Condensed Matter Theory I   WS 2022/2023

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Sheet 3
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Category A

1. Nearly free electrons (10 + 10 = 20 points)

The one-dimensional Hamiltonian

$$H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + U\cos^2\left(\frac{\pi x}{a}\right).$$

describes electrons in a periodic $\cos^2$-shaped potential with lattice constant a. We assume in this task that the strength U of the potential is sufficiently small to be treated perturbatively, i.e., within the approximation of nearly free electrons which was discussed in the lecture. We will now derive the band structure $E_{n,k}$ of this model.

(a) Perform perturbation theory to second order for crystal momenta at which the unperturbed solutions are non-degenerate.

(b) Now calculate the leading-order corrections to the electron energies at the degeneracy points in reciprocal space. Draw a sketch of the entire band structure.

Category B

2. $\vec{\mathbf{k}}\cdot\vec{\mathbf{p}}$-Method (10 + 10 = 20 points)

We derived the following Schrödinger equation in the lecture,

$$\left(E_k - \frac{\hbar^2(\vec{k}-i\vec{\nabla})^2}{2m}\right)u_{\vec{k}}(\vec{r}) = U(\vec{r})u_{\vec{k}}(\vec{r})\ .$$

Here, $u_{\vec{k}}(\vec{r})$ is the periodic part of the Bloch wave function, $\psi_k(\vec{r}) = u_k(\vec{r})e^{i\vec{k}\vec{r}}$. The periodic crystal potential is $U(\vec{r}) = U(\vec{r}+\vec{R})$, m is the mass of an electron, and $\vec{k}$ is the quasi-momentum (wave vector) in the first Brillouin zone. We assume that this equation has been solved for a certain quasi-momentum $\vec{k}_0$, i.e., all eigenstates $u_{n,\vec{k}_0}(\vec{r})$ and all eigenenergies $E_{n,\vec{k}_0}$ are known (n is the band index).

We will calculate now the eigenenergies and eigenstates for a state with quasi-momentum $\vec{k} = \vec{k}_0 + \delta\vec{k}$ where $\delta\vec{k}$ is small. Using perturbation theory and assuming no degeneracy at $\vec{k}_0$, calculate:

(a) the group velocity in the band n at the quasi-momentum $\vec{k}_0$;

(b) the effective mass tensor in the band n at the quasi-momentum $\vec{k}_0$.

3. Wannier functions (10 points)

The Wannier functions $w_n(\vec{r})$ are given by

$$w_n(\vec{r}) = V_{\mathrm{uc}} \int_{1.\mathrm{BZ}} \frac{d^3k}{(2\pi)^3} \psi_{n,\vec{k}}(\vec{r}) \,,$$

where $\psi_{n,\vec{k}}(\vec{r})$ are Bloch states and V_{uc} is the volume of the unit cell. Show that the Wannier functions $\{w_n(\vec{r} - \vec{R}),\ n = 1, 2, 3, \ldots,\ \vec{R} \in \text{Bravais lattice}\}$ form a complete orthonormal system, cf. (1.97) and (1.98) in the lecture notes.