Institut für Theoretische Festkörperphysik
Karlsruher Institut für Technologie

Prof. Dr. M. Garst
Dr. J. Masell
Dr. S. Sorn

Condensed Matter Theory 1 — Exercise 6

Winter term 2023/24

https://ilias.studium.kit.edu/goto.php?target=crs_2219528
To be discussed on: *Thursday 2023/12/07*

1. Magnetic unit cell for 2D electrons in a uniform magnetic field

We consider the Landau problem of an electron in two dimensions placed inside a uniform magnetic field B. We will see how the magnetic field introduces a length scale which leads to a magnetic unit cell and, thereby, enables the application of the Bloch theorem. To see this, consider the quantum mechanical Hamiltonian

$$H = \frac{1}{2m_e}\left(\pi_x^2 + \pi_y^2\right) \ , \tag{1}$$

where $\pi_i = p_i + eA_i$ is the mechanical momentum operator with $i = x, y$ and $e > 0$. Choose the symmetric gauge for the vector potential $A_i = (-B/2)\sum_{j=x,y}\epsilon_{ij}x_j$. ϵ_{ij} is the two-dimensional version of the Levi-Civita symbol, i.e., $\epsilon_{xy} = -\epsilon_{yx} = 1$ and $\epsilon_{xx} = \epsilon_{yy} = 0$.

a) Using the commutation relation between the position operator and the canonical momentum operator, $[x_i, p_j] = \mathrm{i}\hbar\delta_{ij}$, show that

$$[\pi_i, \pi_j] = \mathrm{i}C\epsilon_{ij} \ , \tag{2}$$

and compute the constant C. Unlike the canonical momentum operators p_i, which commute with one another, the mechanical momentum operators π_i do not commute. Show also that they do not commute with the Hamiltonian either by computing $[\pi_i, H]$.

b) Application of the Bloch theorem in two dimensions requires a translation operator along the x-direction and a translation operator along the y-direction, both of which commute with each other as well as the Hamiltonian. The first step to construct the translation operators is to define $\tilde{\pi}_i = p_i - eA_i$. Show that

$$[\tilde{\pi}_i, \tilde{\pi}_j] = -\mathrm{i}C\epsilon_{ij}, \tag{3}$$

$$[\tilde{\pi}_i, \pi_j] = 0, \tag{4}$$

$$[\tilde{\pi}_i, H] = 0. \tag{5}$$

c) The magnetic translation operator along the i-th direction is $T_i(d) = e^{-\mathrm{i}\tilde{\pi}_i d/\hbar}$ where d is a distance. Show that the magnetic translation operators act on the wavefunction as

$$T_x(d)\psi(x, y) = e^{ieA_x d/\hbar}\psi(x - d, y) \tag{6}$$

$$T_y(d)\psi(x, y) = e^{ieA_y d/\hbar}\psi(x, y - d) \tag{7}$$

for the symmetric gauge for the vector potential A_i. Show that $T_i(d)$ commutes with

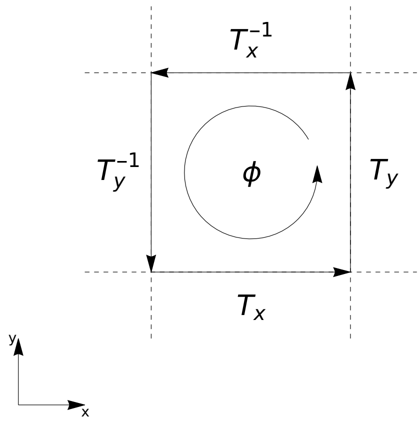

Figure 1: Schematic plot of the magnetic translation operations, $T_y^{-1}T_x^{-1}T_yT_x = e^{2\pi i\phi/\phi_0}$, along a loop encircling a magnetic flux ϕ.

the Hamiltonian, $[T_i(d), H] = 0$.

