Electrons in crystals
Final written test
academic year 2008/2009
December 16, 2008

(*Time: 3 hours*)

Exercise 1: *Free electrons - Sommerfeld model*

Copper (Cu) in normal temperature and pressure conditions is a metal with FCC structure and mass density of about 8.96 g cm^{-3}. It has an average mass number of 63.55 and Fermi energy of 7.00 eV.

1. From the given Fermi energy, derive the density n of the free electrons.
2. Using the Sommerfeld expansion, calculate the electronic contribution to the specific heat at room temperature.
3. Using now its mass density and its mass number, calculate the *atomic* density n_{at}. Using this result and the result in (1), calculate the average number of free electrons per atom. Is it what you would expect?

Exercise 2: *Bravais lattices with basis*

The copper-oxide high-Tc superconductors contain CuO_2 planes that can be idealized as shown in Figure (a).

1. Write a possible choice of basis vectors, descrive and sketch the primitive cell.
2. Assuming that the atomic form factors are such that $f_{Cu} = 2f_O$, calculate the geometrical structure factor S($\mathbf{K}$) on the reciprocal lattice vectors, and specify for which $\mathbf{K}$ it is maximum and for which ones it vanishes.
3. There are other compounds having a similar structure, but with non equivalent atoms in the oxigen positions, as indicated in Figure (b). Specify in this case which is the primitive cell, the lattice parameter and the basis vectors of the reciprocal space.

Exercise 3: *Band structures for free electrons*

Consider the BCC lattice.

1. Plot the contours of the I Brillouin zone in the $k_x k_y$ plane, specifying the relevant point.
2. Write explicitly the expression of the first energy band $\mathcal{E}_1(\mathbf{k})$ 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 plot it in the reduced zone scheme.
3. Calculate and plot the other three lowest bands, $\mathcal{E}_n(\mathbf{k})$ for $n = 2, 3, 4$.

Exercise 4: *Graphene band structure in tight-binding approximation*

Graphene is a single graphite sheet, which can be represented therefore with a 2D honeycomb lattice (consider $\hat{z}$ perpendicular to the sheet). It is interesting to consider the two bands (the highest valence and the lowest conduction band) originating from the p_z orbitals of the carbon atoms (therefore, due to pp_π bonding).
Following the tight-binding approach, we seek for solutions of the full Schroedinger equation which are Bloch sums built on the p_z orbitals of the carbon atoms in one and in the other site $i = 1, 2$ of the primitive cell: $\Psi_i(\mathbf{r}) = \sum_{\mathbf{R}} \mathrm{e}^{i\mathbf{k}\cdot\mathbf{R}} \phi_{p_z}(\mathbf{r} - \mathbf{R} - \tau_\mathbf{i})$ (analogous to the eq. (10.6) of the textbook).

1. Write the basis vectors and the atomic basis inside the primitive cell in real space and the vectors of the reciprocal lattice.
2. Using the tight-binding method, with only NN interactions and no overlap, write explicitly the eigenvalue equation $det|\langle\Psi_i|H|\Psi_j\rangle - \delta_{ij}\mathcal{E}(\mathbf{k})|$=0 and show that

$$\mathcal{E}(\mathbf{k}) = E_{p_z} - \beta \mp \gamma\sqrt{1 + 4cos\frac{ak_x}{2}cos\frac{\sqrt{3}}{2}ak_y + 4cos^2\frac{ak_y}{2}}$$

   with the obvious meaning of the terms E_{p_z}, β, γ.
3. Calculate and sketch $\mathcal{E}(\mathbf{k})$ along the lines M-Γ-K, where M= $\left(\frac{2\pi}{\sqrt{3}a}, 0\right)$, K= $\left(\frac{2\pi}{\sqrt{3}a}, \frac{2\pi}{3a}\right)$ and $\Gamma = (0, 0)$ and show that, since there is one π electron per atom, graphene is a zero-gap semiconductor.

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.
- When required, numerical evaluations should be given exactly with 3 significant figures, if not otherwise indicated.