INSTITUTE FOR THEORETICAL CONDENSED MATTER PHYSICS

Condensed Matter Theory I WS 2022/2023

Prof. Dr. A. Shnirman		Sheet 8
Dr. D. Shapiro, Dr. H. Perrin	Tutorial:	22.12.2022

Category A

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

In this exercise we practice solving the Boltzmann equation using the example of a system with spin-orbit interaction. We construct a model collision integral and attempt solving the resulting Boltzmann equation. As a result, we obtain the physics of the so-called Edelstein effect. Note, that this is not a true theory of the spin-orbit interaction, but rather an exercise: the collision integral we are using here is incorrect. (A true kinetic theory of systems with spin-orbit interaction has not been worked out yet – it is an important topic in current research).

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 $\Omega(\boldsymbol{p})$ 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 semiclassically, i.e. $\rho \to \rho_{\sigma_1 \sigma_2}(\boldsymbol{r}, \boldsymbol{p}, t)$.

We introduce an homogeneous electric field (no magnetic field). The kinetic equation can now be derived. We consider time variation 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 definition where the time derivative of an operator is given by its commutator with the Hamiltonian. This way in a spatially homogeneous systems one arrives at the equation

$$rac{\partial
ho}{\partial t} + i ig[oldsymbol{\Omega}(oldsymbol{p}) \cdot oldsymbol{\sigma},
ho ig] - e oldsymbol{E} rac{\partial
ho}{\partial oldsymbol{p}} = I[
ho].$$

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 semiclassically.
 Solution:

Consider the kinetic equations describing a particle with spin. The density matrix evolves due to non commutation relation with the Hamiltonian. Moreover, we must add a collision term in the evolution equation which is not taken into account in the Hamiltonian.

$$\frac{d\rho}{dt} = i[\rho, H] + I[\rho]$$

Treating the phase space variables r and p as number we obtain:

$$\frac{\partial \rho}{\partial t} + \boldsymbol{v} \frac{\partial \rho}{\partial \boldsymbol{r}} + \dot{\boldsymbol{p}} \frac{\partial \rho}{\partial \boldsymbol{p}} = i[\rho, H] + I[\rho].$$

Finally, using the explicit form of the Hamiltonian

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

we find

$$rac{\partial
ho}{\partial t} + i[\Omega(\boldsymbol{p})\boldsymbol{\sigma},
ho] - e\boldsymbol{E} rac{\partial
ho}{\partial \boldsymbol{p}} = I[
ho].$$

(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 S. Use the τ -approximation to evaluate the collision integral.

Solution:

Here we use the explicit form for a density matrix where the phase space part is treated semiclassically

$$\rho = \frac{1}{2}f(t,p) + \boldsymbol{S}(t,p)\boldsymbol{\sigma},$$

where f(t, p) is the usual (charge) distribution function, S(t, p) is the spin distribution function, and the first term is proportional to the unit matrix (no texplicitly written).

Substituting the above density matrix into the kinetic equation we find

$$\frac{1}{2}\frac{\partial f}{\partial t} + \frac{\partial S}{\partial t}\boldsymbol{\sigma} + i[\boldsymbol{\Omega}(\boldsymbol{p})\boldsymbol{\sigma}, \boldsymbol{S}\boldsymbol{\sigma}] - \frac{1}{2}eE_{\alpha}\frac{\partial f}{\partial p_{\alpha}} - eE_{\alpha}\frac{\partial S}{\partial p_{\alpha}}\boldsymbol{\sigma} = I[\rho].$$

The commutator can be simplified using the properties of the Pauli matrices

$$[\mathbf{\Omega}(\mathbf{p})\boldsymbol{\sigma}, \mathbf{S}\boldsymbol{\sigma}] = \Omega_i(\mathbf{p})S_j[\sigma_i, \sigma_j] = 2i\Omega_i(\mathbf{p})S_j\epsilon_{ijk}\sigma_k = 2i[\mathbf{\Omega}(\mathbf{p})\times\mathbf{S}]\boldsymbol{\sigma}$$

