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Einführung in die Theoretische Festkörperphysik

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Exercise 7

(Due date: 09.12.2019)

Hint: On this exercise sheet you need the wave functions of electrons in a periodic potential, the so-called Bloch functions $\psi_{n\vec{k}}(\vec{r})$. They can be written:

$$\psi_{n\vec{k}}(\vec{r}) = u_{n\vec{k}}(\vec{r})e^{i\vec{k}\cdot\vec{r}}$$

where $u_{n\vec{k}}(\vec{r})$ is a lattice-periodic function with dimension $L^{-3/2}$. The determination of the wave function is thus reduced to the determination of $u_{n\vec{k}}(\vec{r})$.

Problem 1 (**Bloch Functions**) (3 points)

The Bloch functions are lattice-periodic functions, and therefore can be converted into the reciprocal space by a Fourier transformation. It may be helpful to express them by dimensionless coefficients $C_{n\vec{k}}(\vec{G})$,

$$u_{n\vec{k}}(\vec{G}) \equiv \frac{C_{n\vec{k}}(\vec{G})}{\sqrt{N\Omega}} \qquad \text{with} \qquad \sum_{\vec{G}} |C_{n\vec{k}}(\vec{G})|^2 = 1,$$

where Ω is the volume per unit cell, and N is the number of unit cells in the crystal. Assume that the spin does not have to be considered as a quantum number of the Bloch states. E_F is an upper limit for the energies to be considered. The electron density per unit cell as a function of the Bloch functions is then given by

$$\rho(\vec{r}) = 2\sum_{n}\sum_{\vec{k}\in \mathrm{BZ}} \Theta(E_F - \epsilon_{n\vec{k}})\,|\psi_{n\vec{k}}(\vec{r})|^2.$$

a) Using the given relations, calculate the normalization of the Bloch states, first per unit cell. How are the Bloch states defined above normalized with respect to the total crystal volume?

b) $N_{\vec{k}}$ is the number of allowed $\vec{k}$ points in the Brillouin zone. Show that the following applies to the number of electrons:

$$N_e = \frac{2}{N_{\vec{k}}}\sum_{n}\sum_{\vec{k}\in \mathrm{BZ}} \Theta(E_F - \epsilon_{n\vec{k}}).$$

c) How many electrons are allowed per band? For the sake of simplicity, consider the case that all relevant band energies are below the energy E_F.

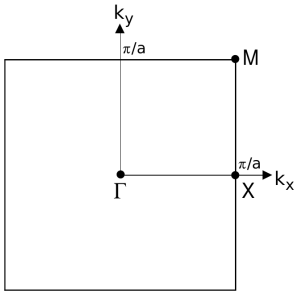
Problem 2 (**Free Electrons on a Square Lattice**) (3 points)

In this task, we sketch the band structure of free electrons on a square lattice, in order to better understand electronic band structures. In the process, we will see that even in this simple situation, the band structures may take a complicated form. Assume the dispersion relation is:

$$E(\vec{k}) = \frac{\hbar^2}{2m}|\vec{q}|^2 = \frac{\hbar^2}{2m}\left|\vec{k} - \vec{G}_0\right|^2$$

$\vec{k}$ is restricted to the first Brillouin zone and $\vec{G}_0$ is a reciprocal lattice vector of the square lattice. Sketch the dispersion relation along the path Γ - M in the Brillouin zone (see below) up to an energy $\frac{5\hbar^2}{4ma^2}$. You can use a computer to do this.

(*Hint:* You must also consider neighboring Brillouin zones with $\vec{G}_0 \neq 0$. In the lecture you will identify this situation with bands of higher energy.)



Problem 3 (**Schrödinger Equation in a Periodic Potential**) (4 points)

In the lecture, a general procedure to solve the Schrödinger equation in a periodic potential $V(\vec{r})$ with Fourier coefficients $V_{\vec{G}}$ was discussed. The Fourier coefficients $u_{\vec{k}}$ of the Bloch wave functions are given by the solution of the following eigenvalue problem:

$$\left(\frac{\hbar^2}{2m}\left(\vec{k}-\vec{G}_0\right)^2-\epsilon\right)c_{\vec{k}-\vec{G}_0}+\sum_{\vec{G}}V_{\vec{G}-\vec{G}_0}c_{\vec{k}-\vec{G}}=0 \quad \text{mit} \quad u_{\vec{k}}(\vec{r})=\sum_{\vec{G}}c_{\vec{k}-\vec{G}}e^{-i\vec{G}\cdot\vec{r}}$$

Consider a one-dimensional crystal with lattice constant a. The potential is given by $V(\vec{r}) = 2V_0 \cos\frac{2\pi x}{a}$. The eigenvalue problem can then be rewritten as follows:

$$\sum_{\vec{G}} M_{\vec{G}_0,\vec{G}}\; c_{\vec{k}-\vec{G}} = \epsilon\; c_{\vec{k}-\vec{G}_0}$$

a) What is the structure of the matrix M? Write an expression for the matrix elements $M_{\vec{G}_0,\vec{G}}$.

b) Write a program to diagonalize the matrix M for $k = 0$. In principal, M is infinitely large. You can restrict yourself to ten neighboring Brillouin zones in positive and negative direction, i.e. $G_0 \in \{-10\frac{2\pi}{a}, \cdots, 10\frac{2\pi}{a}\}$. The diagonalization yields the energy eigenvalues ϵ and the eigenfunction coefficients c_{k-G_0}. Use this to calculate the Bloch wave function of the band with minimal energy.

c) Plot the modulus of the wave function of the band with lowest energy as a function of x. Use the following parameters: $V_0 = 100,\ a = 1,\ \hbar = 1,\ m = 1$. In the case of such a strong potential you can expect the wave functions to be localized.