Theorie der Kondensierten Materie I WS 2015/16

Prof. Dr. A. Shnirman
PD Dr. B. Narozhny, Dr. I. Protopopov

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1. Conductivity of the 2D tight-binding modell

(5 + 5 = 10 Punkte)

(a) The conductivity as derived from the Boltzmann equation reads

$$\sigma_{\alpha\beta} = -2e^2\tau \int \frac{d^2k}{(2\pi)^3} \frac{\partial f_0}{\partial \epsilon} v_\alpha v_\beta \tag{1}$$

Here

$$v_\alpha = \frac{\partial \epsilon(k)}{\partial k_\alpha} = E_1 a \sin k_\alpha a \tag{2}$$

To compute the integral we take into account that at low temperatures $\partial f_0/\partial\epsilon = -\delta(\epsilon - \mu)$ and also that $d^3k = dSd\epsilon/|v|$, where dS is the area element on the surface of constant energy (in our case surfaces of constant energy are lines and dS is just a line element). We also note that $|v| = \sqrt{v_x^2 + v_y^2} = E_1 a\sqrt{\sin^2 ak_x + \sin^2 ak_y}$. Thus,

$$\sigma_{\alpha\beta} = 2e^2\tau E_1 a \int \frac{dS}{4\pi^2} \frac{\sin ak_\alpha \sin ak_\beta}{\sqrt{\sin^2 ak_x + \sin^2 ak_y}} \tag{3}$$

Due to symmetry

$$\sigma_{xy} = \sigma_{yx} = 0, \qquad \sigma_{xx} = \sigma_{yy} \tag{4}$$

so we limit ourself to the computation of σ_{xx}.
We have

$$\sigma_{\alpha\beta} = 2e^2\tau E_1 a \int \frac{dS}{4\pi^2} \frac{\sin^2 ak_x}{\sqrt{\sin^2 ak_x + \sin^2 ak_y}} \tag{5}$$

The integration goes over the Fermi surface of the system which, at half-filling, is just a square with one of the sides $k_y = \pi/a - k_x$ $(0 < k_x < \pi/a)$ and the other three sides related by symmetry to the one mentioned. The line element $dS = \sqrt{2}k_x$. Thus,

$$\sigma_{xx} = 8\sqrt{2}e^2\tau E_1 a \int_0^{\pi/a} \frac{dk_x}{4\pi^2} \frac{\sin^2 ak_x}{\sqrt{\sin^2 ak_x + \sin^2 a(\pi/a - k_x)}} = \frac{2e^2}{\pi^2}\tau E_1 a \int_0^{\pi/a} dk_x \sin ak_x = \frac{4e^2}{\pi^2}\tau E_1 \tag{6}$$

We note that the density corresponding to half-filling is

$$n = 2\frac{1}{2}\frac{(2\pi/a)^2}{4\pi^2} = \frac{1}{a^2}. \tag{7}$$

Here the leading factor of 2 comes from spin. Thus

$$\sigma_{xx} = \frac{4e^2}{\pi^2}\tau E_1 = \frac{ne^2\tau}{\pi^2/4E_1 a^2}. \tag{8}$$

(b) We now need to compare the result from the previous section to the prediction of the Drude model.

$$\sigma_{xx} = \frac{ne^2\tau}{m^*} \tag{9}$$

Comparing Eq. (8) to Eq. (9) we find

$$m^* = \frac{\pi^2}{4E_1a^2} \tag{10}$$

Note that the expansion of the dispersion relation near $k = 0$ would lead to the estimate that is parametrically the same

$$\epsilon(k) = \frac{E_1a^2}{2}k^2 + \text{const.}, \qquad m^* = \frac{1}{E_1a^2}. \tag{11}$$

2. Boltzmann equation in the presence of spin-orbit interaction

$(5+5+5+5 = 20$ Punkte $\quad + \quad 5+5 = 10$ Bonuspunkte)

(a) Let us consider a simple spin. Its density matrix is a 2×2 matrix ρ. Its equation of motion is

$$\frac{d\rho}{dt} = i\,[\rho, H]\,, \tag{12}$$

where H, a 2×2 matrix, is the Hamiltonian of the system. The diagonal elements of ρ give the probabilities to find the system in a state with z-projection of the spin being equal to $\pm 1/2$. For example, the average value of s_z is given by

$$\langle s_z\rangle = \operatorname{tr}\rho s_z = \frac{1}{2}\left(\rho_{11} - \rho_{22}\right) \tag{13}$$

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 definite projection s_x.

