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Übungen zur Festkörpertheorie I — WS03/04

2. Übungsblatt

Electronic Band Structure

1. Tight–binding Model and Density of States

   We consider a d-dimensional cubic lattice ($d = 1, 2, 3$) with a lattice constant a (=length of primitive lattice vectors) and with a single atom on each lattice site $\vec{R}_i$. Each atom has one atomic orbital $\Psi_i(\vec{r}) = \Psi(\vec{r} - \vec{R}_i)$ with energy ε_0. The matrix elements of the kinetic energy are

$$\left\langle \Psi_i \left| \frac{\hbar^2 \nabla^2}{2m} \right| \Psi_j \right\rangle = \begin{cases} -t_{ij} < 0 & , \quad i, j \text{ nearest neighbors} \\ 0 & , \quad \text{else} \end{cases}$$

   a) Write down the Hamiltonian matrix H in the basis of atomic orbitals $\{\Psi_i\}$.

   b) Show that H is diagonalized by Fourier transformation with respect to the positions i, j and determine the band energy $\varepsilon_{\vec{k}}$ and the group velocity $v_{\vec{k}}$ for $d = 1, 2, 3$.

   c) Sketch for the two-dimensional case ($d = 2$) the lines of constant energy $\varepsilon_{\vec{k}} = const.$ in the 1st Brillouin zone. In particular, draw the constant energy lines in the band center, $\varepsilon_{\vec{k}} = \varepsilon_0$.

   d) Calculate the density of states (DOS) $N(\varepsilon)$ (per spin direction) for $d = 1, 2, 3$ dimensions. Determine the positions and the shape of the van Hove singularities for each case.

      Remark: For $d = 2, 3$ $N(\varepsilon)$ cannot be given in a closed form. In these cases, calculate $N(\varepsilon)$ only in the vicinity of the van Hove singularities.

   e) Discuss why the shape of the van Hove singularities at the band edges is characteristic for the dimension d and does *not* depend on the lattice structure.

— Please turn —

2. Electrons in a weak periodic potential - perturbation theory

We consider an electron (free dispersion $\varepsilon_{\vec{q}}^{(0)} = \hbar^2 q^2/2m$) moving in a weak periodic potential

$$U(\vec{r}) = \sum_{\vec{K}} U_{\vec{K}} \, \mathrm{e}^{i\vec{K}\cdot\vec{r}} \,,$$

where $\vec{K}$ is a reciprocal lattice vector. The Bloch wave function is $\Psi_{\vec{q}}(\vec{r}) = \sum_{\vec{K}} c_{\vec{K}+\vec{q}} \exp[i(\vec{q}+\vec{K})\cdot\vec{r}]$. We choose without loss of generality the zero of the energy scale such that $U_0 = 0$.

a) Determine the Schrödinger equation in reciprocal space (compare lecture).

b) Calculate the linear correction to the wave function $\Psi_{\vec{q}}(\vec{r})$ due to the periodic potential $U(\vec{r})$, i.e. calculate the coefficients $c_{\vec{K}+\vec{q}}$ of the wave function in $O(U_{\vec{K}})$. Assume here that $\Psi_{\vec{q}}(\vec{r})$ is not nearly degenerate with another wave function $\Psi_{\vec{q}+\vec{K}}(\vec{r})$ for any reciprocal lattice vector $\vec{K}$ (1st order non-degenerate perturbation theory).

   Hint: Verify that the linear correction to the energy $\varepsilon_{\vec{q}}^{(0)}$ vanishes. Then calculate the coefficient $c_{\vec{K}+\vec{q}}$ (for arbitrary, fixed $\vec{K}$) of the corrected wave function $\Psi_{\vec{q}}$ in $O(U_{\vec{K}})$ from the Schrödinger equation in reciprocal space, and note that only the coefficient $c_{\vec{q}}$ is of $O(U_{\vec{K}}^0)$.

c) Using the result of b), calculate the shift of the energy of $\Psi_{\vec{q}}$ in $O(U_{\vec{K}}^2)$.

d) Assume now that $\vec{q}$ is close to a Brillouin zone boundary, so that $\Psi_{\vec{q}}(\vec{r})$ and $\Psi_{\vec{q}+\vec{K}}(\vec{r})$ are (nearly) degenerate for exactly one reciprocal latice vector $\vec{K}$. Determine the wave functions $\Psi_{\vec{q}}(\vec{r})$ $\Psi_{\vec{q}+\vec{K}}(\vec{r})$ in the periodic potential as well as their energies.

e) Draw the dispersion relation $\varepsilon_{\vec{q}}$ in the presence of the periodic potential in the extendend, the reduced and in the periodic zone scheme. Show that at a Brillouin zone boundary the component of the group velocity $\vec{v}_{\vec{q}}$ perpendicular to the zone boundary is zero. Give an interpretation of this result in terms of the form of the corresponding Bloch wave function at the zone boundary.