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Spin–orbit scattering effects on magnetoresistance in a quasi-two-dimensional disordered electron system

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Abstract

Making use of the diagrammatic techniques in perturbation theory, we have investigated theoretically the spin–orbit scattering effects in a layered quasi-two-dimensional disordered electron system. The analytical expressions for the magnetoconductivities due to weak-localization effects have been obtained as functions of elastic, inelastic and spin–orbit scattering times. The relevant dimensional crossover, from three-dimensional to two-dimensional behaviour, with decreasing interlayer coupling has been discussed, and the condition for the crossover has been obtained.

1. Introduction

For the last two decades, Anderson localization of disordered electron systems by elastic scattering from static impurities has been a topic of serious study [1, 2]. According to the scaling theory of the pioneering work of Abrahams *et al* [3], all electronic states in one- and two-dimensional (1D and 2D) disordered systems are localized irrespective of the degree of randomness, while in three-dimensional (3D) systems there exist metal–insulator transitions due to Anderson localization. (It must of course be mentioned at this point that recent experiments [4] have found a metal–insulator transition also in a 2D disordered system; however, this is probably due to the interference of interaction effects and does not play a role in the present context.) In recent years, however, quasi-2D electron systems have attracted a great deal of attention because of their unique physical properties. A positive magnetoresistance due to suppression of antilocalization in a CdTe/Hg_{1-y}Cd_yTe superlattice has been studied experimentally by Moyle, Cheung and Ong [5]. Szott, Jedrzejek and Kirk have completed the measurements and made extended studies of negative magnetoresistance effects in a GaAs/Al_xGa_{1-x}As superlattice [6]. Another example of a quasi-2D electron system is the layered high- T_c cuprates. The logarithmic increase of resistivity with decreasing temperature in a magnetic field suppressing superconductivity in La_{2-x}Sr_xCuO₄ [7] and La-doped Bi₂Sr₂CuO₇ [8] is attributed to weak-localization effects [2]. These experimental results provide motivation for a theoretical investigation of weak-localization effects in quasi-2D

disordered electron systems [9–13]. In a recent work [13], Abrikosov calculated the quantum interference corrections for a quasi-2D metal to the conductivity as a function of temperature and magnetic field, and discussed the dimensional crossover from 3D to 2D behaviour with decreasing interlayer coupling.

Weak localization is a quantum effect that results from constructive interference between closed electron paths and their time-reversed counterparts. This constructive interference increases the probability of backscattering and results in an increase in resistivity over the classical Drude value. In this work, we will study theoretically the spin–orbit scattering effects on the weak localization in a quasi-2D disordered electron system, which were not considered in the above-mentioned theoretical works. In the presence of spin–orbit scatterings, the quantum interference becomes suppressed due to the rotation of the electron spin [2]. Therefore spin–orbit scatterings must have a very important influence on the transport properties of a quasi-2D system, as well as on the dimensional crossover from 3D to 2D behaviour. By means of the diagrammatic techniques in perturbation theory, we will calculate the magnetoresistance due to weak-localization effects for a quasi-2D disordered electron system in the presence of spin–orbit scatterings, and discuss the relevant dimensional crossover from 3D to 2D behaviour with decreasing interlayer coupling.

In section 2, we will present the model for a layered quasi-2D disordered electron system, and calculate the Boltzmann conductivities of this model. In perturbation theory, the so-called cooperon (particle–particle propagator) is responsible for weak-localization effects; therefore we will, in section 3, derive the expression for a cooperon in the presence of spin–orbit scatterings in a magnetic field perpendicular to the layers. The evaluation of the weak-localization corrections to the magnetoconductivities will be presented in section 4. Finally a brief summary is given in section 5.

2. The model for a quasi-2D disordered electron system

Let us consider a quasi-2D disordered electron system with the following energy spectrum:

$$\epsilon_k = k_{\parallel}^2/2m - t \cos(k_z a) \quad (1)$$

where $\mathbf{k}_{\parallel} = (k_x, k_y)$ and k_z are wavevectors along the planar and z -directions respectively, m is the in-plane effective mass, a is the period of the structure along the z -axis, t is the interlayer hopping energy which is assumed to be much smaller than the Fermi energy ϵ_F . It is easily shown that the Fermi surface of this model is a slightly corrugated cylinder, the density of states per spin at the Fermi energy is $N = m/2\pi a$ and the electron density is given by $n = k_F^2/2\pi a$ with $k_F = mv_F = \sqrt{2m\epsilon_F}$.

