# LULEÅ UNIVERSITY OF TECHNOLOGY Applied Physics

Course code	F0053T
Examination date	2018-09-01
Time	9.00 - 14.00 (5  hours)

### Examination in: FASTA TILLSTÅNDETS FYSIK MED KVANTMEKANIK / QUANTUM MECHANICS AND SOLID STATE PHYSICS Total number of problems: 5 Teacher on duty: Hans Weber Tel: (49)2088, Room E163 Examiner: Hans Weber Tel: (49)2088, Room E163

Allowed aids: Fysika(lia), Physics Handbook, Beta, calculator, COLLECTION OF FORMULAE for Solid state physics and COLLECTION OF FORMULAE for Quantum Physics.

Define notations and motivate assumptions and approximations. Present the solutions so that they are easy to follow. Maximum number of point is 15 p. 7.5 points are required to pass the examination. Grades 3: 7.5, 4: 9.5, 5: 12.0

### 1. Crystal structure

The crystal structure below represents a 2 dimensional crystal. It consists of 4 kinds of atoms marked by the 4 letters q,p,d and b. The '....' in the figure mark a periodic continuation.

q	р	d b	q p	d b	q p	d b
d	b	q p	d b	q p	d b	q p
q	р	d b	q p	d b	q p	d b
d	b	q p	d b	q p	d b	q p
	•		•			
	•					

For the shown crystal structure indicate:

- (a) The rectangular unit cell.
- (b) The primitive unit cell.
- (c) The basis of letters associated with each lattice point.

(3p)



Figure 1: Principal scetch of the experiment showing the angle  $\beta$ 



Figure 2: Bragg peaks for a sample of unknown structure.

### 2. Bragg scattering

The diffraction pattern of a polycrystalline mono atomic powder is shown in figure 2 below. The X-rays used is the  $K_{\alpha 1}$  line from copper (Cu). The angle  $\beta$  (see figure 1) can be controlled between 0° and 90°. The outcome of the experiment is presented in figure 2, where the intensity (I) of the deflected beam is presented as a function of  $\beta$ .

From the data in the figure determine the structure (sc, fcc, bcc or diamond) of the sample. (3p)

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#### 3. A primitive cell consisting of two atoms

The structure of NaCl is FCC with the basis one Na at (0,0,0) and one Cl at  $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ . The lattice constant of the cubic unit cell is a = 5.65 Å. The velocity of sound for a transverse acoustic wave in the [111] direction is  $2.75 \cdot 10^3$  m/s. As each (111) plane in NaCl only consists of atoms of the same kind one can treat lattice vibrations with a simple one dimensional model where each plane is represented by one atom.

- (a) Make a drawing of the one dimensional crystal and determine the size of the primitive unit cell in terms of the lattice constant *a*, and sketch the dispersion relation (in the [111] direction) on a principal level.
- (b) Use the group velocity  $v = \partial \omega / \partial K$ , and the expansion of the dispersion relation

$$\omega^2 = C \frac{M_1 + M_2}{M_1 M_2} \pm C \sqrt{\left(\frac{M_1 + M_2}{M_1 M_2}\right)^2 - \frac{4\sin^2(Kd/2)}{M_1 M_2}},$$

to calculate the spring constant C.

(c) The crystal is exposed to light and there are several possible ways a photon can interact with the crystal. One is that the photon is absorbed creating a phonon conserving energy and momentum. Calculate the appropriate photon wave length for this process. (3p)

#### 4. **Misc.**

- a) Evaluate the commutator  $[y^2, p_y^2]$ .
- b) The ion Be<sup>3+</sup> has the nuclear charge +4 but only one electron. How much energy does it take to excite the electron from the ground state to the level 2s? Give a numerical value in electron Volts (eV)!
- c) The wave function of a hydrogen atom in an eigenstate to the Hamilton operator is:

$$\Psi(r,\theta,\phi) = \frac{1}{81\sqrt{6\pi}} (1/a_{\mu})^{3/2} (r^2/a_{\mu}^2) e^{-r/3a_{\mu}} [3\cos^2\theta - 1],$$

where  $a_{\mu}$  is the Bohr radius (with the reduced mass). Determine the quantum numbers n, l och  $m_l$ .

(3p)

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### 5. Hydrogen atom

Consider a hydrogen atom whose wave function at t = 0 is the following superposition of energy eigenfunctions  $\psi_{nlm_l}(\mathbf{r})$ :

$$\Psi(\mathbf{r}, t=0) = \frac{1}{\sqrt{15}} \left( 3\psi_{100}(\mathbf{r}) - 2\psi_{210}(\mathbf{r}) + \psi_{310}(\mathbf{r}) - \psi_{322}(\mathbf{r}) \right)$$

- (a) Is this wave function an eigenfunction of the parity operator  $\hat{\Pi}$  ?
- (b) What is the probability of finding the system in the ground state? In the state (210)? In the state (310)? In the state (322)? In any other state?
- (c) What is the expectation value of the energy (in eV); of the operator  $\mathbf{L}^2$  (in units of  $\hbar^2$ ); of the the operator  $L_z$  (in units of  $\hbar$ ).