

Theorie der Kondensierten Materie I WS 2018/2019

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Blatt 6

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Lösungsvorschlag

1. Boltzmann equation in the presence of spin-orbit interaction:

(a) *Derive the kinetic equation for a system with SO interaction*

Consider first a single spin. It can be described by a 2×2 density matrix ρ satisfying the equation of motion

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

where the Hamiltonian H is also a 2×2 matrix. The diagonal elements of ρ give the probabilities to

find the system in a state with $s_z = \pm 1/2$:

$$\langle s_z \rangle = \text{Tr} \rho s_z = (\rho_{11} - \rho_{22})/2.$$

The off-diagonal elements of ρ take into account the possibility to find the spin in a state which is a coherent superposition of the states with $s_z = \pm 1/2$, e.g. a state with a definite projection of s_x .

Consider now the kinetic equations describing a particle with spin. Now, the density matrix involves not only spin variables, but also phase space variables. Treating the latter semiclassically, we find

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

As a result, the kinetic equation has the form

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

Finally, using the explicit form of the Hamiltonian

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

we find

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

(b) *Spin and charge distribution functions*

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

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

where $f(t, p)$ is the usual (charge) distribution function, $\mathbf{S}(t, p)$ is the spin distribution function, and the first term is proportional to the unit matrix (not explicitly written).

Substituting the above density matrix into the kinetic equation we find

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

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

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

This way we find the matrix equation

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

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

$$\frac{\partial f}{\partial t} - eE_\alpha \frac{\partial f}{\partial p_\alpha} = \text{Tr}I[\rho],$$

$$\frac{\partial S_i}{\partial t} - 2[\boldsymbol{\Omega}(\mathbf{p}) \times \mathbf{S}]_i - eE_\alpha \frac{\partial S_i}{\partial p_\alpha} = \frac{1}{2}\text{Tr}\sigma_i I[\rho].$$

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

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

Substituting this into the above kinetic equations we find

$$\frac{\partial f}{\partial t} - eE_\alpha \frac{\partial f}{\partial p_\alpha} = -\frac{\delta f}{\tau},$$

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

(c) *Rashba spin-orbit coupling*

For the case of the Rashba coupling,

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

the vector product in the kinetic equations has the form

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

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

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

(d) *Equilibrium distribution function*

The Hamiltonian

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

has the following eigenvalues

$$\epsilon_\pm(p) = \frac{p^2}{2m} \pm \alpha p.$$

Without writing down the eigenvectors, we may relate the Hamiltonian in the diagonal form to the original basis using a unitary transformation

$$H = U^+ \left[\frac{p^2}{2m} + \alpha p \sigma_z \right] U,$$

with

$$U^+ \alpha p \sigma_z U = \mathbf{\Omega}(\mathbf{p})\boldsymbol{\sigma}.$$

The equilibrium occupation numbers of the eigenstates are given by the Fermi functions $n_F[\epsilon_\sigma(p)]$. Hence the equilibrium density matrix in the basis of the eigenstates is given by

$$\tilde{\rho}_0 = \frac{1}{2} \left\{ n_F[\epsilon_+(p)] + n_F[\epsilon_-(p)] + \sigma_z (n_F[\epsilon_+(p)] - n_F[\epsilon_-(p)]) \right\}.$$

The density matrix in the original basis can be found using the same unitary rotation

$$\rho_0 = U^+ \tilde{\rho}_0 U = \frac{1}{2} \left\{ n_F[\epsilon_+(p)] + n_F[\epsilon_-(p)] + (n_F[\epsilon_+(p)] - n_F[\epsilon_-(p)]) \frac{\mathbf{\Omega}(\mathbf{p})\boldsymbol{\sigma}}{\alpha p} \right\}.$$

Reading off the expressions for the charge and spin distributions we find (with $\epsilon = p^2/(2m)$)

$$\begin{aligned}f_0 &= n_F[\epsilon_+(p)] + n_F[\epsilon_-(p)] \xrightarrow{\alpha \rightarrow 0} 2n_F(\epsilon), \\ \mathbf{S}_{\perp,0} &= (n_F[\epsilon_+(p)] - n_F[\epsilon_-(p)]) \frac{\mathbf{\Omega}(\mathbf{p})}{\alpha p} \xrightarrow{\alpha \rightarrow 0} n'_F(\epsilon) \mathbf{\Omega}(\mathbf{p}), \\ S_{z,0} &= 0.\end{aligned}$$

