

Midterm Examination in FYS3410

28.03.2010

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 specific planes in a triclinic crystal as shown in Fig.1. What are Miller indices of the planes?

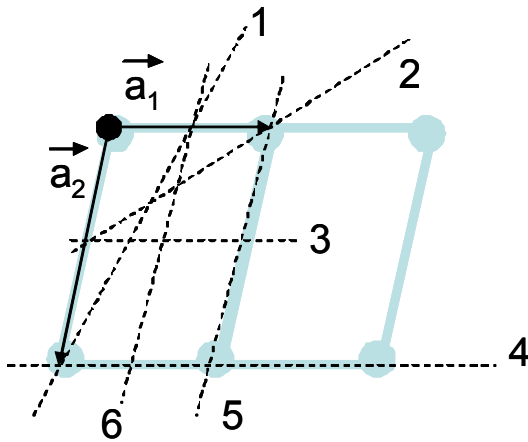


Fig.1. Three-dimensional lattice (thick grey lines) with basis vectors $\vec{a}_1, \vec{a}_2, \vec{a}_3$ containing different planes (labelled with numbers). Vector \vec{a}_3 is directed toward the reader. The origo is marked with a dark spot where \vec{a}_1 and \vec{a}_2 are originated.

1.2 Make a drawing representing reciprocal lattice points corresponding to the 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.

1.3 Consider the reciprocal lattice vector \vec{G} corresponding to the (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 diffraction experiment (applying a wavelength $\lambda = 1.54 \text{ \AA}$) is conducted using a cubic crystal (having a lattice parameter $a = 5 \text{ \AA}$) as shown in a cross section in Fig.2 in the reciprocal space. Is there any Bragg condition ($\lambda = 2d_{hkl} \sin \theta$) satisfied in Fig.2? Explain using Ewald sphere concept. In addition, explain what limits the detection of high index plains in a diffraction experiment in general and conclude if diffractions from (444) planes may be potentially detected in the experimental conditions in Fig.2.

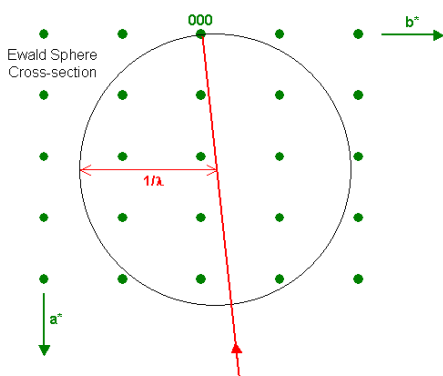


Fig.2. Schematics of a diffraction experiment in a cubic crystal.

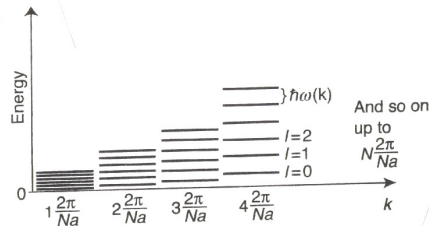
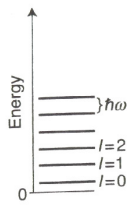
Note, that $d_{hkl} = a/\sqrt{(h^2 + k^2 + l^2)}$ in a cubic crystal.

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 as well as the group velocity (v_g) in the first Brillouin zone (for example investigate the long wave limit, magnitudes of ω and v_g at the centre and boundaries of the first Brillouin zone, etc). Illustrate – qualitatively – in the drawing how the dispersion would change accounting for two sorts of atoms (having different mass) per primitive cell.

2.2 Make a motivation for quantization of vibrations in a periodic crystal applying Born – von Karman boundary conditions and evaluate progress/limitations of Dulong-Petit, Einstein, and Debye models for explaining temperature dependence of the heat capacity. A possible strategy – when attacking the questions – may include an illustration in terms of Fig.3.

Energy level diagram for one harmonic oscillator



Energy level diagram for a chain of atoms with one atom per unit cell and a length of N unit cells

Fig.3. Schematics illustrating quantization of vibration phenomena (phonons) in periodic structures that may be explained and used when answering to problem 2.2. Note: Dulong and Petit used a classical approach and discovered that the heat capacity for many solids was independent of temperature ($\sim 25 \text{ J/mol} \cdot \text{K}$ specifically when measuring above room temperature).

2.3 Provide a qualitative explanation of the T^3 -Debye law comparing the fraction of phonon modes occupied at a given temperature T versus all modes within the Debye cut-off wavevector K_D .

2.4 The thermal conductivity coefficient κ is given by $\kappa = \frac{1}{3} C_V \Lambda$, where C_V is the heat capacity and Λ is the phonon mean free path. Consider temperature dependences for C_V , Λ , and κ at low/high temperature limits and fill Table I (assume pure crystal so that Λ is inversely proportional to the number of phonons provided by the Planck distribution, $\langle n \rangle = 1/[\exp(\hbar\omega/k_B T) - 1]$). Make a plot illustrating temperature dependence of κ and elaborate on “normal” versus “umklapp” processes.

Table I

	C_V	Λ	κ
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 (ε_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 μ 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.

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