

## **Midterm Examination in FYS3410**

10.03.2010

Duration: 3 hours

No in-advance prepared helping materials are allowed to be used during the examination. No books are allowed except standard reference books listing mathematical formulas if needed. Calculators are allowed.

The present examination measures the level of understanding reached by students on 3 fundamental topics of Solid State Physics as addressed in the lectures/seminars within FYS3410 and in accordance with the course syllabus based on selective chapters of Kittel's book. All examination questions are organized within the following topics:

1. Periodic lattice and x-ray diffraction
2. Vibrations and phonons
3. Free electron Fermi gas

Each topic contains questions of different levels of complexity and a full answer to each topic provides 1/3 of a full score.

## FYS3410 Topic 1: Crystalline lattice and x-ray diffraction

1.1 Consider a family of planes in a cubic crystal in Fig.1. What are Miller indices of the planes?

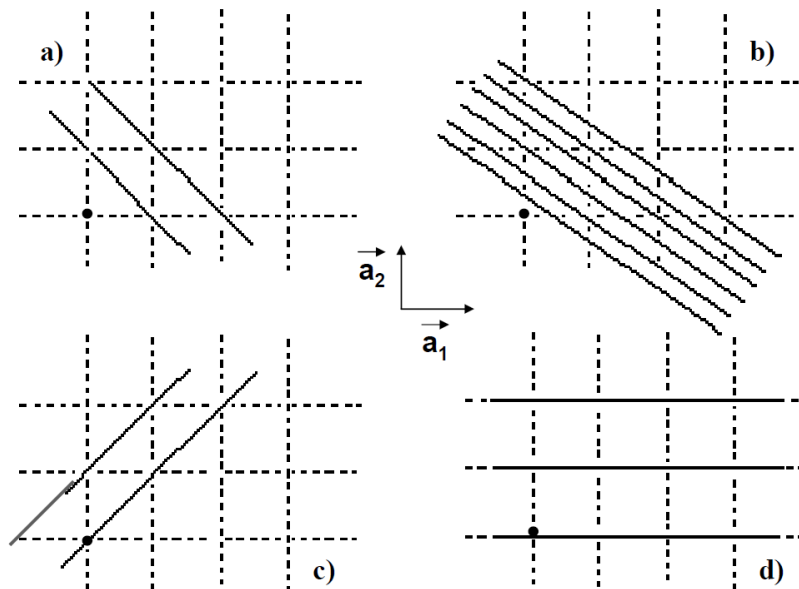


Fig.1. Three-dimensional lattice (dashed lines) with basis vectors  $\vec{a}_1, \vec{a}_2, \vec{a}_3$  containing different families of planes. Vector  $\vec{a}_3$  is normal to the page plane and is directed toward the reader. The magnitude of all basis vectors is  $a$ . The origo is marked with a dark spot in all four panels.

1.2 Make a drawing representing reciprocal lattice points corresponding to the families of planes in Fig.1 in the reciprocal space. In order to make the drawing more quantitative, note

that the reciprocal lattice vector may be given as  $\vec{G} = \frac{2\pi}{d_{hkl}} \vec{n}_{hkl}$ , where  $\vec{n}_{hkl}$  is a normal to a hkl-plane and  $d_{hkl}$  is a distance between hkl-planes: 
$$d_{hkl} = \frac{a}{\sqrt{(h^2 + k^2 + l^2)}}$$

1.3 Consider the reciprocal lattice vector  $\vec{G}$  corresponding to the family of (010) planes in the drawing produced when solving problem 1.2 and an x-ray wave having wavevector  $\vec{k}$ . Prove that diffraction is not taking place for any  $k_G < 1/2|\vec{G}|$  where  $k_G$  is a projection of  $\vec{k}$  vector on  $\vec{G}$  direction. Tip: develop Laue equation  $\Delta\vec{k} = \vec{G}$  to the form of  $2\vec{k} \cdot \vec{G} = \vec{G} \cdot \vec{G}$  and draw the Bragg plane cutting vector  $\vec{G}$ . Generalize the argument to the rest of the nearest to origo reciprocal points and introduce the Brillouin zone concept on the same graph.

1.4 A reflection from the (111) planes of a cubic crystal was observed at an angle  $\theta = 11.2^\circ$  using Cu K $\alpha$  radiation ( $\lambda = 1.5418 \text{ \AA}$ ). What is the length of the side of the unit cell? List and provide short clarifications on factors limiting the number of reciprocal lattice points observed in diffraction experiments. Remember Bragg law  $n\lambda = 2d_{hkl} \sin \theta$

## FYS3410 Topic 2: Vibrations and phonons

**2.1** Assume one atom of mass  $m$  per primitive cell in a linear lattice of  $N$  atoms with a lattice parameter  $a$  and an elastic constant  $c$ . Accounting for nearest neighbour interactions only, the dispersion law is given by  $\omega^2 = \frac{4c}{m} \sin^2 \frac{ka}{2}$ . Analyze and sketch the dispersion law in the first Brillouin zone.

**2.2** Apply periodic (Born – von Karman) boundary conditions for the lattice introduced in problem 2.1 and show that the density of modes (states) is given by

$$D(\omega) = \frac{2N}{\pi} \cdot \frac{1}{\sqrt{\omega_0^2 - \omega^2}} \text{ where } \omega_0^2 = \frac{4c}{m}. \text{ Use the graph from the problem 2.1 for correlating}$$

$\Delta k$  obtained from Born – van Karman treatment of elastic waves and the actual  $\Delta\omega$  interval.