(e) *Linear response solution*

Consider the equations for the spin distribution function in the steady state. Introducing small deviations from equilibrium,

$$\mathbf{S}_\perp = \mathbf{S}_{\perp,0} + \delta\mathbf{S}_\perp, \quad S_z = \delta S_z,$$

we linearize the equations for the spin distribution function. For the purpose of linearizing, it is important to understand that both $\delta\mathbf{S}$ and \mathbf{E} are small quantities (deviations from equilibrium). In particular, we disregard terms like $E_\alpha \delta S_z$ as those are of second order in small quantities. We find

$$\begin{aligned} 2\alpha \mathbf{S}_{\perp,0} \mathbf{p}^0 + 2\alpha \delta\mathbf{S}_\perp \mathbf{p} &= \delta S_z / \tau, \\ 2\alpha \mathbf{p} \delta S_z - eE_\alpha \frac{\partial \mathbf{S}_{\perp,0}}{\partial p_\alpha} &= -\delta\mathbf{S}_\perp / \tau, \end{aligned}$$

where the first term vanishes, since $\mathbf{S}_{\perp,0} \propto \boldsymbol{\Omega}(\mathbf{p})$ and $\boldsymbol{\Omega}(\mathbf{p}) \perp \mathbf{p}$. Clearly, in the absence of the electric field the solution is zero, $\delta\mathbf{S} = 0$, proving that we have the correct equilibrium distribution. We can use the second equation to eliminate $\delta\mathbf{S}_\perp$ from the first; then, solving for δS_z , we find,

$$\delta S_z = \frac{-2\alpha\tau^2 e}{1 + 4\alpha^2 p^2 \tau^2} \mathbf{E} \cdot \mathbf{S}_{\perp,0},$$

where we have used the general relation (product rule of differentiation) $(\partial_{p_\alpha} \mathbf{S}_{\perp,0}) \cdot \mathbf{p} = \partial_{p_\alpha} (\mathbf{S}_{\perp,0} \mathbf{p}) - \mathbf{S}_{\perp,0} \cdot \partial_{p_\alpha} \mathbf{p}$ which reduces to $(\partial_{p_\alpha} \mathbf{S}_{\perp,0}) \cdot \mathbf{p} = -(\mathbf{S}_{\perp,0})_\alpha$, due to $\mathbf{S}_{\perp,0} \perp \mathbf{p}$. Inserting the result for δS_z into the second equation, we find

$$\delta\mathbf{S}_\perp = e\tau E_\alpha \frac{\partial \mathbf{S}_{\perp,0}}{\partial p_\alpha} + \frac{4e\alpha^2 \tau^3}{1 + 4\alpha^2 \tau^2 p^2} (\mathbf{E} \cdot \mathbf{S}_{\perp,0}) \mathbf{p}.$$

(f) *Average spin polarization*

The average spin is given by

$$\langle \mathbf{s} \rangle = \int \frac{d^2 p}{(2\pi)^2} \text{Tr} \rho \mathbf{s} = \int \frac{d^2 p}{(2\pi)^2} \mathbf{S}.$$

Given that δS_z is an odd function of the momentum components p_α , we conclude that

$$\langle s_z \rangle = 0.$$

The planar polarization we calculate choosing the x -direction along the in-plane electric field,

$$\mathbf{E} = (E, 0, 0).$$

In this case, only the y -component of the magnetization is nonzero. For weak spin-orbit coupling ($\alpha \rightarrow 0$) we find

$$\langle s_y \rangle = 4eE\alpha^3 \tau^3 \int \frac{d^2 p}{(2\pi)^2} \frac{p_y^2}{1 + 4\alpha^2 \tau^2 p^2} n'_F(p^2/2m).$$

At $T = 0$,

$$n'_F(p^2/2m) = -\frac{1}{v_F}\delta(p - p_F),$$

and the integral can be easily evaluated, e.g. in polar coordinates.

The final result is given by

$$\langle s_y \rangle = -\frac{1}{\pi}eEm\frac{\alpha^3\tau^3 p_F^2}{1 + 4\alpha^2\tau^2 p_F^2}.$$