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Crossover from the weak to strong-field behavior of the longitudinal interlayer magnetoresistance in quasi-two-dimensional conductors

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We investigate the monotonic growth of longitudinal interlayer magnetoresistance $\overline{R}_{zz}(B_z)$, analytically and numerically in the self-consistent Born approximation. We show that in a weak magnetic field the monotonic part of $\overline{R}_{zz}(B_z)$ is almost constant and starts to grow only above the crossover field B_c, when the Landau levels (LL) become isolated, i.e., when the LL separation becomes greater than the LL broadening. In higher field $B_z >> B_c$, $\overline{R}_{zz}(B_z) \propto B_z^{1/2}$ in agreement with previous works.

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73.43.Qt Magnetoresistance;
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74.72.–h Cuprate superconductors.

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1. Introduction

Magnetoresistance (MR) in strongly anisotropic layered metals is extensively studied during last decades, because it provides a powerful tool to determine the electronic properties of various layered materials, including high-temperature superconductors [1–11], organic metals (see, e.g., Refs. 12–14 for recent reviews), heterostructures [15] etc. The standard three-dimensional theory of MR [13,16–18], based on the τ-approximation, is not valid in the two-dimensional (2D) electron system because of the high Landau-level (LL) degeneracy (see, e.g., Refs. 19, 20 or Refs. 21, 22 for review) even in the fields insufficient for the quantum Hall effect (QHE) [23,24]. In strongly anisotropic layered quasi-2D metals, when the interlayer transfer integral t_z is less than the LL separation $\hbar\omega_c = \hbar eB/m^*c$, the standard MR theory [13,16–18] is also inapplicable. In particular, it predicts only a transverse MR, while the strong longitudinal interlayer MR $R_{zz}(B_z)$ is observed in various compounds as a general feature of quasi-2D conductors [25–34]. In spite of a considerable theoretical attention to MR in quasi-2D compounds [35–40], this longitudinal interlayer MR has been explained only recently [41–43] in the high-field limit, when the LLs do not overlap, i.e., when the LL separation $\hbar\omega_c$ is greater than the LL broadening $2\Gamma_0 = \hbar/\tau$, while $t_z \ll \Gamma_0$. Qualitatively, the longitudinal interlayer MR $R_{zz}(B_z) \propto B_z^{1/2}$ originates from the monotonic growth of the LL width $\Gamma(B_z) \propto B_z^{1/2}$, well-known in a 2D electron system [19]. This LL width, being equal to the imaginary part of electron self-energy $|\mathrm{Im}\Sigma|$, enters the denominator of the interlayer conductivity similarly to the scattering rate [41–43]. Various LL shapes give slightly different coefficients $\eta \sim 1$ in the high-field dependence of $R_{zz}(B_z)$ [43]:

$$R_{zz}(B_z)/R_{zz}(0) = \eta\sqrt{\hbar\omega_c/\Gamma_0}. \qquad (1)$$

The Lorenztian LL shape gives $\eta = \sqrt{4/\pi}$, the non-crossing (or single-site) approximation [44] gives $\eta = 3\sqrt{\pi}/8$ [45], while the self-consistent Born approximation (SCBA) gives $\eta = \sqrt{\pi/4}$ (see below). In Ref. 46 the calculation of $R_{zz}(B_z)$ was generalized to a finite $t_z \gtrsim \Gamma_0$ in the high-field limit $\hbar\omega_c > 4t_z$. The behavior at $\hbar\omega_c \lesssim \Gamma$ is still unknown. The smooth dependence

$$R_{zz}(B_z) \propto \left[\left(\hbar\omega_c/\Gamma_0\right)^2 + 1\right]^{1/4}, \qquad (2)$$

assumed in Refs. 34, 41 to compare with experimental data, does not have a theoretical substantiation. The aim of this paper is to calculate longitudinal interlayer magnetoresistance at $\hbar\omega_c \lesssim \Gamma$.