Note the identity:  $\cos(\arcsin x) = \sqrt{1 - x^2}$ . Make a sketch of the  $D(\omega) = \frac{2N}{\pi} \cdot \frac{1}{\sqrt{\omega_0^2 - \omega^2}}$  function

and illustrate by drawing in the same graph how  $D(\omega)$  would change having 2 atoms with different masses per primitive cell.

**2.3** What is the density of states Einstein used in his analysis of heat capacity? Correlate – qualitatively – the characteristic frequency used by Einstein ( $\omega_E$ ) with the sketch of  $D(\omega)$  produced when solving problem 2.2. Further, Einstein temperature can be determined as  $\Theta_E = \hbar\omega_E/k_B$ , where  $k_B$  is a Boltzmann constant. Make a rough estimate of  $\Theta_E$  (order-of-magnitude accuracy is acceptable). The velocity of sound ( $\sim 5 \times 10^3$  m/s) and a lattice parameter typical for common crystals, say  $a = 3 \times 10^{-8}$  cm, may be applied when estimating  $\Theta_E$ . Analyze the trends for  $\Theta_E$  provided by changes in the mass of atoms and the strength of the elastic constant. It is known that at sufficiently low temperatures almost all phonons are in their ground states. What difference in phonon occupation a small rise in temperature going to make in terms of Einstein formalism? When answering the last question the magnitudes of  $\hbar\omega_E$  and  $k_B T$  may be compared and considering the occupation probabilities may provide a basis for conclusions.

$$\hbar = 6.58 \times 10^{-16} \text{ eV} \cdot \text{s}$$

$$k_B = 8.61 \times 10^{-5} \text{ eV} \cdot \text{K}^{-1}$$

**2.4** The thermal conductivity coefficient  $\kappa$  is given by  $\kappa = \frac{1}{3} C_V \Lambda$ , where  $C_V$  is the heat capacity and  $\Lambda$  is the phonon mean free path. Consider temperature dependences for  $C_V$ ,  $\Lambda$ , and  $\kappa$  at low/high temperature limits and fill Table I. Make a plot illustrating temperature dependence of  $\kappa$ .

Table I

	$C_V$	$\Lambda$	$\kappa$
low T			
high T			

### FYS3410 Topic 3: Free Electron Fermi gas

**3.1** The free electron Fermi gas (FEFG) is described in terms of an independent electron orbital model, where the density of orbital's (electron states) is derived solving a free particle

Schrödinger equation  $-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)\psi_{\vec{k}}(\vec{r}) = \varepsilon_{\vec{k}}\psi_{\vec{k}}(\vec{r})$  for wavefunction in a form of

travelling plane wave  $\psi_{\vec{k}}(\vec{r}) = \exp(i\vec{k} \cdot \vec{r})$  applying periodic (Born – von Karman) boundary conditions in 3 dimensions (e.g. in  $x$ -direction  $\psi(x+L, y, z) = \psi(x, y, z)$  where  $L$  is a period). Assuming  $N$  to be a number of free electrons in a system in a ground state derive expressions for: the Fermi energy ( $\varepsilon_F$ ), the magnitude of the wavevector at the Fermi surface ( $k_F$ ), and the density of states ( $D(\varepsilon)$ ). If needed use the identity  $\exp(ix) = \cos x + i \sin x$  when considering allowed values of  $k$ . Note,  $m$  is a rest mass of an electron.

**3.2** Sketch the density of states,  $D(\varepsilon)$ , for FEFG in the ground state obtained when solving problem 3.1. Account for the Fermi-Dirac distribution of electrons

$$f(\varepsilon, \mu, T) = \frac{1}{\exp\left(\frac{\varepsilon - \mu}{k_B T}\right) + 1}$$

and make a modification in your graph, showing how the

electron density of states changes with increasing temperature. How do you understand the quantity  $\mu$  which a chemical potential? For example, what is the chemical potential at  $T = 0$ ?

**3.3** Classical statistical mechanics predicts that a free particle should have a heat capacity of  $\frac{3}{2}k_B$  where  $k_B$  is a Boltzmann constant. If  $N$  atoms each give one valence electron to the electron gas, as considered in problems 3.1 and 3.2, then the electronic contribution to the heat capacity should be  $\frac{3}{2}k_B N$ , just as for atoms in a monoatomic gas. Calculate  $\frac{3}{2}k_B N$  for a mole to use as a reference. On the other hand experiments usually tell that the actual electronic contribution to the heat capacity is in the order of 0.01 of the classical  $\frac{3}{2}k_B N$  value. Use the graph obtained when solving problem 3.2 and make an estimate of total electronic thermal kinetic energy and the corresponding heat capacity accessible for FEFG. Importantly, avoid the complicated integration of the  $D(\varepsilon) \cdot f(\varepsilon, \mu, T)$  product – make a motivated estimate! Using this estimate, calculate, at room temperature  $T = 300K$ , the electronic heat capacity in potassium characterized with an electron concentration of  $1.4 \times 10^{22} \text{ cm}^{-3}$ . Note, it is convenient to introduce the quantity  $T_F = \varepsilon_F / k_B$  called Fermi temperature.

$$\begin{aligned} \hbar &= 6.58 \times 10^{-16} \text{ eV} \cdot \text{s} & k_B &= 8.61 \times 10^{-5} \text{ eV} \cdot \text{K}^{-1} & m &= 9.1 \times 10^{-31} \text{ Kg} \\ N_A &= 6.02 \times 10^{23} \text{ mole}^{-1} & 1 \text{ eV} &= 1.6 \times 10^{-19} \text{ J} \end{aligned}$$