Condensed Matter Physics I
II partial written test
academic year 2011/2012
January 16, 2012

(*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: *Tight bindings energy bands and density of states*

Consider a two-dimensional material whose crystalline structure is a square lattice with spacing a. The expression for a s-band considering no overlap, only nearest-neighbor hopping (γ is the hopping integral), and setting the reference level at zero, is:

$$E(\vec{k}) = -2\gamma(cos(ak_x) + cos(ak_y))$$

1. Sketch the band dispersion in the direction $k_x = k_y$. Indicate the value and position of the minimum band gap.
2. Show that close to the bottom and top band edges, contours of constant energy are circles in k-space.
3. Write the expression of the density of states. Calculate the value of the density of states at the band edges.
4. Show that the density of states of this band has a logarithmic singularity at $E = 0$ $(*)$
5. Sketch the density of states as a function of energy for the whole band.
6. Consider that this 2D material has a conduction and a valence band, where:

$$E_c(\vec{k}) = 6\alpha - 2\alpha(\cos(ak_x) + \cos(ak_y))$$

$$E_v(\vec{k}) = -2\alpha + \alpha(\cos(ak_x) + \cos(ak_y))$$

Sketch the density of states as a function of energy for the whole of both the conduction and the valence band.

$(*)$ You might find useful the integral:

$$\int \frac{dx}{\sin(ax)} = \frac{1}{a} \ln \frac{1 - \cos(ax)}{\sin(ax)}$$

Exercise 2: *Effective masses and density of levels*

Consider bulk Silicon, whose conduction band minima E_c are near the Brillouin zone boundary along $\langle 100 \rangle$ directions. Assume a parabolic conduction band with ellipsoidal constant energy surfaces around the minima, described by:

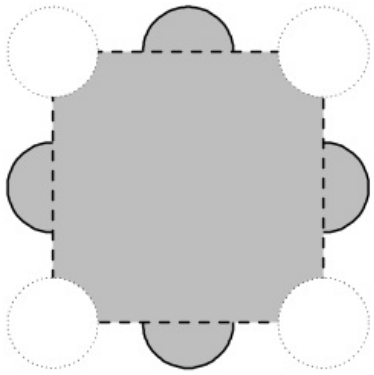
$$E(\mathbf{k}) = E_c + \frac{\hbar^2}{2}\left(\frac{k_\ell^2}{m_\ell^*} + \frac{k_t^2}{m_t^*} + \frac{k_t^2}{m_t^*}\right)$$

(t=transverse, ℓ=longitudinal, with $m_\ell^* = 0.98 m_0$ $m_t^* = 0.19 m_0$, where m_0 is the free electron mass; $\vec{k}$ is with respect to the location of the minima).

1. How many equivalent minima there are?
2. Write the expression of the density of states $g(E)$ around one of the conduction band minima, in terms of E_c, m_ℓ^*, m_t^*.
3. Calculate the number of states per unit energy for an energy 100 meV above the conduction band bottom, in a 100 × 100 × 10 nm piece of silicon. Write the result in units of eV^{-1}.

Exercise 3: *Semi metals*

Bismuth is a "semi metal"; it has the second lowest thermal conductivity (after mercury) and the highest Hall coefficient, a high electrical resistance (or low electrical conductivity) (look for instance at Tab 1.2 and 1.6 of A&M book!).
The unit cell is rhombohedral with two atoms (see Tab 7.5 A&M book), so it *could* be an insulator. However, there is a little band overlap that makes the situation similar to the case of a divalent metal with simple cubic lattice, whose Fermi-surfaces in (k_x, k_y) plane is shown in the figure. We refer therefore for simplicity to this case.



1. Make the same picture using the repeated zone scheme. Which part of the Fermi-surface can be described as electron-like and which as hole-like?
2. By which factor is the specific heat of the electrons at low temperatures ($k_B T << E_F$) smaller than the electronic specific heat in the model of free electrons? For numerical estimations use the following data: the radius of the electronic Fermi-sphere is $k_e = 0.1 G_0$, where G_0 is the shortest reciprocal lattice vector; the bands in the vicinity of E_F are parabolic with effective masses $m_e = m_h = 0.1 m_0$.
3. Why is the conductivity of such metals smaller than in the model of free electrons?