Electrons in crystals
Final written test
academic year 2009/2010
January 25, 2010

(*Time: 3 hours)*

Exercise 1: *Sommerfeld model of free electrons*

The Sommerfeld model is very accurate in describing the properties of the elemental solid Na. The structure is BCC with lattice parameter a_0=4.23 Å.

1. The Fermi sphere is fully contained in the first Brillouin zone or not? Justify numerically the answer.

2. What about all the other elemental solids made of the atoms of the I column of the periodic table? Justify numerically the answer.

3. These solids are metallic or not? Justify the answer.

4. Consider now Cu, whose valence electron is $4s^1$ and the crystal structure of the solid phase which is FCC. If the Sommerfeld theory would apply also to Cu (*), would the Fermi sphere be fully contained in the first Brillouin zone or not? Justify numerically the answer. (* important distortions of the Fermi surface with respect to a perfect sphere are instead present).

5. Consider then Ca, in the same row of Cu, which is divalent and crystallizes in a FCC structure, too. On the basis of this information only, could you exclude the possibility for it to be insulator?

6. Which is the volume of its Fermi sphere (if the Sommerfeld model would be applied) with respect to the first Brillouin zone? Would you expect the Fermi surface to intersect the zone faces or not?

Exercise 2: *Bravais lattices and structure factors*

Consider a scattering experiment from a 3D elemental cubic solid. It is possible to determine precisely the structure (BCC or FCC, we exclude SC which is very rare) by comparing the diffraction patterns in some relevant directions, for instance (101), (222) and (110). (*Hint: consider the same underlying 3D cubic structure with proper atomic basis, with one atom always at the origin*)

1. Calculate the structure factor for BCC in $\mathbf{k}=2\pi/a(101)$, $\mathbf{k}=2\pi/a(222)$, $\mathbf{k}=2\pi/a(110)$.
2. Calculate the structure factor for FCC in the same $\mathbf{k}$'s.
3. What could you conclude ?

Exercise 3: *Tight binding bands and Electron Dynamics*

1. Derive the expression for the energy band of a BCC crystal with cube edge a in a tight-binding model assuming one s orbital per atom and nearest neighbor interaction of strength γ. (*Hint: it could be convenient for the following to keep the exponential form instead of sin and cos functions)*
2. Use the above energy band to answer the following questions: Let an electron at rest ($\mathbf{k}$ =0 at t = 0) feel a uniform electric field $\mathbf{E}$ constant in time. Find its trajectory in real space. That is, derive the expression for x(t), y(t) and z(t).
3. Sketch the trajectory for $\mathbf{E}$ in a [110] direction.

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.