|\phi(r+a) >$. Assume $\gamma < 0$.

1. Where is the Fermi energy?
2. Consider small displacements of the atoms with respect to their ideal positions, (-1)$^n\delta$ along the chain direction for the n-th atom. Show that the hopping integrals are alternating $\gamma + \Delta$ and $\gamma - \Delta$, where $\Delta = 2\delta|\frac{d\gamma}{da}|$. What is the band structure in this case? Is the system metallic or insulating?

Exercise 4: *Electrons in 2D crystals*

Consider a 2-d rectangular lattice with sides a and b (consider $a < b$), with energy dispersion:

$$E(k_x, k_y) = E_0 + 2t_1 cos(ak_x) + 2t_2 cos(bk_y)$$

1. What is the reciprocal lattice? Draw the first Brillouin zone.
2. Plot the constant energy contours around the maxima and the minima, assuming $t_1 > t_2 > 0$. Is this physically reasonable? Justify your answer.