Let us consider spin–orbit scatterings. If an electron with spin σ is scattered by a potential $u\delta(\mathbf{r})$ from the state \mathbf{k} into the state \mathbf{k}' , the Born amplitude of the scattering is given by $u[1 + i\eta(\mathbf{k} \times \mathbf{k}') \cdot \boldsymbol{\sigma}]$ with η being a small constant. The impurity-averaged retarded and advanced Green's functions for the conduction electrons are given by

$$G^{RA}(\mathbf{k}, \omega) = (\omega - \xi_k \pm i/2\tau)^{-1} \quad (2)$$

where $\xi_k = \epsilon_k - \epsilon_F$ and $\tau^{-1} = \tau_0^{-1} + \tau_i^{-1} + \tau_{so}^{-1}$, with τ_0 , τ_i and τ_{so} being the elastic, inelastic and spin–orbit scattering times respectively. Using the Born approximation, we have $\tau_0^{-1} = 2\pi N n_i u^2$ and

$$\tau_{so}^{-1} = \sum_{\mu} (\tau_{so}^{\mu})^{-1} = 2\pi N n_i u^2 \eta^2 \sum_{\mu} \langle (\mathbf{k} \times \mathbf{k}')_{\mu}^2 \rangle_F$$

where n_i is the concentration of impurities and $\langle (\mathbf{k} \times \mathbf{k}')_{\mu}^2 \rangle_F$ represents the average over the Fermi surface [14]. The inelastic scattering time τ_i depends on the temperature due to

electron–electron or electron–phonon interactions. In the weak-disorder regime, n_i is assumed to be so small that $\epsilon_F^{-1} \ll \tau_0 \ll \tau_{so}, \tau_i$.

The diffusion constant and the mean free path along the μ -direction are defined by $D_\mu = \langle v_\mu^2 \rangle_F \tau$ and $l_\mu = (D_\mu \tau)^{1/2}$ respectively, where $\langle v_\mu^2 \rangle_F$ represents the mean square velocity on the Fermi surface. Making use of the dispersion relation (1), one can easily obtain $D_\parallel = v_F^2 \tau / 2$ and $D_z = t^2 a^2 \tau / 2$. The Boltzmann dc conductivities can be easily calculated through the well-known Einstein relation $\sigma_\mu = 2e^2 N D_\mu$, yielding $\sigma_\parallel = ne^2 \tau / m$ and $\sigma_z = e^2 m a t^2 \tau / 2\pi$.

It is important to emphasize that both Boltzmann theory and weak-localization theory are correct within the region where the quasiclassical approximation is valid; therefore we must distinguish two different cases:

- (i) $\tau^{-1} \ll t \ll \epsilon_F$, meaning that $l_\parallel \gg \lambda_F$ (Fermi wavelength) and $l_z \gg a$; in this case the quasiclassical method is valid for all directions;
- (ii) $t \lesssim \tau^{-1} \ll \epsilon_F$, meaning that $l_\parallel \gg \lambda_F$ and $l_z \lesssim a$; in this case the quasiclassical method is valid only for the planar direction.

3. The cooperon in the presence of spin-orbit scatterings and the magnetic field

Let us consider an external magnetic field perpendicular to the layers, which is described by the vector potential $\mathbf{A} = (-Hy, 0, 0)$. We assume that the field is weak enough that $\tau \ll \tau_H$ with $\tau_H = c/4eHD_\parallel$, which means that the in-plane mean free path is much shorter than the magnetic length. It is favourable to perform the calculation in real space instead of momentum space. The vector potential modifies the phase of the wavefunctions of electrons which results in a partial destruction of the quantum interference. Then the Green's functions in the presence of the magnetic field are given by [15]

$$\tilde{G}^{RA}(\mathbf{r}, \mathbf{r}'; \omega) = G^{RA}(\mathbf{r}, \mathbf{r}'; \omega) \exp \left[ie \int_r^{r'} \mathbf{A}(s) \cdot d\mathbf{s} \right] \quad (3)$$

where the integral is along a straight line connecting \mathbf{r} and \mathbf{r}' , and where \tilde{G}^{RA} and G^{RA} are the Green's functions in the presence or absence, respectively, of a magnetic field. The cooperon responsible for weak-localization effects is the particle–particle propagator, which can be diagrammatically represented as in figure 1. The dashed lines with crosses represent the impurity-averaged amplitude, which can be expressed by [14]

$$W_{\alpha\alpha', \beta\beta'} = (2\pi N \tau_0)^{-1} \left[\delta_{\alpha\alpha'} \delta_{\beta\beta'} - \sum_\mu (\tau_0 / \tau_{so}^\mu) \sigma_{\alpha\alpha'}^\mu \sigma_{\beta\beta'}^\mu \right] \quad (4)$$

