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Theoretical Condensed Matter Physics
Exercise 2

(Submission: 02.11.18, discussion: 05./07.11.18)

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,

$$\frac{d\sigma}{d\Omega} = \frac{2\pi}{\hbar}\left|M_{\mathbf{q}}\right|^2 = \frac{2\pi}{\hbar}\left|\int_V d^3r U_b(\mathbf{r}) e^{-i\mathbf{q}\mathbf{r}} \frac{1}{V}\sum_{\mathbf{R}_i\in\mathcal{B}} e^{-i\mathbf{q}\mathbf{R}_i}\right|^2 \tag{1}$$

where $\mathbf{q} = \mathbf{k}_f - \mathbf{k}_i$ is the momentum transfer during the scattering process from the initial to the final state, $|\mathbf{k}_i\rangle \to |\mathbf{k}_f\rangle$.

$$U_b(\mathbf{r}) = \sum_{j\in \text{basis}} V_j \delta^3\left(\mathbf{r} - \mathbf{r}_j\right) \tag{2}$$

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

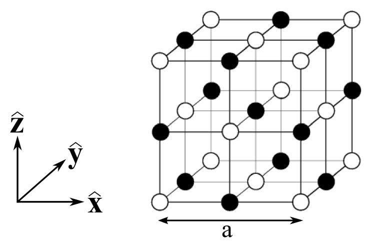

Figure 1: NaCl structure

(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, an a (positively charged) Na ion at $\frac{a}{2}\hat{\mathbf{x}}$. A set of primitive basis vectors for the fcc-lattice is given by

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

Calculate the basis vectors of the corresponding reciprocal lattice by

$$\mathbf{k}_i = 2\pi\frac{\epsilon_{ijk}\left(\mathbf{a}_j \times \mathbf{a}_k\right)}{\mathbf{a}_1 \cdot \left(\mathbf{a}_2 \times \mathbf{a}_3\right)}\ , \qquad i,\ j,\ k = 1,\ 2,\ 3 \ \ \text{(sum convention).}$$

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.

2.2 Bloch Functions and Wannier Functions (8 points)

In the lecture the Bloch functions $\psi_{n,\mathbf{k}}(\mathbf{r})$ were introduced, where $\mathbf{r}$ is the function variable and $\mathbf{k}$ is the quantum number labeling each Bloch state. Additionally we introduced the Wannier functions by considering now $\mathbf{k}$ as a variable and Fourier transforming $\psi_{n,\mathbf{k}}(\mathbf{r})$ with respect to $\mathbf{k}$:

$$W_{n,\mathbf{R}}(\mathbf{r}) = \int_{1\mathrm{BZ}} \frac{d^d k}{V_{\mathrm{BZ}}} e^{-i\mathbf{k}\cdot\mathbf{R}} \psi_{n,\mathbf{k}}(\mathbf{r}) \ ,$$

where $\mathbf{R} \in \mathcal{B}$ is a lattice vector of the Bravais lattice $\mathcal{B}$ in position space and V_{BZ} the volume of the 1st Brillouin zone.

(a) Show $W_{n,\mathbf{R}}(\mathbf{r}) = W_{n,0}(\mathbf{r} - \mathbf{R})$.

(b) Prove that both $\{\psi_{n,\mathbf{k}}(\mathbf{r}) | \mathbf{k} \in 1BZ\}$ and $\{W_{n,\mathbf{R}}(\mathbf{r}) | \mathbf{R} \in \mathcal{B}\}$ are a complete set of orthonormal basis functions of the lattice-function space.

(c) What follows for $W_{n,\mathbf{R}}(\mathbf{r})$ in the case that the Bloch functions $\psi_{n,\mathbf{k}}(\mathbf{r})$ are plane waves? Subsequently, discuss qualitatively the behavior of $W_{n,\mathbf{R}}(\mathbf{r})$ for the case that the Bloch functions $\psi_{n,\mathbf{k}}(\mathbf{r})$ are nearly plane waves, i.e., that their lattice-periodic part $u_{n\mathbf{k}}(\mathbf{r})$ is "nearly" a constant function of $\mathbf{r}$? For what cases will the Wannier function basis in general be most useful?