Condensed Matter Physics I
II partial written test
academic year 2012/2013
January 14, 2013

(*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 binding*

Consider a two-dimensional material whose crystalline structure is a square lattice with spacing a.

1. Show that the expression for a s-band considering no overlap, nearest-neighbors (NN) and next-nearest-neighbors (NNN) hopping (t_{NN} and t_{NNN} are the corresponding hopping integrals), and setting the reference level at zero, is:

$$E(\mathbf{k}) = -2t_{NN}(\cos(ak_x) + \cos(ak_y)) - 4t_{NNN}\cos(ak_x)\cos(ak_y)$$

2. Consider $t_{NN} = t_{NNN} = t > 0$. Calculate the values and positions of the minima and the maxima of the band in the Brillouin zone.

3. Sketch the band dispersion along the $\Gamma - X - W - \Gamma$ line, where $X = \left(\frac{\pi}{a}, 0\right)$ and $W = \left(\frac{\pi}{a}, \frac{\pi}{a}\right)$.

4. Calculate the Fermi energy for two electrons per lattice site.

5. Calculate the effective mass tensor in Γ and W and discuss the character of the charge carriers in those points.

6. Consider only NN hopping. Calculate the Fermi energy for (i) one and (ii) two electrons per lattice site and in both cases make a sketch of the Fermi "surfaces" (lines) in the first Brillouin zone.

Exercise 2: *Density of states in 1D and 2D*

Consider a 1D lattice with lattice constant a. Suppose that the dispersion relation in the conduction band is expressed as

$$E(k) = E_0 + 4\gamma sin^2\left(\frac{ka}{2}\right)$$

with γ being a (positive) constant.

1. Calculate the effective electron mass m^* in the extrema of the band, specifying if it is electron-like or hole-like.

2. Calculate (write explicitly the expression) the electronic density of states $g(E)$. Calculate its minimum and make a sketch of $g(E)$.

3. Calculate the Fermi energy in case of half filling of the band.

4. Consider now a 2D lattice. Suppose that the band dispersion around the minimum is *linear* (i.e., it has a relativistic character), $E(\mathbf{k}) = \alpha|\mathbf{k}|$, instead of the standard parabolic expansion. [This is for instance the case of the celebrated graphene, a single layer of graphite, not around Γ but other $\mathbf{k}$ points.] Describe and sketch the constant energy "surfaces" (lines) in the (k_x, k_y) plane.

5. Calculate the velocity and describe clearly its direction. Make a sketch in the (k_x, k_y) plane.

6. Calculate the density of states $g(E)$ around the minimum of the band. Which would be the result in case of a standard quadratic dispersion? Comment the difference.