This way we find the matrix equation

$$\frac{1}{2}\frac{\partial f}{\partial t} + \frac{\partial S}{\partial t}\boldsymbol{\sigma} - 2[\boldsymbol{\Omega}(\boldsymbol{p}) \times \boldsymbol{S}]\boldsymbol{\sigma} - \frac{1}{2}eE_{\alpha}\frac{\partial f}{\partial p_{\alpha}} - eE_{\alpha}\frac{\partial \boldsymbol{S}}{\partial p_{\alpha}}\boldsymbol{\sigma} = I[\rho].$$

The matrix equation can be reduced to a set of scalar equations by multiplying the equation by the Pauli matrices and evaluating the trace. We find

$$\frac{\partial f}{\partial t} - eE_{\alpha}\frac{\partial f}{\partial p_{\alpha}} = \operatorname{Tr} I[\rho],$$
$$\frac{\partial S_{i}}{\partial t} - 2[\boldsymbol{\Omega}(\boldsymbol{p}) \times \boldsymbol{S}]_{i} - eE_{\alpha}\frac{\partial S_{i}}{\partial p_{\alpha}} = \frac{1}{2}\operatorname{Tr}\sigma_{i}I[\rho].$$

Finally, let us assume the simplest τ -approximation for the collision integral

$$I[\rho] = -\frac{\delta\rho}{\tau} = -\frac{\delta f}{2\tau} - \frac{\delta S\sigma}{\tau}.$$

Substituting this into the above kinetic equations we find

$$\frac{\partial f}{\partial t} - eE_{\alpha}\frac{\partial f}{\partial p_{\alpha}} = -\frac{\delta f}{\tau},$$
$$\frac{\partial S_i}{\partial t} - 2[\mathbf{\Omega}(\mathbf{p}) \times \mathbf{S}]_i - eE_{\alpha}\frac{\partial S_i}{\partial p_{\alpha}} = -\frac{\delta S_i}{\tau}$$

(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

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

Substitute the Rashba form of the spin-orbit coupling in the equations obtained above.

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

Solution:

For the case of the Rashba coupling,

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

the vector product in the kinetic equations has the form

$$\boldsymbol{\Omega} \times \boldsymbol{S} = \alpha(-p_x S_z, -p_y S_z, p_x S_x + p_y S_y) = -\alpha \boldsymbol{p} S_z + \alpha (\boldsymbol{S}_{\perp} \cdot \boldsymbol{p}) \boldsymbol{e}_z,$$

where $S_{\perp} = (S_x, S_y)$ and e_z is the unit vector in the z-direction. The equations for the spin distribution function now have the form

$$\frac{\partial S_z}{\partial t} - 2\alpha \mathbf{S}_{\perp} \cdot \mathbf{p} - eE_{\alpha} \frac{\partial S_z}{\partial p_{\alpha}} = -\frac{\delta S_z}{\tau}, \\ \frac{\partial \mathbf{S}_{\perp}}{\partial t} + 2\alpha \mathbf{p} S_z - eE_{\alpha} \frac{\partial \mathbf{S}_{\perp}}{\partial p_{\alpha}} = -\frac{\delta \mathbf{S}_{\perp}}{\tau}.$$

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, $\varepsilon = \frac{\hbar^2 k^2}{2m}$, 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.

Solution:

The electric current follows from the Boltzmann equation on the distribution function:

$$\vec{j} = \frac{\tau e}{T} \int \frac{dp_x dp_y dp_z}{(2\pi\hbar)^3} \vec{v_p} (\epsilon_{\vec{p}} - \varepsilon_F) \frac{\partial f_0}{\partial \epsilon} (\vec{v_p} \cdot \vec{\nabla}T).$$