d) Show that

$$T_x(d_x)\tilde{\pi}_y T_x^{-1}(d_x) = \tilde{\pi}_y + eBd_x \tag{8}$$

$$T_y(d_y)\tilde{\pi}_x T_y^{-1}(d_y) = \tilde{\pi}_x - eBd_y \ . \tag{9}$$

One can thus also view, for example, $T_x(d_x)$ as a translation operator for the $\tilde{\pi}_y$ operator. Using this result, show that

$$T_x(d_x)T_y(d_y) = e^{-i2\pi\phi/\phi_0}T_y(d_y)T_x(d_x) \ , \tag{10}$$

where $\phi = Bd_xd_y$ is the magnetic flux enclosed by the rectangular area defined by d_x and d_y, and $\phi_0 = 2\pi\hbar/e$ is the magnetic flux quantum. This implies that consecutive application of magnetic translations around a closed loop leads to a phase factor determined by the magnetic flux enclosed by the loop, see Fig.1.

e) Assuming that $d_x = d_y = d$, compute the commutator $[T_x(d), T_y(d)]$. For which values of d does the commutator vanish? The smallest non-zero d defines the magnetic length as well as a square-shaped magnetic unit cell. With all these, we have set a stage for an application of the Bloch theorem. The resulting band structure can be identified with the Landau levels. Compute the degeneracy of each Landau level.

2. Model of free electrons

In the model of free spin-1/2 electrons, the interaction of the conduction electrons with the ionic potential is neglected and the electrons are considered as a free Fermi gas. This exercise shall familarize you with the effect of a weak lattice potential on the free electron energy spectrum.

a) For a two-dimensional square lattice with the lattice constant a, determine the concentration of free electrons at which the third Brillouin zone starts to get filled.

b) Consider a monoatomic monovalent (giving a single electron per atom) fcc material, whose electrons are approximated as a free electron gas. Show that the ratio of the Fermi sphere volume to the volume of the first Brillouin zone is 1/2. Do you get a metal or an insulator in this case when the periodic potential is treated in lowest order perturbation theory?

3. Weak periodic potential

In momentum space, the Schrödinger equation in the presence of a periodic potential has the following form

$$\left(\frac{\hbar^2 k^2}{2m_0} - \varepsilon\right)\psi_{\vec{k}} + \sum_{\vec{G}} V_{\vec{G}}\psi_{\vec{k}-\vec{G}} = 0 \; . \tag{11}$$

Here, $V_{\vec{G}} = V_{\text{PUC}}^{-1}\int_{V_{\text{PUC}}} V(\vec{r})e^{-i\vec{G}\cdot\vec{r}}\mathrm{d}\vec{r}$ is the Fourier component of the periodic potential with the translational invariance of the underlying Bravais lattice, $V(\vec{r}) = V(\vec{r}+\vec{R})$. $\vec{R}$ and $\vec{G}$ denote points of the Bravais and reciprocal lattices, respectively. If the potential is weak, $|V_{\vec{G}}| \ll \hbar^2k^2/(2m_0)$, then one can use for an N-fold degenerate point $\vec{k}_d$ in the first Brillouin zone the N-component approximation and apply degenerate perturbation theory. N is the number of degenerate solutions $\vec{G}$ such that $\hbar^2(\vec{k}_d - \vec{G})^2/2m_0 = \hbar^2\vec{k}_d^2/2m_0$. This problem illustrates an estimate of the energy gaps caused by the lattice potential.

a) For a one-dimensional symmetrical potential $V(x) = V(-x)$, show that the m-th energy gap is $\Delta\varepsilon_m \approx |2V_G|$, with the reciprocal lattice vector $G = 2\pi m/a$.

b) For the two-dimensional potential $V(x,y) = 4U\cos(2\pi x/a)\cos(2\pi y/a)$, determine the energy gap for the point $\vec{k}_d = \frac{\pi}{a}(1,1)^T$ at the corner of the first Brillouin zone.