2. Analytical calculations

We apply the same "weakly incoherent" [35] model as in Refs. 41–43, i.e., we start from isolated 2D metallic layers with disorder, taken into account, at least in the self-consistent Born approximation, and consider the interlayer tunneling as a weakest perturbation in the minimal non-vanishing order. The interlayer conductivity is calculated using the Kubo formula [47] in the second order in the interlayer tunneling t_z, taking into account only two adjacent conducting layers. As was shown in Ref. 46, this approach is valid at $t_z \ll \Gamma, \hbar\omega_c$. The positions of short-range impurities on adjacent layers are assumed to be uncorrelated, which allows the independent averaging over disorder for each conducting layer. Then the interlayer conductivity $\sigma_{zz}(B_z)$ is expressed via the disorder-averaged electron Green's functions $\langle G_R(\mathbf{r}, j, \varepsilon)\rangle = \langle G_R(\mathbf{r}_1 - \mathbf{r}_2, j, \varepsilon)\rangle$ on 2D conducting layer with number j (see Eq. (12) of Ref. 43):

$$\sigma_{zz} = \frac{2\sigma_0\Gamma_0}{\pi\nu_{2D}} \int d^2\mathbf{r} \int d\varepsilon[-n_F'(\varepsilon)] \times$$

$$\times \langle \mathrm{Im}\, G_R(\mathbf{r}, j, \varepsilon)\rangle \langle \mathrm{Im}\, G_R(\mathbf{r}, j+1, \varepsilon)\rangle, \qquad (3)$$

where $n_F'(\varepsilon) = -1/\{4T\cosh^2[(\varepsilon-\mu)/2T]\}$ is the derivative of the Fermi distribution function, μ is the chemical potential,

$$\sigma_0 = e^2 t_z^2 \nu_{2D} d/\hbar\Gamma_0 \qquad (4)$$

is the interlayer conductivity without magnetic field,

$$\nu_{2D} = 2g_{LL}/\hbar\omega_c = m^*/\pi\hbar^2 = \nu_{3D} d$$

is the 2D density of states (DoS) at the Fermi level in the absence of magnetic field per two spin components, d is the interlayer distance, and $g_{LL} = eB_z/2\pi\hbar c$ is the LL degeneracy per unit area.

The 2D metallic electron system in a perpendicular magnetic field in the point-like impurity potential has been extensively studied [19–24,44,48–53]. In the self-consistent single-site approximation [44], which takes into account all diagrams without intersection of impurity lines [54], the coordinate electron Green's function, averaged over impurity configurations, is given by

$$G(\mathbf{r}_1, \mathbf{r}_2, \varepsilon) = \sum_{n,k_y} \Psi^{0*}_{n,k_y}(r_2)\Psi^0_{n,k_y}(r_1) G(\varepsilon, n), \qquad (5)$$

where $\Psi^0_{n,k_y}(r_1)$ are the 2D electron wave functions in a perpendicular magnetic field [55], and the 2D electron Green's function $G(\varepsilon, n)$ does not depend on k_y:

$$G(\varepsilon, n) = \frac{1}{\varepsilon - \hbar\omega_c(n+1/2) - \Sigma(\varepsilon)}, \qquad (6)$$

where we have used that the 2D electron dispersion in magnetic field $\varepsilon_{2D}(n) = \hbar\omega_c(n+1/2)$, and $\Sigma(\varepsilon)$ is the electron self-energy part due to the scattering by impurities.

In a perpendicular-to-layers magnetic field the integration over coordinate in Eq. (3) with the Green's functions (5) reduces to the normalization of the wave functions and gives (see Eq. (14) of Ref. 43)

$$\sigma_{zz} = \frac{\sigma_0\Gamma_0\hbar\omega_c}{\pi} \int d\varepsilon\left[-n_F'(\varepsilon)\right] \sum_n \left|\mathrm{Im}\, G(\varepsilon, n)\right|^2 \qquad (7)$$

with $\mathrm{Im}\, G(\varepsilon, n)$ given by Eq. (6). After substitution of Eq. (6) to Eq. (7), and introducing the notations

$$\alpha \equiv 2\pi(\varepsilon - \mathrm{Re}\Sigma(\varepsilon))/\hbar\omega_c, \quad \gamma \equiv 2\pi\left|\mathrm{Im}\,\Sigma(\varepsilon)\right|/\hbar\omega_c, \qquad (8)$$

the sum over n in Eq. (7) gives

$$\frac{\sigma_{zz}}{\sigma_0} = \int d\varepsilon \frac{-n_F'(\varepsilon)\Gamma_0}{\left|\mathrm{Im}\,\Sigma(\varepsilon)\right|} \left[\frac{\left|\sinh\gamma\right|}{\cosh\gamma + \cos\alpha} - \right.$$

$$\left. - \gamma \frac{\cos\alpha\cosh\gamma + 1}{[\cosh\gamma + \cos\alpha]^2}\right] \qquad (9)$$

in agreement with Eqs. (19)–(21) of Ref. 37 or with Eq. (C3) of Ref. 56.