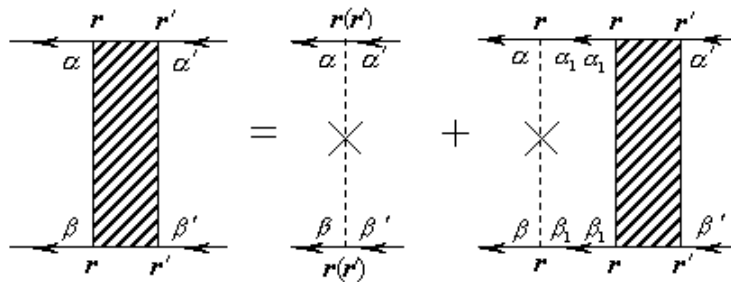


Figure 1. Diagrams for the cooperon.

where σ^μ ($\mu = x, y, z$) are the Pauli matrices, and the first and second terms in equation (4) correspond to normal and spin-orbit scatterings respectively. The cooperon is described by the following equation:

$$C(\mathbf{r}, \mathbf{r}'; \omega)_{\alpha\alpha', \beta\beta'} = W_{\alpha\alpha', \beta\beta'} \delta(\mathbf{r} - \mathbf{r}') + \sum_{\alpha_1 \beta_1} \int d^3 r_1 W_{\alpha\alpha_1, \beta\beta_1} K(\mathbf{r}, \mathbf{r}_1; \omega) C(\mathbf{r}_1, \mathbf{r}'; \omega)_{\alpha_1 \alpha', \beta_1 \beta'} \quad (5)$$

where the kernel $K(\mathbf{r}, \mathbf{r}_1; \omega)$ is defined by

$$K(\mathbf{r}, \mathbf{r}_1; \omega) = \tilde{G}^R(\mathbf{r}, \mathbf{r}_1; \omega) \tilde{G}^A(\mathbf{r}, \mathbf{r}_1; 0). \quad (6)$$

In order to compute $C(\mathbf{r}, \mathbf{r}'; \omega)_{\alpha\alpha', \beta\beta'}$ in equation (5), we shall try to solve the following integral equation:

$$\int d^3 r' K(\mathbf{r}, \mathbf{r}'; \omega) \psi(\mathbf{r}') = K(\omega) \psi(\mathbf{r}). \quad (7)$$

If ω is so small that $\omega\tau \ll 1$, one can solve equation (7) using a method similar to the one applied to a purely 2D system [15], obtaining the eigenfunctions and eigenvalues of the kernel $K(\mathbf{r}, \mathbf{r}'; \omega)$ as follows:

$$\psi_{nq_x q_z}(\mathbf{r}) = \exp(iq_x x) \psi_n(y - cq_x/2eH) \phi_{q_z}(z) \quad (8)$$

$$K(n, q_z; \omega) = 2\pi N\tau [1 + i\omega\tau - (n + 1/2)\tau/\tau_H - (2l_z/a)^2 \sin^2(q_z a/2)] \quad (9)$$

where ψ_n is the eigenfunction of an oscillator and $\phi_{q_z}(z)$ is the Bloch wavefunction along the z -direction. Now we can expand $K(\mathbf{r}, \mathbf{r}'; \omega)$ and $C(\mathbf{r}, \mathbf{r}'; \omega)_{\alpha\alpha', \beta\beta'}$ in terms of the eigenfunctions (8), obtaining

$$K(\mathbf{r}, \mathbf{r}'; \omega) = \sum_{nq_x q_z} K(n, q_z; \omega) \psi_{nq_x q_z}(\mathbf{r}) \psi_{nq_x q_z}^*(\mathbf{r}') \quad (10)$$

$$C(\mathbf{r}, \mathbf{r}'; \omega)_{\alpha\alpha', \beta\beta'} = \sum_{nq_x q_z} C(n, q_z; \omega)_{\alpha\alpha', \beta\beta'} \psi_{nq_x q_z}(\mathbf{r}) \psi_{nq_x q_z}^*(\mathbf{r}'). \quad (11)$$