Here, f_0 is the Fermi distribution function in the equilibrium. Consider an isoenergy surface S in momentum space for a certain energy ε . The surface is defined by the equa-

surface S in momentum space for a certain energy ε . The integral over \vec{p} now reads as $\int d^3 \vec{p} = \int_0^\infty d\varepsilon \oint_{\epsilon_{\vec{p}}=\varepsilon} dS$. In d dimensions, for isotropic spectrum we have for the velocities, $\oint_{\epsilon_{\vec{p}}=\varepsilon} \vec{p} v_{p_{\alpha}} v_{p_{\beta}} dS = \delta_{\alpha,\beta} \frac{v^2(\varepsilon)}{d} \oint_{\epsilon_{\vec{p}}=\varepsilon} dS$,

where the velocity at this energy is $v(\varepsilon) = \sqrt{\frac{2\varepsilon}{m}}$. As long as no variables now do not depend on \vec{p} , we can calculate surface integral over momenta $\epsilon_{\vec{p}} = \varepsilon$ and introduce the density of states $\nu(\varepsilon)$. As a result, we replace the integral over momentum as follows, $\int \frac{d^3 \vec{p}}{(2\pi\hbar)^3} \to \int \nu(\varepsilon) d\varepsilon$. Then, the current now reads

$$\vec{j} = -\left[\frac{\tau e}{dT}\int v^2(\varepsilon)\nu(\varepsilon)(\varepsilon-\varepsilon_F)\frac{-\partial f_0(\varepsilon)}{\partial\varepsilon}d\varepsilon\right]\vec{\nabla}T$$

The term in square braces is nothing but the thermoelectric coefficient η . To calculate it, we use the Sommerfeld expansion for low temperatures $T \ll \varepsilon_F$:

$$\frac{-\partial f_0(\varepsilon)}{\partial \varepsilon} \approx \delta(\varepsilon - \varepsilon_F) + \frac{\pi^2 T^2}{6} \delta''(\varepsilon - \varepsilon_F).$$

Integrating over ε , we find

$$\eta = \frac{\pi^2 e \tau T}{3d} \left. \frac{\partial (v^2(\varepsilon)\nu(\varepsilon))}{\partial \varepsilon} \right|_{\varepsilon = \varepsilon_F}$$

As mentioned above, $v(\varepsilon) \propto \varepsilon^{\frac{1}{2}}$. The density of states in d dimensions, is $\nu(\varepsilon) \propto \varepsilon^{\frac{1}{2}}$. $\varepsilon^{\frac{d}{2}-1}$. Then, the combination $v^2(\varepsilon)\nu(\varepsilon) \propto \varepsilon^{\frac{d}{2}}$ has $\frac{d}{2}$ in the exponent. Its derivative is $\frac{\partial(v^2(\varepsilon)\nu(\varepsilon))}{\partial\varepsilon} = \frac{d}{2}\frac{v^2(\varepsilon)\nu(\varepsilon)}{\varepsilon}.$ Finally, we have for any dimension:

$$\eta = \frac{\pi^2 e \tau T v_F^2 \nu_F}{6\varepsilon_F}$$

Category B

3. Conductivity of the tight-binding model

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

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

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 diagonale elements of the quasiclassical electrical conductivity tensor at half filling. Suppose that $k_B T \ll \mu$.

Solution: The conductivity is given by:

$$\sigma_{\alpha,\beta} = -2e^2\tau \int \frac{\mathrm{d}^2k}{(2\pi)^2} \frac{\partial f_0}{\partial \epsilon} v_\alpha v_\beta$$

If $k_B T \ll \mu$, the Fermi-Dirac distribution is at lowest order:

$$\frac{\partial f_0}{\partial \epsilon} \simeq -\delta(\epsilon - \mu)$$

One can transform the integration variable $(k_x, k_y) \to (k_x, \epsilon)$. The Jacobian of the transformation is $|v_y|^{-1}$.

$$\sigma_{y,y} = \frac{e^2 \tau}{2\pi^2} \int \mathrm{d}k_x d\epsilon \delta(\epsilon - \mu) |v_y|$$

At half filling $\mu = 0$, therefore at $\epsilon = 0$ $k_y = \frac{\pi}{a} - k_x$ for one quadrant.

$$\sigma_{y,y} = \frac{2e^2\tau\epsilon_1 a}{\pi^2} \int_0^{\pi/a} \mathrm{d}k_x \sin(\pi - k_x a) = \frac{4e^2\tau\epsilon_1}{\pi^2}$$

The expression is similar for $\sigma_{x,x}$ because $|v_x| = |v_y|$ at $\epsilon = 0$

(10 points)