The expressions for interlayer conductivity σ_{zz} contain the electron self-energy $\Sigma(\varepsilon)$ coming from the scattering on impurity potential $V_i(\mathbf{r})$. The impurities are assumed to be short-range (point-like) and randomly distributed with volume concentration n_i:

$$V_i(\mathbf{r}) = U\sum_i \delta^3(\mathbf{r} - \mathbf{r}_i). \qquad (10)$$

The scattering by impurity potential given by Eq. (10) is spin-independent. In the self-consistent single-site (non-crossing) approximation the electron self energy satisfies the following equation [44]:

$$\Sigma(\varepsilon) = \frac{n_i U}{1 - UG(\varepsilon)}, \qquad (11)$$

where the Green's function

$$G(\varepsilon) = \sum_{n,k_y,k_z} G(\varepsilon, n) = \frac{g_{LL}}{d}\sum_n G(\varepsilon, n) = \qquad (12)$$

$$= -\frac{\pi g_{LL}}{\hbar\omega_c d}\tan\left[\pi\frac{\varepsilon - \Sigma(\varepsilon)}{\hbar\omega_c}\right]. \qquad (13)$$

The summation over k_y in Eq. (12) gives the LL degeneracy g_{LL} and the summation over k_z gives $1/d$. It is convenient to use the normalized electron Green's function

$$g(\varepsilon) \equiv G(\varepsilon)\hbar\omega_c d/\pi g_{LL}. \qquad (14)$$

To obtain the monotonic growth of longitudinal interlayer magnetoresistance, the self-consistent Born approximation (SCBA) is sufficient, which gives

$$\Sigma(\varepsilon) - n_i U = n_i U^2 G(\varepsilon) = \Gamma_0 g(\varepsilon). \quad (15)$$

instead of Eq. (11). Here we used that the zero-field level broadening is

$$\Gamma_0 = \pi n_i U^2 \nu_{3D} = \pi n_i U^2 g_{LL}/d\hbar\omega_c.$$

Below we also neglect the constant energy shift $n_i U$ in Eq. (15), which does not affect physical quantities as conductivity.

Equations (13)–(15) give the following equations on $g \equiv g(\varepsilon)$:

$$\mathrm{Im}g = \frac{\sinh(2\pi\Gamma_0 \mathrm{Im}g/\hbar\omega_c)}{\cosh(2\pi\Gamma_0 \mathrm{Im}g/\hbar\omega_c) + \cos(2\pi\varepsilon^*/\hbar\omega_c)}, \quad (16)$$

$$\mathrm{Re}g = \frac{-\sin(2\pi\varepsilon^*/\hbar\omega_c)}{\cosh(2\pi\Gamma_0 \mathrm{Im}g/\hbar\omega_c) + \cos(2\pi\varepsilon^*/\hbar\omega_c)}. \quad (17)$$

where

$$\varepsilon^* \equiv \varepsilon - \mathrm{Re}\Sigma^R(\varepsilon) = \varepsilon - \Gamma_0 \mathrm{Re}g(\varepsilon). \quad (18)$$

These equations can be written also for $\Sigma^R(\varepsilon)$. With notations $\gamma_0 = 2\pi\Gamma_0/\hbar\omega_c$, $\gamma \equiv 2\pi \mathrm{Im}\Sigma^R(\varepsilon)/\hbar\omega_c$, $\alpha \equiv 2\pi\varepsilon^*/\hbar\omega_c$, $\delta \equiv -2\pi\,\mathrm{Re}\,\Sigma^R(\varepsilon)/\hbar\omega_c = 2\pi(\varepsilon^* - \varepsilon)/\hbar\omega_c$, Eqs. (13) and (15) give

$$\frac{\gamma}{\gamma_0} = \frac{\sinh(\gamma)}{\cosh(\gamma) + \cos(\alpha)}, \quad (19)$$

$$\delta \equiv \alpha - \frac{2\pi\varepsilon}{\hbar\omega_c} = \frac{\gamma_0 \sin(\alpha)}{\cosh(\gamma) + \cos(\alpha)}. \quad (20)$$

The solution of Eq. (19) gives $\mathrm{Im}\,\Sigma(\alpha)$, while Eq. (20) allows to find $\alpha(\varepsilon)$ and $\mathrm{Re}\,\Sigma(\varepsilon)$. Equation (9), (19) and (20) will be used for numerical calculations in the next section.

