
Exercise 5 for Theoretical Solid State Physics in Summer 2023

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1. One-dimensional potentials (10 points)

The Fourier coefficients $\psi_{\vec{k}-\vec{G}}$ of the energy eigenfunctions $\psi_{\vec{k}}(\vec{r}) = \sum_{\vec{G}} \psi_{\vec{k}-\vec{G}} e^{i(\vec{k}-\vec{G})\vec{r}}$ are related among each other by the lattice potential $V(\vec{r}) = \sum_{\vec{G}} V_{\vec{G}} e^{i\vec{G}\vec{r}}$ due to the Schrödinger equation in Fourier space. In the lecture the following system of equations was derived:

$$\left(\frac{\hbar^2 (\vec{k} - \vec{G})^2}{2m} - E \right) \psi_{\vec{k}-\vec{G}} + \sum_{\vec{G}'} V_{\vec{G}'-\vec{G}} \psi_{\vec{k}-\vec{G}'} = 0$$

Consider now cases of one-dimensional periodic lattices with lattice parameter a .

- Calculate the energy bands of the “empty lattice”, i.e. $V_{\vec{G}} \rightarrow 0$ for all \vec{G} . Draw a picture of the band structure in the first Brillouin zone.
- For the periodic potential $V(x) = V_0 \cos \frac{2\pi x}{a}$ only two coefficients $V_{\vec{G}}$ do not vanish. Calculate all energy gaps in first order perturbation theory. Where are they located in Fourier space? Draw a picture of the band structure and compare it with the “empty lattice”.
- Calculate the coefficients $V_{\vec{G}}$ and all gaps in first order perturbation theory (V_0 small) for the potential $V(x) = -aV_0 \sum_{n \in \mathbb{Z}} \delta(x - an)$ (Kronig-Penney model). Draw the shape of energy bands.

2. Dynamics of band electrons (4 points)

The Hamiltonian of an electron in energy band n exposed to an electro-magnetic field is given by

$$H_n = E_n \left(\vec{p} - \frac{e}{c} \vec{A} \right) + e\phi(\vec{r}).$$

Show the relations

$$\begin{aligned}\dot{\vec{r}} &= \vec{\nabla}_{\vec{k}} E_n(\vec{k}), \\ \dot{\vec{k}} &= \frac{e}{c} \dot{\vec{r}} \times \vec{B} + e\vec{E}.\end{aligned}$$

Hint: Prove first that $[k_\alpha, k_\beta] = i\frac{e}{c}\epsilon_{\alpha\beta\gamma}B_\gamma$.

3. Landau quantization (6 points)

Consider a free electron with mass m and charge e in a magnetic field $\vec{B} = B\vec{e}_z$. The Hamiltonian H is given by

$$H = \frac{1}{2m} \left(\vec{p} - \frac{e}{c} \vec{A} \right)^2.$$

The Landau gauge $\vec{A} = Bx\vec{e}_y$ fulfills $\vec{B} = B\vec{e}_z$ and $\vec{p}\vec{A} = \vec{A}\vec{p}$.

(a) Show that the energy eigenvalues are given by

$$E_{n,k_y,k_z} = \hbar\omega_0 \left(n + \frac{1}{2} \right) + \frac{\hbar^2 k_z^2}{2m},$$

where $\omega_0 = \frac{|e|B}{mc}$ is called the cyclotron frequency.

Hint: Show that the Hamiltonian transforms into

$$H = \frac{p_x^2}{2m} + \frac{m\omega_0^2}{2} \left(x - \frac{p_y}{m\omega_0} \right)^2 + \frac{p_z^2}{2m}$$

and that the ansatz $\psi(\vec{r}) = \phi(x) e^{ik_y y} e^{ik_z z}$ leads to the Schrödinger equation for the one-dimensional harmonic oscillator. How does the solution depend on the wavenumber k_y ?

(b) Determine the degree of degeneracy. Assume periodic boundary conditions in y -direction, $k_y = \frac{2\pi l_y}{L_y}$, $l_y \in \mathbb{N}$ and use the condition, that the midpoint of the oscillator x_0 is restricted to $0 \leq x_0 \leq L_x$.