Condensed Matter Physics I
II written test
academic year 2009/2010
January 12, 2011

(*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: *Electrons in periodic structures*

1. Consider free electrons (”empty lattice”) in a 2D square lattice. Write the expression and plot the energy bands along a path from Γ to the midpoint X of a side of the first Brillouin zone, to the corner (L) and back to Γ. Give in particular the value of the band at the high symmetry points listed above. Show that E(L) is higher than E(X) by a factor of 2.

2. Consider a 2D square lattice solid made of divalent atoms. Calculate the Fermi energy E_F, and report it in the plot obtained in (1) and draw the corresponding Fermi surface (circle) in (k_x, k_y) space with respect to the Brillouin zones.

3. Consider now a 3D simple cubic lattice. Which is the ratio between the value of the first energy band (i) at a corner (R) of the first Brillouin zone and (ii) at the midpoint of a side or (iii) of a face of the zone in this case?

4. Write the expression and a *detailed* plot (*) the *first two* bands along a path from Γ to the corner (R) of the first Brillouin zone. Give in particular the value of the bands at Γ and R. (* *show where is the minimum of each band*)

5. Consider a 3D cubic lattice solid made of divalent atoms. Calculate the Fermi energy E_F, and discuss the occupation of the first two bands. *(Note that the studying the bands along Γ–R is not enough...)*

6. If we now consider a non zero crystalline potential which opens a gap at the Bragg plane, is it possible for a solid in (5) to be an insulator? In case of positive answer, which is the condition?

Exercise 2: *Weak potential*

Consider a square lattice in 2D with the crystal potential

$$U(x,y) = -2U_0 \left[cos\left(\frac{2\pi}{a}x\right) cos\left(\frac{2\pi}{a}y\right)\right].$$

1. Calculate the Fourier transform $U_{\mathbf{G}}$ for a generic $\mathbf{G}$ of the reciprocal lattice (*Hint: write trigonometric functions in terms of exponentials*).
2. Which is to the first order in U_0 the effect on the energy bands at $\mathbf{G_1}/2$, where $\mathbf{G_1}$ (one of the star of) the shortest reciprocal lattice vectors?
3. What can you say about the effect of this potential at the corner of the Brillouin zone?

Exercise 3: *Tight-binding model*

1. Consider a FCC lattice with a s-band given by:

$$E(k) = E_s - \beta - 4\gamma \left(cos\frac{k_x a}{2} cos\frac{k_y a}{2} + cos\frac{k_y a}{2} cos\frac{k_z a}{2} + cos\frac{k_z a}{2} cos\frac{k_x a}{2} \right)$$

2. Write the expression of the Bloch velocity for this band.
3. Show explicitly that the velocity for $\mathbf{k}$ lying on the face of the Brillouin zone containing X=$\frac{2\pi}{a}(1,0,0)$ is parallel on such face *(the answer will be considered valid only if fully justified by calculations)*