Let us now turn to the discussion of a particle with spin and corresponding kinetic equation. If we neglect first the possibility to have spin coherence and approximate the matrix ρ (which is now also aa function of r, p and t) by its diagonal elements the kinetic equation should have the form

$$\frac{d\rho}{dt} \equiv \frac{\partial\rho}{\partial t} + \mathbf{v}\frac{\partial\rho}{\partial\mathbf{r}} + \dot{\mathbf{p}}\frac{\partial\rho}{\partial\mathbf{p}} = I[\rho] \tag{14}$$

Equation (14) neglects the evolution of the density matrix of the particle due to rotation of the spin. The spin rotation can be taken into account by analogy with equation Eq. (12). We write, limiting ourself to the space-independent density matrixes,

$$\frac{d\rho}{dt} \equiv \frac{\partial\rho}{\partial t} + \dot{\mathbf{p}}\frac{\partial\rho}{\partial\mathbf{p}} = i[\rho, H] + I[\rho], \tag{15}$$

where $H = p^2/2m + \mathbf{\Omega}(\mathbf{p})\sigma$ is the Hamiltonian of the system. Computing now the commutator we get

$$\frac{\partial\rho}{\partial t} + i\left[\mathbf{\Omega}(\mathbf{p})\sigma, \rho\right] - e\mathbf{E}\frac{\partial\rho}{\partial\mathbf{p}} = I[\rho], \tag{16}$$

where we have explicitly written down $\dot{\mathbf{p}} = -e\mathbf{E}$ for a particle in an electric field.

(b) We now substitute the

$$\rho = \frac{f(t,p)}{2} + \mathbf{S}(\mathbf{t},\mathbf{p})\sigma. \tag{17}$$

into kinetic equation. We get

$$\frac{1}{2}\frac{\partial f}{\partial t} + \frac{\partial \mathbf{S}}{\partial t}\sigma + i\left[\boldsymbol{\Omega}(\mathbf{p})\sigma, \mathbf{S}\sigma\right] - \frac{1}{2}eE_\alpha\frac{\partial f}{\partial p_\alpha} - eE_\alpha\frac{\partial \mathbf{S}}{\partial p_\alpha}\sigma = I[\rho] \tag{18}$$

We have

$$[\boldsymbol{\Omega}(\mathbf{p})\sigma, \mathbf{S}\sigma] = \Omega_i(\mathbf{p})S_j\left[\sigma_i, \sigma_j\right] = 2i\Omega_i(\mathbf{p})S_j\epsilon_{ijk}\sigma_k = 2i(\boldsymbol{\Omega}(\mathbf{p}) \times \mathbf{S})\cdot\sigma, \tag{19}$$

where ϵ_{ijk} is the fully antisymmetric tensor. We thus have

$$\frac{1}{2}\frac{\partial f}{\partial t} + \frac{\partial \mathbf{S}}{\partial t}\sigma - 2(\boldsymbol{\Omega}(\mathbf{p}) \times \mathbf{S})\cdot\sigma - \frac{1}{2}eE_\alpha\frac{\partial f}{\partial p_\alpha} - eE_\alpha\frac{\partial \mathbf{S}}{\partial p_\alpha}\sigma = I[\rho] \tag{20}$$

