Examination in Condensed Matter Physics I, FK3004, 7.5 hp

Saturday, March 28, 2009, 09.00-15.00.

Allowed help:

- periodic table and fundamental constants (distributed)

- formula sheet (distributed)

- pocket calculator, BETA / mathematics handbook or similar

Instructions:

All solutions should be easy to read and have enough details to be followed. The use of nontrivial formulas from the formula sheet should be explained. *Summarize each problem* before its solution, so that the solution becomes self-explained. State any assumptions or interpretation of a problem formulation.

Good luck! / A.R.

1. Graphene is a two-dimensional crystal consisting of sp^2 -hybridized carbon atoms forming a honeycomb structure. The carbon-carbon bond length is 1.415 Å.

a. Describe the crystal structure (Bravais lattice and basis) of graphene and determine the lattice parameter(s). (2p)

b. Graphite consists of graphene layers stacked with a distance of 3.35 Å. In diamond, the carbon atoms are sp³-hybridized, with a nearest-neighbor distance of 1.5445 Å. The diamond structure can be seen as two merged *fcc* lattices. Determine the density of graphite and diamond. (2p)

2. Consider a metal at room temperature, whose electrons follow the free electron model.

a. Discuss the difference between the metal's Fermi energy and chemical potential. Find an expression for this difference. (1.5p)

b. Find an expression for the electronic density of states. Explain all steps clearly with words. (1.5p)

c. According to the equipartition theorem, a classical monoatomic gas should have a heat capacity $C = 3Nk_B/2$, where N is the number of atoms and k_B is the Boltzmann constant. The heat capacity of conduction electrons in a metal is much smaller, indicating the need of new physics (quantum mechanics). Motivate why the electronic heat capacity is so low. (1p)

3. The orthorhombic crystal system can be described by lattice vectors $\mathbf{a_1} = a\hat{x}$, $\mathbf{a_2} = b\hat{y}$, and $\mathbf{a_3} = c\hat{z}$, where $a \neq b \neq c$ and \hat{x} , \hat{y} , and \hat{z} are unit vectors in the cartesian coordinate system. The base-centered orthorhombic Bravais lattice has a basis of two atoms, **0** and $(\mathbf{a_1} + \mathbf{a_2})/2$, in the traditional cell. It is one of four Bravais lattices in the system, the other being the simple orthorhombic, the body-centered orthorhombic, and the face-centered orthorhombic.

a. Determine the reciprocal lattices of the simple orthorhombic and the base-centered orthorhombic lattices. (1.5p)

b. In x-ray experiments, a vanishing structure factor corresponds to destructive interference. For a face-centered cubic lattice, the condition for diffraction is that the Miller indices (hkl) should be all even or all odd. Find the corresponding condition for diffraction to occur in the base-centered orthorhombic lattice. (1.5p)

c. Find the k-volume of the first Brillouin zone of the base-centered orthorhombic Bravais lattice. (1p)

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4. a. Explain briefly the following concepts related to lattice vibrations: Phonon, dispersion relation, optical branch, Debye model, Umklapp process. (2p)

b. Copper has a sound velocity $v_s = 3560$ m/s and a lattice parameter a = 3.61 Å. Estimate the highest vibration frequency of phonons in Cu and discuss the probability that a mode of this frequency is excited at room temperature. (2p)

5. In a certain material with simple cubic structure and lattice parameter a, a tight-binding description of the lowest-lying energy band is given by

$$\varepsilon(\mathbf{k}) = \alpha - 2\gamma(\cos k_x a + \cos k_y a + \cos k_z a)$$

where $\mathbf{k} = (k_x, k_y, k_z)$ and α and γ are constants.

a. Calculate the effective mass at Γ of the 1st Brillouin zone for the material. (1p)

b. In the absence of scattering, the electrons will start to oscillate if an electrical field is applied to the material. Calculate the expected oscillation frequency of these so called Bloch oscillations if a field $E_x = 10^5$ V/cm is applied. (2p)

c. Assume that the Fermi level lies at $\varepsilon_F = \alpha + 2\gamma$. Make a simple two-dimensional sketch of the Fermi surface of the 1st Brillouin zone. (1p)

6. a. Use Hund's rules to obtain the spectoscopic notation $({}^{2S+1}L_J)$ of the ground states of Cr^{2+} , that has electron configuration [] $3d^4$, and Yb³⁺ with configuration [] $4f^{13}5s^25p^6$. (1p) b. A free spin paramagnet with J = 1/2 displays a magnetization

$$M = \mu_B (N_{\uparrow} - N_{\downarrow}) = \mu_B N \frac{e^x - e^{-x}}{e^x + e^{-x}}$$

where N is the total number of spins and $x = \mu_B B/k_B T$. Find a corresponding expression for a free spin paramagnet with J = 1. Also calculate the magnetization in high fields and susceptibility in low fields for the system. (2p)

c. Discuss an experiment that could tell the difference between a superconductor and a very good normal conductor. (0.5p)

d. Describe the isotope effect of superconductors. (0.5p)