Substituting equations (10) and (11) into equation (5), we obtain

$$C(n, q_z; \omega)_{\alpha\alpha', \beta\beta'} = W_{\alpha\alpha', \beta\beta'} + K(n, q_z; \omega) \sum_{\alpha_1 \beta_1} W_{\alpha\alpha_1, \beta\beta_1} C(n, q_z; \omega)_{\alpha_1 \alpha', \beta_1 \beta'}. \quad (12)$$

We expect the expression for the cooperon to have the same structure as the scattering amplitude, assuming that

$$C(n, q_z; \omega)_{\alpha\alpha', \beta\beta'} = (2\pi N\tau)^{-1} \left(A \delta_{\alpha\alpha'} \delta_{\beta\beta'} + \sum_{\mu} B_{\mu} \sigma_{\alpha\alpha'}^{\mu} \sigma_{\beta\beta'}^{\mu} \right). \quad (13)$$

Substituting equations (4), (9) and (13) into (12), one can calculate the values of A and B_{μ} , which yields

$$\begin{aligned} \sum_{\alpha\beta} C(n, q_z; \omega)_{\alpha\beta, \beta\alpha} &= (2\pi N\tau)^{-1} (2A + 2 \sum_{\mu} B_{\mu}) \\ &= (2\pi N\tau)^{-1} \{ 2[F(n, q_z; \omega) + \lambda_1]^{-1} \\ &\quad + [F(n, q_z; \omega) + \lambda_2]^{-1} - [F(n, q_z; \omega) + \lambda_3]^{-1} \} \end{aligned} \quad (14)$$

where

$$\lambda_1 = \tau/\tau_i + 2\tau/\tau_{so}^{\parallel} + 2\tau/\tau_{so}^z \quad \lambda_2 = \tau/\tau_i + 4\tau/\tau_{so}^{\parallel} \quad \lambda_3 = \tau/\tau_i$$

and

$$F(n, q_z; \omega) = (n + 1/2)\tau/\tau_H + (2l_z/a)^2 \sin^2(q_z a/2) - i\omega\tau.$$

Equation (14) is an expression for the cooperon which has a different form from that for a 3D system with anisotropic effective masses due to the special structure of the energy spectrum in the quasi-2D system, and will be used in the following calculation.

4. Magnetoresistance due to weak-localization effects

The calculation for conductivities in the quasiclassical approximation can be easily performed by means of the Kubo formalism. In the presence of a magnetic field, the quantum interference correction to the conductivity along the μ -direction is given by [2, 15]

$$\sigma_{\mu}^{[WL]} = (e^2/2\pi) \sum_{\mathbf{k}} \sum_{nq_x q_z} \sum_{\alpha\beta} v_{\mu}(\mathbf{k}) v_{\mu}(-\mathbf{k}) |G^R(\mathbf{k}, 0)|^4 C(n, q_z; \omega)_{\alpha\beta, \beta\alpha} \quad (15)$$

where $\omega \ll \tau^{-1}$ is the frequency of the applied field and $v_{\mu}(\mathbf{k}) = \partial\epsilon_{\mathbf{k}}/\partial k_{\mu}$ is the velocity of electrons along the μ -direction. We can easily perform the integrations over \mathbf{k} and q_x , getting

$$\frac{\sigma_{\mu}^{[WL]}}{\sigma_{\mu}} = -\frac{eH\tau^2}{\pi c} \sum_{n=0}^{\tau_H/\tau} \sum_{q_z} \sum_{\alpha\beta} C(n, q_z; \omega)_{\alpha\beta, \beta\alpha}. \quad (16)$$

Substituting equation (14) into (16), we get the general expression for the relative corrections to the conductivities:

$$\begin{aligned} \frac{\sigma_{\mu}^{[WL]}}{\sigma_{\mu}} = & -\frac{\omega_c \tau a}{\pi} \sum_{n=0}^{\tau_H/\tau} \sum_{q_z} \{2[F(n, q_z; \omega) + \lambda_1]^{-1} \\ & + [F(n, q_z; \omega) + \lambda_2]^{-1} - [F(n, q_z; \omega) + \lambda_3]^{-1}\} \end{aligned} \quad (17)$$

where $\omega_c = eH/mc$ is the cyclotron frequency. In order to discuss the dimensional crossover from 3D to 2D behaviour, we will set $\omega = 0$ and study several limiting cases.