Equation (20) is still a matrix one. To reduce it to a set of scalar equations we use the orthogonality of the Pauli matrixes

$$\mathrm{tr}\,\sigma_i\sigma_j = 2\delta_{i,j}, \qquad i,j = 0,\ldots 3, \qquad \sigma_0 \equiv 1. \tag{21}$$

For example, taking trace of the both sides of Eq. (20) we find

$$\frac{\partial f}{\partial t} - eE_\alpha\frac{\partial f}{\partial p_\alpha} = \mathrm{tr}\,I[\rho] \tag{22}$$

Likewise, multiplying both sides of Eq. (20) by σ_i, $i = 1,2,3$, and taking trace we find

$$\frac{\partial S_i}{\partial t} - 2(\boldsymbol{\Omega}(\mathbf{p}) \times \mathbf{S})_i - eE_\alpha\frac{\partial S_i}{\partial p_\alpha} = \frac{1}{2}\mathrm{tr}\,I[\rho]\sigma_i \tag{23}$$

Let us now assume that the collision integral can be written in the τ-approximation as

$$I[\rho] = -\frac{1}{\tau}\delta\rho \equiv -\frac{1}{\tau}(\rho - \rho_0) \equiv -\frac{1}{\tau}\left(\frac{1}{2}\delta f + \delta\mathbf{S}\cdot\sigma\right) \tag{24}$$

We then find

$$\frac{\partial f}{\partial t} - eE_\alpha\frac{\partial f}{\partial p_\alpha} = -\frac{\delta f}{\tau} \tag{25}$$

$$\frac{\partial S_i}{\partial t} - 2(\boldsymbol{\Omega}(\mathbf{p}) \times \mathbf{S})_i - eE_\alpha\frac{\partial S_i}{\partial p_\alpha} = -\frac{\delta S_i}{\tau} \tag{26}$$

(c) We can now consider the case of the Rashba coupling $\boldsymbol{\Omega} = \alpha(p_y, -p_x, 0)$. In this case

$$\Omega \times S = \alpha(-p_xS_z, -p_yS_z, p_xS_x + p_yS_y) \equiv -\alpha\mathbf{p}S_z + \alpha(\mathbf{S}_\perp\cdot\mathbf{p})\,\mathbf{e}_z. \tag{27}$$

Here $\mathbf{e}_z$ is a unit vector in z-direction and $\mathbf{S}_\perp = (S_x, S_y)$. Equations (26) now can be written as

$$\frac{\partial S_z}{\partial t} - 2\alpha\mathbf{S}_\perp\cdot\mathbf{p} - eE_\alpha\frac{\partial S_z}{\partial p_\alpha} = -\frac{\delta S_z}{\tau}, \tag{28}$$

$$\frac{\partial \mathbf{S}_\perp}{\partial t} + 2\alpha\mathbf{p}S_z - eE_\alpha\frac{\partial \mathbf{S}_\perp}{\partial p_\alpha} = -\frac{\delta\mathbf{S}_\perp}{\tau} \tag{29}$$

This is our final set of equations.

(d) Let us now compute the equilibrium density matrix ρ_0. Our Hamiltonian $H = p^2/2m + \mathbf{\Omega}(\mathbf{p})\sigma$ has eigenenergies $\epsilon_\sigma(p) = \frac{p^2}{2m} + \sigma|\mathbf{\Omega}(\mathbf{p})|$, where $\sigma = \pm 1$ and $|\mathbf{\Omega}(\mathbf{p})| = \alpha|\mathbf{p}|$. In particular, there exist a unitary matrix $U(p)$ such that

$$H = U^+(p)\left[\frac{p^2}{2m} + \alpha|p|\sigma_z\right]U(p), \qquad U^+(p)\alpha|p|\sigma_z U(p) = \mathbf{\Omega}(\mathbf{p})\sigma \tag{30}$$

