

## Condensed Matter Theory I — WS09/10

### Exercise 2

(Please return your solutions before Fr. 6.11., 12:00 h)

#### 2.1. Reciprocal lattice and scattering experiments (12 points)

For a crystal with basis the differential scattering cross section is, as discussed in the lecture,

$$\frac{d^2\sigma}{d\Omega} = \frac{2\pi}{\hbar} |M_{\mathbf{q}}|^2 = \frac{2\pi}{\hbar} \left| \underbrace{\int_V d^3r U_b(\mathbf{r}) e^{-i\mathbf{q}\mathbf{r}}}_{\text{form factor } F(\mathbf{q})} \underbrace{\frac{1}{V} \sum_{\mathbf{R}_i \in \mathbb{B}} e^{-i\mathbf{q}\mathbf{R}_i}}_{\text{structure factor } S(\mathbf{q})} \right|^2 \quad (1)$$

where  $\mathbf{q} = \mathbf{k}_f - \mathbf{k}_i$  is the momentum transfer during the scattering process.

$$U_b(\mathbf{r}) = \sum_j V_j \delta^3(\mathbf{r} - \mathbf{r}_j) \quad (2)$$

is the scattering potential created by the atoms of the basis located at positions  $\mathbf{r}_j$  (it is assumed for simplicity that each atom creates a  $\delta$ -like potential of strength  $V_j$ ).  $\mathbf{R}_i$  are the position vectors of the Bravais lattice  $\mathbb{B}$  and  $V$  is the volume of the crystal.

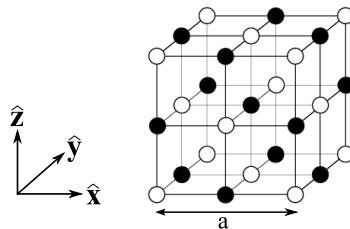


Figure 1: NaCl structure

- a) We consider the NaCl structure as shown in Fig. 1. This crystal can be described as an fcc-lattice with lattice constant  $a$  and a basis which consists of a (negatively charged) Cl ion at the origin and a (positively charged) Na ion at  $\frac{a}{2}\hat{\mathbf{x}}$ . A set of basis vectors for the fcc-lattice is given by

$$\begin{aligned} \mathbf{a}_1 &= \frac{a}{2}(\hat{\mathbf{y}} + \hat{\mathbf{z}}) \\ \mathbf{a}_2 &= \frac{a}{2}(\hat{\mathbf{z}} + \hat{\mathbf{x}}) \\ \mathbf{a}_3 &= \frac{a}{2}(\hat{\mathbf{x}} + \hat{\mathbf{y}}) \end{aligned}$$

Calculate the the basis vectors of the corresponding reciprocal lattice by

$$\mathbf{k}_i = 2\pi \frac{\epsilon_{ijk}(\mathbf{a}_j \times \mathbf{a}_k)}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}.$$

What kind of lattice is spanned by  $\mathbf{k}_1$ ,  $\mathbf{k}_2$  and  $\mathbf{k}_3$ ? We consider electron diffraction, i.e.  $V_2 = -V_1$ . Calculate the scattering amplitude  $M_{\mathbf{q}}$  for this crystal and show that all Bragg reflexes with  $\mathbf{q} = \mathbf{K} = m_1\mathbf{k}_1 + m_2\mathbf{k}_2 + m_3\mathbf{k}_3$ , with

$$(m_1 + m_2 + m_3) = \text{even}$$

vanish. Why does this happen?

b) Sketch the  $\mathbf{q}$  dependence of the scattering cross section along the x-axis.

The forward scattering cross section for a diffraction experiment on a one-dimensional crystal is shown in Fig. 2, i.e. every 3rd Bragg reflex is extinguished by the basis. Again, the atomic potentials are expected to be pointlike (2). Furthermore we assume that the atoms are placed equidistantly.

c) Use (1) to investigate the structure of the basis and calculate the potential strengths  $V_j$ .

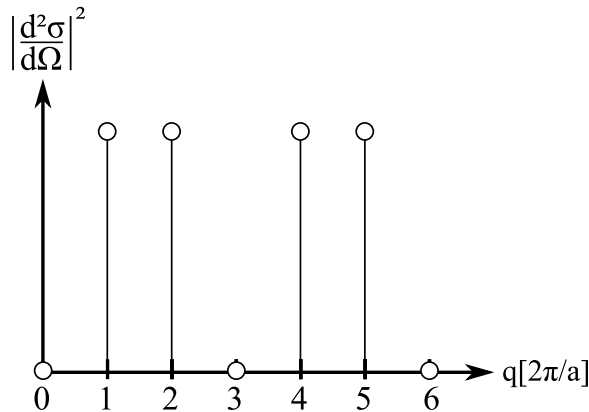


Figure 2: Observed cross section

## 2.2. Bandstructure calculation: weak periodic potential (10 points)

In this exercise we want to study the effect of a periodic potential in the limit of a very weak one. We will see that it creates a band structure with energy gaps at the Brillouin zone boundaries in  $k$ -space.

We start our calculation with a free electron system ( $\epsilon_k^0 = \frac{k^2}{2m}$ ) and treat the periodic potential in 2nd order perturbation theory.

a) Use Bloch's theorem to express the potential and the electron wave function as a Fourier series over all reciprocal lattice vectors and over all  $k$ -vectors in the 1st Brillouin zone, respectively. Write down the Schrödinger equation in  $k$ -space (compare lecture).

- b) Calculate the energy shift  $\Delta E_k^{(1)}$  in 1st order perturbation theory and show that it is a constant, which we will define to be 0.
- c) Continue with 2nd order perturbation theory: Is there an energy degeneracy for some values of  $k$ ? Diagonalize the Hamiltonian in the degenerate Hilbert subspace and show that the potential creates an energy gap at the Brillouin zone boundaries. Calculate this gap.
- d) Draw the dispersion relation  $\varepsilon_k$  in the presence of a weak periodic potential in the extended and in the reduced zone scheme.

### 2.3. Bloch Functions and Wannier Functions

(8 points)

In the lecture the Bloch functions  $\psi_{n,\vec{k}}(\vec{r})$  were introduced. These functions are a mixed representation depending both on  $\vec{k}$  and on  $\vec{r}$ . Additionally we introduce now a pure real space representation by Fourier transform of  $\psi_{n,\vec{k}}(\vec{r})$  (Wannier function):

$$W_{n,\vec{R}}(\vec{r}) = \int_{\text{1.BZ}} \frac{d^d k}{V_{BZ}} e^{-i\vec{k}\cdot\vec{R}} \psi_{n,\vec{k}}(\vec{r}) \quad V_{BZ} : \text{Vol. of 1.BZ}$$

- a) Show  $W_{n,\vec{R}}(\vec{r}) = W_n(\vec{r} - \vec{R})$  and prove that both  $\{\psi_{n,\vec{k}}(\vec{r})\}$  and  $\{W_{n,\vec{R}}(\vec{r})\}$  are a complete set of orthonormal functions.
- b) What follows for  $W_{n,\vec{R}}(\vec{r})$  in the case that  $\{\psi_{n,\vec{k}}(\vec{r})\}$  are nearly plane waves? In which case are these Wannier functions therefore relevant?