2.1. High-field limit

In the high-field limit, the monotonic growth of longitudinal interlayer MR $R_{zz}(B_z)$, given by Eq. (1), was calculated for the Lorentzian LL shape in Refs. 41, 42. In Ref. 43 $R_{zz}(B_z)$ was calculated in the noncrossing approximation, but the coefficient η in Eq. (24) of Ref. 43 is greater than the correct value by a factor 4/3 [45]. Following the procedure of Ref. 43, we calculate $R_{zz}(B_z)$ in the SCBA at $\hbar\omega_c \gg \Gamma_0$ to compare with the numerical results in Sec. 3. At $\hbar\omega_c \gg \Gamma_0$ the summation over n in Eq. (12) is restricted to only one LL $n = n_F$ on the Fermi level and gives the equation for $G(\Delta\varepsilon) = (g_{LL}/d)G(\varepsilon, n_F)$:

$$G(\Delta\varepsilon) = g_{LL}/d/\left[\Delta\varepsilon - n_i U^2 G(\Delta\varepsilon)\right], \quad (21)$$

where we have used Eq. (15) and the notation $\Delta\varepsilon = \varepsilon - \hbar\omega_c(n_F + 1/2) - n_i U$. This equation yields

$$\mathrm{Im}G(\Delta\varepsilon, n_F) = \frac{\pi}{2\Gamma_0\hbar\omega_c}\sqrt{4\hbar\omega_c\Gamma_0/\pi - (\Delta\varepsilon)^2}, \quad (22)$$

which is nonzero only at $|\Delta\varepsilon| < E_1 \equiv \sqrt{4\hbar\omega_c\Gamma_0/\pi}$. Substituting Eq. (22) to Eq. (7) and keeping only one LL at the Fermi level, after averaging over MQO period we get

$$\sigma_{zz} = \frac{\sigma_0\Gamma_0}{\pi}\left(\frac{\pi}{2\Gamma_0\hbar\omega_c}\right)^2 \int_{-E_1}^{E_1} d\varepsilon\left[E_1^2 - (\Delta\varepsilon)^2\right] =$$

$$= \frac{\sigma_0\Gamma_0}{\pi}\left(\frac{\pi}{2\Gamma_0\hbar\omega_c}\right)^2 \frac{4E_1^3}{3} = \sigma_0\sqrt{\frac{4\Gamma_0}{\pi\hbar\omega_c}}, \quad (23)$$

corresponding to $\eta = \sqrt{\pi/4}$ in Eq. (1).

3. Numerical results and discussion

Substituting the solutions of Eqs. (19) and (20) into Eq. (9) one can calculate interlayer conductivity σ_{zz} numerically in the SCBA in the full interval of magnetic field. The result is shown in Figs. 1 and 2. As one can see from Fig. 2, in high field the calculated dependence $R_{zz}(B_z) \approx \sqrt{\pi\hbar\omega_c/4\Gamma_0} \propto B_z^{1/2}$ in agreement with Eq. (23) and Refs. 41–43, 46. From Fig. 1 one can clearly see, that the drop of interlayer conductivity $\sigma_{zz}(B_z)$ starts not from zero field, but from some critical field B_c, where $\hbar\omega_c \approx \Gamma_0/2$. At this field in SCBA the Landau levels become isolated, i.e. the LL separation $\hbar\omega_c$ exceeds the LL broadening 2Γ (see Fig. 3). Below this field, at $B < B_c$, $\sigma_{zz}(B_z)$ is flat within the accuracy of our calculation. This means, that the field dependence of the monotonic part of longitudinal MR $\bar{R}_{zz}(B_z)$ is not a simple analytic function, as was assumed

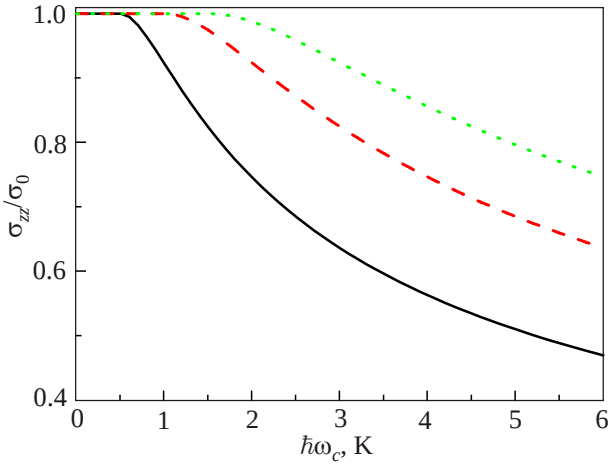

Fig. 1. (Color online) Average interlayer conductivity σ_{zz} as function of the LL separation $\hbar\omega_c \propto B_z$, calculated numerically using Eqs. (19), (20) and (9) for three different values $\Gamma_0 = 1$ K (solid black line), $\Gamma_0 = 2$ K (dashed red line), and $\Gamma_0 = 3$ K (dotted green line).