The occupation numbers of the eigenstates of our Hamiltonian at equilibrium are given by just the Fermi distribution, $n(p,\sigma) = n_F(\epsilon_\sigma(p))$. This means that the equilibrium density matrix in the basis of eigenstates takes the form

$$\tilde{\rho}_0 = n_F\left[\frac{p^2}{2m} + \alpha|p|\sigma_z\right] = \frac{n_F(\epsilon_+(p)) + n_F(\epsilon_-(p))}{2} + \frac{n_F(\epsilon_+(p)) - n_F(\epsilon_-(p))}{2}\sigma_z \tag{31}$$

The density matrix in the original basis is then given by

$$\rho_0 = U^+\tilde{\rho}_0 U = n_F\left[\frac{p^2}{2m} + \alpha|p|\sigma_z\right] = \frac{n_F(\epsilon_+(p)) + n_F(\epsilon_-(p))}{2} + \frac{n_F(\epsilon_+(p)) - n_F(\epsilon_-(p))}{2\alpha|p|}\mathbf{\Omega}(\mathbf{p})\sigma \tag{32}$$

where $\epsilon_\pm(p) = p^2/2m \pm \alpha|p|$.

Equation (32) is equivalent to the statement that

$$\rho_0 = n_F(H) \equiv n_F\left(p^2/2m + \mathbf{\Omega}(\mathbf{p})\sigma\right). \tag{33}$$

A particular case of of Eq. (32) that will be interesting for us is the limit of small α. In this situation Eq. (32) gives (to first order)

$$\rho_0 \approx n_F(p^2/2m) + n_F'(p^2/2m)\mathbf{\Omega}(\mathbf{p})\sigma. \tag{34}$$

Here n_F' stands for the derivative of the Fermi distribution with respect to energy. Obviously, we can get the same answer from Eq. (33).

Equation (32) can be now translated to the expressions for f_0 and $\mathbf{S}_0$. We just need to use orthogonality of the Pauli matrixes. We get

$$f_0 = n_F(\epsilon_+(p)) + n_F(\epsilon_-(p)), \tag{35}$$

$$\mathbf{S}_{\perp 0} = \frac{n_F(\epsilon_+(p)) - n_F(\epsilon_-(p))}{2\alpha|p|}\mathbf{\Omega}(\mathbf{p}) \equiv G(|p|)\mathbf{\Omega}(\mathbf{p}), \tag{36}$$

$$S_{z0} = 0. \tag{37}$$

In the limit of small α this reduces to

$$f_0 = 2n_F(\epsilon), \tag{38}$$

$$\mathbf{S}_{\perp 0} = n_F'(\epsilon)\mathbf{\Omega}(\mathbf{p}), \qquad G(|p|) = n_F'(\epsilon), \tag{39}$$

$$S_{z0} = 0. \tag{40}$$

Here, $\epsilon = p^2/2m$.

(e) Let us now solve the kinetic equation within the linear response approximation. We consider only equations for $\mathbf{S}$. We consider stationary problem and set all the time derivatives to zero. We also take into account that $S_{z0} = 0$. We then obtain the set of linearized equations

$$2\tau\alpha\, \mathbf{S}_{\perp 0} \cdot \mathbf{p} + 2\tau\alpha\, \delta\mathbf{S}_\perp \cdot \mathbf{p} \;=\; \delta S_z, \tag{41}$$

$$2\alpha\mathbf{p}\, \delta S_z - eE_\alpha \frac{\partial \mathbf{S}_{\perp 0}}{\partial p_\alpha} \;=\; -\frac{\delta \mathbf{S}_\perp}{\tau} \tag{42}$$

Note that the product $\mathbf{S}_{\perp 0} \cdot \mathbf{p}$ vanishes due to Eq. (39). Tis garatees that at $E = 0$ our kinetic equation has the solution $\delta\mathbf{S} = 0$ so we have found correct equilibrium distribution function.

