Universität Bonn 27.10.2005
Physikalisches Institut
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Condensed Matter Theory I — WS05/06

Exercise 2

(Please return your solutions before 08.11., 13:00 h)

2.1. Reciprocal Lattice and Scattering Experiments (8 points)

In this exercise the relation between the reciprocal lattice and a scattering experiment should be clarified. For this purpose consider a crystal described by a Bravais lattice $\mathcal{B}$ with basis, whose reciprocal lattice $\mathcal{R}$ is spanned by $\vec{b}_1, \vec{b}_2, \vec{b}_3$. The scattering potential created by the crystal is $V(\vec{r}) = \sum_{i=1}^{N} \rho(\vec{r} - \vec{R}_i)$ (N: number of lattice points, $\vec{R}_i$: lattice vector, $\rho(\vec{r})$: scattering potential of the basis).

a) A helpful tool to describe directions and planes in a crystal is the notation of Miller indices (see lecture). Consider now a crystal plane described by the Miller indices (hkl). Show that the reciprocal lattice vector $\vec{G} = h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3$ is perpendicular to (hkl). Show additionally that the distance $d(hkl)$ of two neighbouring planes is given by $d(hkl) = 2\pi/|\vec{G}|$

Let's continue with our studies about a scattering experiment. For that purpose consider an incoming plane wave, which is elastically scattered off the crystal (Fig. 1). We will analyse the process in 1st order pertubation theory (Born approximation).

b) Write down the scattering amplitude in terms of the incoming and outgoing plane wave functions and the scattering potential $V(\vec{r})$. Show that the difference between the incoming wavevector $\vec{k}_i$ and a possible outgoing wavevector $\vec{k}_o$ is a reciprocal lattice vector:

$$\Delta\vec{k} \equiv \vec{k}_i - \vec{k}_o \in \mathcal{R} \qquad \text{(Laue condition)}$$

c) Conclude the Bragg condition: (λ: wave length)

$$2\,d(hkl)\,\sin\theta \;=\; n\lambda \quad , n \in \mathbb{N}$$

d) Show that the scattering amplitude for $\Delta\vec{k} = \vec{G}$ factorizes as:

$$F_{\vec{G}} \;=\; \frac{N}{V} \underbrace{\sum_{j=1}^{n} e^{-i\vec{G}\cdot\vec{r}_j}}_{\text{structure factor}} \quad \underbrace{\int_{\substack{\text{unit}\\\text{cell}}} d^3r \;\; \rho_j(\vec{r})\, e^{-i\vec{G}\cdot(\vec{r}-\vec{r}_j)}}_{\text{form factor}}$$

How does the scattering intensity follow from the amplitude?

2.2. Bandstructure Calculation I: Weak Periodic Potential (8 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 ($\varepsilon_k^0 = \frac{k^2}{2m}$) and treat the periodic potential in 2nd order pertubation 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 pertubation theory and show that it is a constant, which we will define to be 0.

c) Continue with 2nd order pertubation 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 ε_k in the presence of a weak periodic potential in the extended and in the reduced zone scheme.

2.3. Bandstructure Calculation II: Tight-Binding Model (6 points)

We will now consider the opposite limit of a very strong periodic potential and start with wave functions, which are nearly atomic wave functions. The Hamiltonian in 2nd quantization reads then (see lecture)

$$H = \sum_{<i,j>} t_{ij}\, c_i^\dagger\, c_j$$

where the sum runs over all nearest neighbour lattice points.

a) Assume $t_{ij} = -t < 0$ and perform a Fourier transformation to show that H becomes diagonal in k-space.

b) Show that for a 3-dimensional cubic lattice the band energy is given by:

$$\varepsilon_k \;=\; \varepsilon_0 \;-\; 2\,t\;(cos(k_x a_x) + cos(k_y a_y) + cos(k_z a_z)) \qquad a_i : \text{lattice basis vectors}$$

and calculate the group velocity $\vec{v}_k$ and effective mass tensor.

c) For the 2-dimensional case, draw the lines of constant energy $\varepsilon_k = const.$ in the first Brillouin zone. Discuss where the group velocity vanishes.

2.4. Bloch Functions and Wannier Functions (4 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):

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

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?

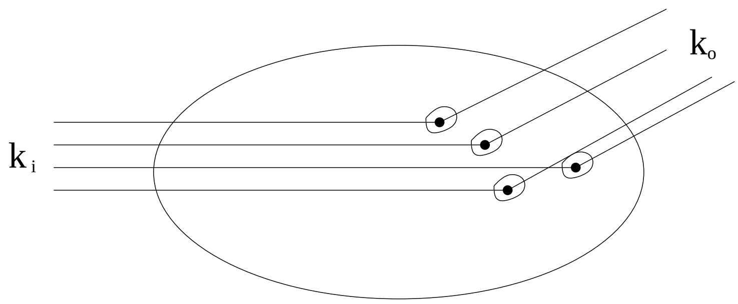

Figure 1: Elastic scattering of a plane wave in 1st order pertubation theory. Black dots shall denote lattice points, the 'circles' around the dots shall denote the basis.