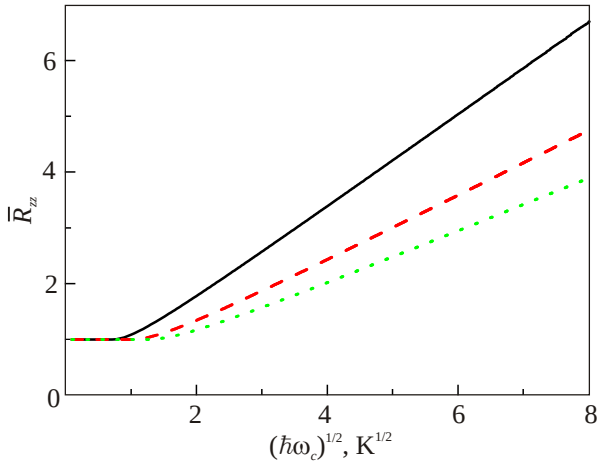

Fig. 2. (Color online) Average interlayer resistance $\bar{R}_{zz}$ as function of a square root of magnetic field $\sqrt{B_z}$, calculated numerically using Eqs. (19), (20) and (9) for three different values Γ_0 = = 1 K (solid black line), Γ_0 = 2 K (dashed red line), and Γ_0 = 3 K (dotted green line). In high field $\hbar\omega_c \gg \Gamma_0$, $\bar{R}_{zz} \propto \sqrt{B_z}$. At low field $\hbar\omega_c < \Gamma_0/2$, $\bar{R}_{zz} \approx$ const.

in Refs. 34, 41 [see Eq. (2)]: within SCBA it is constant at $B < B_c$ and starts to grow at $B > B_c$, reaching the dependence $R_{zz}(B_z) \propto B_z^{1/2}$ at $\hbar\omega_c \gg \Gamma_0$. Such crossover from low-field flat to the high-field increasing MR $\bar{R}_{zz}(B_z)$ was observed in the strongly anisotropic quasi-2D organic metal β″-(BEDT-TTF)$_2$ $SF_5CH_2CF_2SO_3$ at $B \approx 8$ T [29].

The predicted crossover of MR at $B = B_c$ needs further theoretical investigation. The SCBA assumes sharp edges of the electron DoS for each LL. It works well as a zero approximation, capturing rough physical effects, such as the monotonic growth of MR $R_{zz}(B_z) \propto B_z^{1/2}$ in strong field.

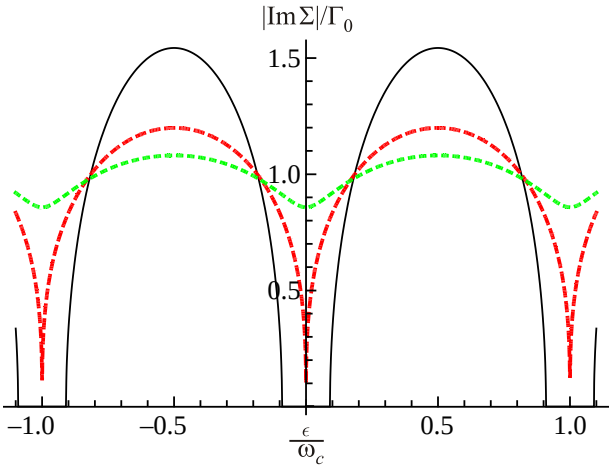

Fig. 3. (Color online) Imaginary part of the electron self energy $\mathrm{Im}\,\Sigma/\Gamma_0$ as function of energy calculated from Eqs. (19) and (20) for three different values of $\hbar\omega_c/\Gamma_0 = 1$ (solid black line), $\hbar\omega_c/\Gamma_0 = 2$ (dashed red line), and $\hbar\omega_c/\Gamma_0 = 3$ (dotted green line). When $\mathrm{Im}\,\Sigma = 0$, the DoS is also zero. The critical field B_c, when the LL become first separated, corresponds to $\hbar\omega_c/\Gamma_0 = 2$.

However, more elaborated theories predict exponential tails of the electronic DoS for each LL [19–24,44,48–53], which may lead to the small deviations from the flat average MR $\bar{R}_{zz}(B_z)$ at $B < B_c$.

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