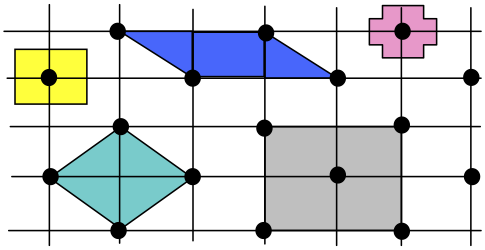
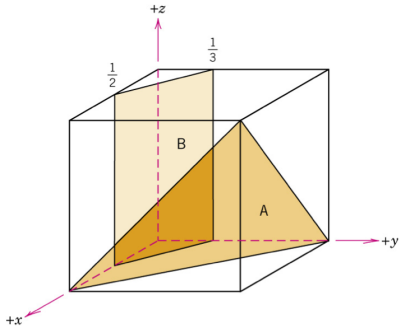
Condensed Matter Physics I
final written test
academic year 2016/2017
February 22, 2017

(*Time: 3 hours*)

Exercise 1: *Crystalline structures*





1. Which of the cells in the left panel of the figure above is/are primitive? Is there a Wigner-Seitz cell in the figure above or not? If yes, indicate it.

2. Which are the Miller indices of the two planes indicated in the right panel?

3. In order to appreciate the role of the surfaces in the nanostructures, consider a material with a simple cubic (SC) structure, and a piece of it made of $n \times n \times n$ SC unit cells. Let S_n be the ratio between the surface atoms and the total number of atoms. In a conventional cubic cell ($n = 1$) there are 8 surface atoms and no inner atoms, so that $S_1 = 1$. Write the expression of S_n as a function of n and show that it is progressively decreasing when n increases.

4. Show that for $n \geq 9$ the number of inner atoms is larger or at least equal to the surface one.

Exercise 2: *Free electron gas*

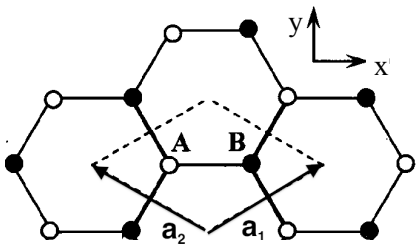
Consider the free electron gas in three dimensions in the Sommerfeld model. The temperature at the core of the Sun is estimated to be of the order of 10^7 K and the concentration of electrons of 10^{32} per cubic meter.

1. Calculate the Fermi energy E_F.

2. Would it be correct to consider this system as a *degenerate* electron gas (Fermi gas with $k_B T << E_F$)? Justify your answer.

Exercise 3: *Tight-binding model of graphene*

Graphene is made by Carbon atoms forming a two-dimensional honeycomb structure, as show in the figure. Let a be the length of the primitive vectors.



1. With reference to the specific choice of the primitive vectors shown in the figure, describe the reciprocal lattice, draw the basis vectors and write their coordinates.

2. Plot the first Brillouin zone, showing that it is an hexagon and that the six corners are located at $\{\mathbf{K}_i\}$ points, with:
$$\mathbf{K}_{1,2} = \left(0, \pm\frac{4\pi}{3a}\right)$$
$$\mathbf{K}_{3,4,5,6} = \left(\pm\frac{2\pi}{\sqrt{3}a}, k_y = \pm\frac{2\pi}{3a}\right)$$

3. In a tight-binding approach, considering only p_z-band and nearest neighbours interaction, the first two electronic bands of graphene are:
$$E(\mathbf{k}) = \pm\gamma\sqrt{1 + 4\cos\left(\frac{\sqrt{3}k_x a}{2}\right)\cos\left(\frac{k_y a}{2}\right) + 4\cos^2\left(\frac{k_y a}{2}\right)}$$
What is the Fermi energy of such system if there is one electron per atom? *(Justify your answer)*

4. Show that $E(\mathbf{K}_i) = E_F$.

5. Consider the behaviour of the bands along the k_y direction from one corner to the opposite one, for instance from $\mathbf{K}_1 = \left(0, -\frac{4\pi}{3a}\right)$ to $\mathbf{K}_2 = \left(0, \frac{4\pi}{3a}\right)$. Make a plot and, considering the leading term, show that it has a linear behaviour close to the corners of the Brillouin zone.

(This trigonometric relationship can be useful: $cos(\alpha + \beta) = cos\alpha\ cos\beta - sin\alpha\ sin\beta$)

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.*