Karlsruhe Institute of Technology

Institute for Theoretical Condensed Matter physics

Condensed Matter Theory I WS 2022/2023

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Sheet 8

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Category A

1. Boltzmann equation in the presence of spin-orbit interaction($10+10+10=30$ Points)

In this exercise we generalize the Boltzmann equation for particles with with spin-orbit interaction. We choose a very simple collision integral and attempt solving the resulting Boltzmann equation.

Consider a system with spin-orbit interaction as described by the Hamiltonian

$$H = \frac{p^2}{2m} + \boldsymbol{\Omega}(\boldsymbol{p}) \cdot \boldsymbol{\sigma},$$

where $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ is the vector of Pauli matrices and $\boldsymbol{\Omega}(\boldsymbol{p})$ is the fictitious "magnetic field" that depends on momentum and thus describes the spin-orbit interaction.

The Boltzmann equation is usually derived within the semiclassical approach, where we treat the quasiparticle momentum as a c-number (and not an operator). However, the electron spin has to be treated quantum-mechanically. This can be achieved by considering the one-particle density matrix which is a 2×2 matrix in spin space. The rest of the variables one can treat semi-classically, i.e. $\rho \to \rho_{\sigma_1\sigma_2}(\boldsymbol{r}, \boldsymbol{p}, t)$.

We consider an homogeneous electric field (no magnetic field) and derive the kinetic equation. We consider the full time derivative of the density matrix and equate it to the collision integral. The quantum-mechanical treatment of the spin variables amounts to using the well-known quantum-mechanical rules, which prescribe the time derivative of an operator to be given by its commutator with the Hamiltonian. This way in a spatially homogeneous systems one arrives at the equation

$$\frac{\partial \rho}{\partial t} + i\big[\boldsymbol{\Omega}(\boldsymbol{p}) \cdot \boldsymbol{\sigma}, \rho\big] - e\boldsymbol{E}\frac{\partial \rho}{\partial \boldsymbol{p}} = I[\rho].$$

Here $[\ldots, \ldots]$ stands for a commutator.

(a) Derive the above equation for a homogeneous system treating the spin variables quantum-mechanically and the momentum semi-classically.

(b) Recall the well-known fact from quantum mechanics: any function of the Pauli matrices is a linear function. Therefore, the 2×2 density matrix can be written as

$$\rho = \frac{f}{2}\,\hat{1} + \boldsymbol{S} \cdot \boldsymbol{\sigma}.$$

Here $\hat{1}$ denotes a unity matrix.

Substitute this expression into the equation for the density matrix and find coupled equations for the charge and spin distribution functions f and $\boldsymbol{S}$. Use the τ-approximation to evaluate the collision integral.

(c) Consider the simplest version of the spin-orbit coupling in two-dimensional systems, the so-called Rashba spin-orbit coupling, which is described by

$$\boldsymbol{\Omega} = \alpha(p_y, -p_x).$$

Write down the Boltzmann equations obtained above for this form of the spin-orbit coupling.

Hint: You are now dealing with a two-dimensional system. The momentum is now a 2D vector, but spin still has three components

Category B

2. Thermoelectric effect (10 Points)

Consider the thermoelectric effect (Mott formula) for a free electron gas. The applied temperature gradient, $\vec{\nabla}T$, induces an electric current,

$$\vec{j} = -\eta\vec{\nabla}T,$$

where η is the thermoelectric coefficient. Consider three-dimensional electron gas with the parabolic dispersion, $\varepsilon = \dfrac{\hbar^2 k^2}{2m}$, which has the given Fermi energy ε_F. Calculate the thermoelectric coefficient, η, for a given temperature T, assuming that the relaxation time τ in the Boltzmann equation is known. Express the result in terms of ε_F, velocity and density of states at the Fermi level, v_F and ν_F.

Without explicit calculations, obtain η for 2D and 1D cases using the representation of η through v_F, ν_F and ε_F found for 3D case.

3. Conductivity of the tight-binding model (10 points)

The dispersion relation of the tight-binding model on the square lattice with lattice constant a has the form

$$\epsilon(\boldsymbol{k}) = -\epsilon_1 \left[\cos(ak_x) + \cos(ak_y)\right].$$

Assume that the relaxation time τ is independent of the momentum. Using equation (268) of lecture notes applied to the 2D case for DC conductivity ($\omega = 0$), derive the diagonal elements of the quasiclassical electrical conductivity tensor at half filling. Suppose that $k_B T \ll \mu$.