Electrons in crystals
Final written test
academic year 2008/2009
January 12, 2009

(*Time: 3 hours)*

Exercise 1: *Examples of Fermi gases*

1. Liquid ^{3}He (it liquifies at about 3 K), the light isotope of helium, has spin 1/2 and so is a fermion. Treating ^{3}He as a perfect gas (which is only approximately right) and noting that its density is 0.081 g cm^3, calculate the Fermi energy E_F . What is the corresponding Fermi temperature (i.e., the Fermi energy expressed in temperature units)?

2. Calculate the Fermi energy for electrons in tungsten (Z=2, density 10.3 g cm^{-3}).

3. Long-chain molecules with some mobile electrons give 1D organic conductors. Derive expressions for E_F for a 1D conductor with n free electrons per unit length. Evaluate E_F for an atomic spacing of 2.5 Å between donor atoms and 0.5 free electron per atom.

Exercise 2: *Bravais lattices with basis and structure factors*

A crystal is formed of two types of atoms, A and B. The atoms are placed in such a way that they form a cubic lattice with the atoms A sitting in the corners and the atoms B sitting in the centers of the cubes. For this crystal:

1. Describe and sketch the primitive cell writing the formula unit (A_nB_m with m=..., m=...?), a possible choice of the primitive translation vectors $\{\mathbf{a}_i\}$ and the basis vectors $\{\mathbf{d}_i\}$; write the primitive translation vectors of the reciprocal lattice $\{\mathbf{b}_i\}$.

2. Assuming that the atomic form factors are f_A and f_B calculate the geometrical structure factor S($\mathbf{K}$) on the reciprocal lattice vectors, and specify the conditions that need to be satisfied to have interference maxima.

3. Show how one can determine experimentally the atomic form factors by measuring the structure factors S(2π/a(1,1,0)) and S(2π/a(1,0,0)).

Exercise 3: *Band structures*

Assume that the dispersion relation of the conduction band of a 1D semiconductor within the first Brillouin zone is cosine-function shaped with (i) a minimum at k= 0, (ii) an amplitude of 25 meV, and (iii) a full-period width of 2π/a = $2\pi/(5\text{Å})$. Assume further that the semiconductor has an energy gap E_g = 2.5 eV and set equal to zero the valence band top.

1. Sketch the dispersion relation of the conduction band within the first Brillouin zone and write the corresponding expression for E($\mathbf{k}$).
2. Calculate the effective mass of electrons near the minimum at k=0.

Exercise 4: *Semiclassical electron dynamics*

Consider a FCC crystal with lattice parameter a and a tight-binding single-orbital s-type energy band $\epsilon(\mathbf{q}) = -4\gamma[cos(q_x a/2)cos(q_y a/2) + cos(q_x a/2)cos(q_z a/2) + cos(q_y a/2)cos(q_z a/2)]$, having properly chosen the zero of the energy. The solid is in a static uniform magnetic field $\mathbf{H} = H\hat{z}$.

1. Write the condition to be satisfied for the orbits in $\mathbf{q}$-space, for $q_z = 0$ and energy $\epsilon(\mathbf{q}) = E$.
2. For such orbits, write explicitely the expression of the velocity in the (x,y) plane for an electron in the given band.
3. For $E = -4\gamma[3 - \delta^2/4]$ and $\delta \ll 1$, sketch the section of the first Brillouin zone and the orbit in the (q_x, q_y) plane and write its expression.
4. Estimate the period of that orbit if $\gamma a^2 = \hbar^2/2m^*$, with $m^* = 0.067m_e$.

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.