If the interlayer hopping energy t is large enough that $\tau^{-1} \ll t \ll \epsilon_F$, meaning that $l_{\parallel} \gg \lambda_F$ and $l_z \gg a$, then the quasiclassical approximation is valid for all directions, and the main contribution to equation (17) arises from $|q_z| \ll l_z^{-1}$. Replacing the summation over q_z by the integral

$$\int_{-l_z^{-1}}^{l_z^{-1}} \frac{dq_z}{2\pi}$$

we get

$$\begin{aligned} \frac{\sigma_{\mu}^{[WL]}(H)}{\sigma_{\mu}} = & -\frac{\omega_c}{\sqrt{2\pi}t} \sqrt{\frac{\tau_H}{\tau}} \sum_{n=0}^{\tau_H/\tau} \left[2 \left(n + \frac{1}{2} + \lambda_1 \frac{\tau_H}{\tau} \right)^{-1/2} \right. \\ & \left. + \left(n + \frac{1}{2} + \lambda_2 \frac{\tau_H}{\tau} \right)^{-1/2} - \left(n + \frac{1}{2} + \lambda_3 \frac{\tau_H}{\tau} \right)^{-1/2} \right]. \end{aligned} \quad (18)$$

When $H \rightarrow 0$, meaning that $\tau_H \rightarrow \infty$, one can replace the summation over n in equation (18) by an integration, obtaining

$$\frac{\sigma_{\mu}^{[WL]}(0)}{\sigma_{\mu}} = -\frac{1}{\sqrt{2\pi}t\epsilon_F\tau^2} [2(\sqrt{1+\lambda_1} - \sqrt{\lambda_1}) + (\sqrt{1+\lambda_2} - \sqrt{\lambda_2}) - (\sqrt{1+\lambda_3} - \sqrt{\lambda_3})]. \quad (19)$$

Combining equations (18) and (19), we obtain the results for magnetoconductivities due to weak-localization effects:

$$\begin{aligned} \frac{\Delta\sigma_{\mu}(H)}{\sigma_{\mu}} = & \frac{\sigma_{\mu}^{[WL]}(H) - \sigma_{\mu}^{[WL]}(0)}{\sigma_{\mu}} \\ = & \frac{\omega_c}{\sqrt{2\pi}t} \sqrt{\frac{\tau_H}{\tau}} \left[2f\left(\lambda_1 \frac{\tau_H}{\tau}\right) + f\left(\lambda_2 \frac{\tau_H}{\tau}\right) - f\left(\lambda_3 \frac{\tau_H}{\tau}\right) \right] \end{aligned} \quad (20)$$

where the function $f(x)$ is defined by

$$f(x) = \sum_{n=0}^{\infty} \left[2(n+1+x)^{1/2} - 2(n+x)^{1/2} - \left(n + \frac{1}{2} + x \right)^{-1/2} \right].$$

The dependence of magnetic field in equation (20) is characteristic behaviour for a 3D system [16].

If the interlayer hopping energy t is small enough that $t \lesssim \tau^{-1} \ll \epsilon_F$, meaning that $l_{\parallel} \gg \lambda_F$ and $l_z \lesssim a$, then the quasiclassical approximation is valid only for the planar direction. Replacing the summation over q_z in equation (17) by the integral

$$\int_{-\pi/a}^{\pi/a} \frac{dq_z}{2\pi}$$

we can get

$$\frac{\sigma_{\parallel}^{[WL]}(H)}{\sigma_{\parallel}} = -\frac{1}{4\pi\epsilon_F\tau} \sum_{n=0}^{\tau_H/\tau} [2F_1(n) + F_2(n) - F_3(n)] \quad (21)$$

where

$$F_l(n) = \left[\left(n + \frac{1}{2} + \lambda_l \frac{\tau_H}{\tau} + t^2 \tau \tau_H \right)^2 - (t^2 \tau \tau_H)^2 \right]^{-1/2} \quad (l = 1, 2, 3).$$

