

Department of physics

# **Examination paper for TFY4220 Solid State Physics**



## **Other information**

*All the subtasks a), b), … are given equal weight.*





**Checked by:**

Date Signature

### *NB! Attachment.*

## **Problem 1**





Figure 1 shows a hypothetical crystal consisting of atoms arranged on a square grid in 2D. *s* denotes the lattice plane spacing in the *x* and *y* directions.

- a) What is a primitive cell? Indicate an example of a primitive unit cell in the arrangement shown in Fig. 1. Write down the basis vectors **a1**, **a<sup>2</sup>** of the primitive cell, expressed by *s*, **i** and **j**, where **i** and **j** denote unit vectors in the *x* and *y* directions.
- b) Define mathematically the 2-dimensional "reciprocal lattice" for the lattice of Fig. 1. *Hint:* A plane normal of length unity can be employed for convenience.

Explain the connection of the reciprocal lattice to Bragg diffraction (Laue conditions).

- c) Sketch the 2-dimensional reciprocal lattice and the first Brillouin zone for the lattice in Fig. 1. How is this zone related to Bragg diffraction?
- d) State and explain Bloch's theorem. Comment shortly on the choice of boundary conditions.

## **Problem 2**

A beam of electrons with kinetic energy 1.0 keV is diffracted by a polycrystalline metal foil. The metal has a simple cubic crystal structure with a lattice constant of 1.0 Å. Given *m*, *q*, *h*, *c*.

- a) Calculate the wavelength of the electron beam. Calculate the Bragg angle for the first order diffraction maximum.
- b) Explain briefly the difference between dark field and bright field imaging in transmission electron microscopy (TEM). What is *diffraction contrast*?

#### **Problem 3**

Harmonic lattice vibrations for a 1-dimensional chain with a 2-atom basis has the following dispersion relation:

$$
\omega^{2} = \gamma \left( \frac{1}{M_{1}} + \frac{1}{M_{2}} \right) \pm \gamma \sqrt{\left( \frac{1}{M_{1}} + \frac{1}{M_{2}} \right)^{2} - \frac{4 \sin^{2} \left( \frac{kb}{2} \right)}{M_{1} M_{2}}}
$$

Here  $\gamma$  is the effective spring constant,  $M_1$  and  $M_2$  the two masses, and *k* is the wave number. The distance between the masses is *b*/2 such that *b* is the repetition distance.

- a) Sketch the dispersion relation. Indicate acoustic and/or optical branches. Are all *k*-values of equal interest?
- b) How is the dispersion relation changed under the assumption that the crystal has a finite number of unit cells *N*? Assume periodic boundary conditions.
- c) Sketch qualitatively the density of states *D* as function of  $\omega$ . Sketch also the group velocity  $v_g$ as function of *k*.
- d) Let  $M_1 = M_2$ . What is the dispersion relation in this case, and what is the relation between this expression and the dispersion relation for a 1-atom basis? *Hint:* Sketch both dispersion relations in the same figure.
- e) Derive Dulong-Petit's classical expression for the heat capacity of a crystal. Then write down an integral expression for the internal energy  $U(T)$  for the phonon modes in a crystal with density of states  $D(\omega)$ .

#### **Problem 4**

a) Free-electron-model for a three-dimensional system: Show that the highest occupied energy at *T* = 0 level for *N* free electrons in a volume *V* can be written

$$
E(N) = A \left( 3\pi^2 \frac{N}{V} \right)^{2/3},
$$

where *A* is a constant. Find an expression for *A*.

b) Use the expression from a) to argue for the following expression for the "density of states» for conduction electrons in metals:

$$
D(E) = \frac{V}{2\pi^2} \left(\frac{2m^*}{\hbar^2}\right)^{\frac{3}{2}} \left(E - E_0\right)^{\frac{1}{2}}.
$$

Then show by integrating over an energy interval  $\Delta E$  that the effective mass  $m^*$  is given by the expression

$$
m^* = \frac{\hbar^2}{2\Delta E} (3\pi^2 N/V)^{2/3}.
$$

Sodium forms a body-centered cubic lattice with lattice constant  $a = 4.25$  Å. Sodium is an alkali metal  $(1<sup>st</sup>$  column of the periodic table).

c) Why is it a better assumption for sodium than for most other metals that the conduction electrons can be described by a free-electron-model? Experimentally one can measure the energy range  $\Delta E$  of the conduction electrons, and one finds  $\Delta E = 3.0$  eV. Calculate the effective mass *m\** for conduction electrons in sodium!

# **Attachment**

Some expressions and constants that may prove useful:

# \_\_\_\_\_ **Physical constants** \_



Mean occupation number for fermions

$$
f(E) = \frac{1}{e^{(E-\mu)/k_B T} + 1}
$$

Mean occupation number for fermions

$$
f(\omega) = \frac{1}{e^{\hbar \omega / k_B T} - 1}
$$

Density of states for free electrons ( $E(k) = E_0 + \hbar^2 k^2 / 2m$ ):

$$
D(E) = \frac{V}{2\pi^2} \left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}} \left(E - E_0\right)^{\frac{1}{2}}
$$

Phonon dispersion relation for a one-atomic basis:

$$
\omega^2 = \frac{4\alpha}{M}\sin^2\frac{ka}{2}
$$