From Eqs. (41) and (42) we now find

$$\delta\mathbf{S}_\perp + 4\alpha^2\tau^2(\delta\mathbf{S}_\perp \cdot \mathbf{p})\, \mathbf{p} \;=\; e\tau E_\alpha \frac{\partial \mathbf{S}_{\perp 0}}{\partial p_\alpha}, \tag{43}$$

$$\delta S_z \;=\; 2\tau\alpha\, \delta\mathbf{S}_{\perp 0} \cdot \mathbf{p}. \tag{44}$$

We multiply both sides of Eq. (43) by $\mathbf{p}$ to get

$$(\delta\mathbf{S}_\perp \cdot \mathbf{p}) = \frac{e\tau E_\alpha}{1 + 4\alpha^2\tau^2p^2}\left(\frac{\partial \mathbf{S}_{\perp 0}}{\partial p_\alpha} \cdot \mathbf{p}\right) = \frac{e\tau E_\alpha}{1 + 4\alpha^2\tau^2p^2}\frac{\partial S_{0\beta}}{\partial p_\alpha} p_\beta$$
$$= \frac{e\tau E_\alpha}{1 + 4\alpha^2\tau^2p^2}\left(\frac{\partial (S_{0\beta}p_\beta)}{\partial p_\alpha} - S_{0\alpha}\right) = -\frac{e\tau(\mathbf{E} \cdot \mathbf{S}_{\perp 0})}{1 + 4\alpha^2\tau^2p^2} \tag{45}$$

Thus,

$$\delta\mathbf{S}_\perp = e\tau E_\alpha \frac{\partial \mathbf{S}_{\perp 0}}{\partial p_\alpha} + \frac{4e\alpha^2\tau^3(\mathbf{E} \cdot \mathbf{S}_{\perp 0})\mathbf{p}}{1 + 4\alpha^2\tau^2p^2}. \tag{46}$$

This is the final result of this exercise.

(f) We now consider the average spin arising in response to the electric field,

$$\langle \mathbf{s} \rangle = \int \frac{d^2p}{(2\pi)^2} \mathrm{tr}\, \rho \mathbf{s} = \int \frac{d^2p}{(2\pi)^2} \mathbf{S}. \tag{47}$$

It is easy to see that $\langle s_z \rangle = 0$. We thus assume that $\mathbf{E} = (E_x, 0, 0)$ and calculate the in-plane spin. With our choice of the direction of electric field we have

$$\delta\mathbf{S}_\perp = e\tau E_\alpha \frac{\partial \mathbf{S}_{\perp 0}}{\partial p_\alpha} + \frac{4e\alpha^3\tau^3E_xG(|p|)p_y\mathbf{p}}{1 + 4\alpha^2\tau^2p^2}. \tag{48}$$

The first term, total derivative, vanishes after integration over momentum. It is easy to see that due toi the symmetry reasons only $\langle s_y \rangle$ is non-zero and given by

$$\langle s_y \rangle = \int \frac{d^2p}{(2\pi)^2} \frac{4e\alpha^3\tau^3G(|p|)E_xp_y^2}{1 + 4\alpha^2\tau^2p^2}, \qquad G(|p|) = \frac{n_F(\epsilon_+(p)) - n_F(\epsilon_-(p))}{2\alpha|p|} \tag{49}$$

We switch to polar coordinates and taking into account that

$$\int_0^{2\pi} \sin^2\phi = \pi \tag{50}$$

we get

$$\langle s_y \rangle = \frac{e\alpha^3\tau^3E_x}{\pi} \int_0^\infty dp \frac{p^3G(|p|)}{1 + 4\alpha^2\tau^2p^2} \tag{51}$$

The integral can be computed explicitly for weak spin-orbit coupling and zero temperature when

$$G|p| = n'_F(p^2/2m) = -\delta(p^2/2m - p_F^2/2m) = -\frac{m}{p_F}\delta(p - p_F) = -\frac{1}{v_F}\delta(p - p_F) \quad (52)$$

We then get

$$\langle s_y \rangle = -\frac{e\alpha^3\tau^3 p_F^3 E_x}{\pi v_F(1 + 4\alpha^2\tau^2 p_F^2)}. \quad (53)$$