When $H \rightarrow 0$, meaning that $\tau_H \rightarrow \infty$, we can replace the summation over n in equation (21) by an integration, obtaining

$$\frac{\sigma_{\parallel}^{[WL]}(0)}{\sigma_{\parallel}} = -\frac{1}{4\pi\epsilon_F\tau} (2F_1 + F_2 - F_3) \quad (22)$$

where

$$F_l = \ln \left[\frac{1 + \lambda_l + t^2 \tau^2 + \sqrt{(1 + \lambda_l + t^2 \tau^2)^2 - (t^2 \tau^2)^2}}{\lambda_l + t^2 \tau^2 + \sqrt{(\lambda_l + t^2 \tau^2)^2 - (t^2 \tau^2)^2}} \right] \quad (l = 1, 2, 3).$$

Combining equations (21) and (22), one can get the expression for the magnetoconductivity along the planar direction:

$$\frac{\Delta\sigma_{\parallel}(H)}{\sigma_{\parallel}} = \frac{1}{4\pi\epsilon_F\tau} \left[2F \left(\lambda_1 \frac{\tau_H}{\tau}, t^2 \tau \tau_H \right) + F \left(\lambda_2 \frac{\tau_H}{\tau}, t^2 \tau \tau_H \right) - F \left(\lambda_3 \frac{\tau_H}{\tau}, t^2 \tau \tau_H \right) \right] \quad (23)$$

where the function $F(x, y)$ is defined by

$$F(x, y) = \sum_{n=0}^{\infty} \left\{ \ln \frac{n+1+x+y + \sqrt{(n+1+x+y)^2 - y^2}}{n+x+y + \sqrt{(n+x+y)^2 - y^2}} - \left[\left(n + \frac{1}{2} + x + y \right)^2 - y^2 \right]^{-1/2} \right\} \\ \approx \psi \left(\frac{1}{2} + x \right) - \ln x \quad (\text{if } x \gg y)$$

with $\psi(x)$ being the well-known digamma function.

In the case of $t \ll \sqrt{\lambda_l}/\tau$, meaning that $\lambda_l \tau_H/\tau \gg t^2 \tau \tau_H$ ($l = 1, 2, 3$), equation (23) changes to

$$\frac{\Delta\sigma_{\parallel}(H)}{\sigma_{\parallel}} = \frac{1}{4\pi\epsilon_F\tau} \left[2\psi \left(\frac{1}{2} + \lambda_1 \frac{\tau_H}{\tau} \right) - 2 \ln \left(\lambda_1 \frac{\tau_H}{\tau} \right) \right. \\ \left. + \psi \left(\frac{1}{2} + \lambda_2 \frac{\tau_H}{\tau} \right) - \ln \left(\lambda_2 \frac{\tau_H}{\tau} \right) - \psi \left(\frac{1}{2} + \lambda_3 \frac{\tau_H}{\tau} \right) + \ln \left(\lambda_3 \frac{\tau_H}{\tau} \right) \right] \quad (24)$$

which is the exact result found for a purely 2D system [2]. From equations (20), (23) and (24), one can see that there exists a dimensional crossover from 3D to 2D behaviour with decreasing interlayer hopping energy.

5. Conclusions

In this work, we have investigated the spin-orbit scattering effects in a quasi-2D disordered electron system. By means of the diagrammatic techniques in perturbation theory, we have calculated the magnetoresistances due to weak-localization effects. The analytical results for the magnetoconductivities have been obtained as functions of the characteristic times: elastic, inelastic and spin-orbit scattering times. We show that all of these scattering times have very important influences on the relevant dimensional crossover from 3D to 2D. In the 3D limit of $t \gg \tau^{-1}$, the relative magnetoconductivities due to weak-localization effects are independent of directions, and have a similar dependence on field to that of an isotropic 3D system. If the interlayer coupling t is small enough that $t \lesssim \tau^{-1}$, the quasiclassical approximation for transport properties is not valid for the z -direction and the planar magnetoconductivity has a very complex dependence on the magnetic field (see equation (23)). In the 2D case of $t \ll \sqrt{\lambda_l}/\tau$, the planar magnetoconductivity is exactly the same as in an isotropic 2D system. Therefore, the relevant dimensional crossover from 3D to 2D occurs in the region $\sqrt{\lambda_l}/\tau \lesssim t \lesssim \tau^{-1}$.

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