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 \( \bar{R}_{zz} (B_z) \), analytically and numerically in the self-consistent Born approximation. We show that in a weak magnetic field the monotonic part of \( \bar{R}_{zz} (B_z) \) 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 \( B_z \gg B_c \), \( \bar{R}_{zz} (B_z) \propto B_z^{1/2} \) in agreement with previous works.

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I. 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 materials (see, e.g., Refs. [12–14] for recent reviews), heterostructures [15] etc. The standard three-dimensional theory of MR [13, 16–18] is also inapplicable. In particular, the Lorenztian LL shape gives slightly different coefficients \( \eta \sim 1 \) in the high-field dependence of \( \bar{R}_{zz} (B_z) \) [18]:

\[
\bar{R}_{zz} (B_z) / \bar{R}_{zz} (0) = \eta \sqrt{\hbar \omega_c / \Gamma_0}.
\]

The Lorenztian LL shape gives \( \eta = \sqrt{4/\pi} \), the non-crossing (or single-site) approximation [18] gives \( \eta = 3\sqrt{\pi}/8 \), while the self-consistent Born approximation (SCBA) [19] gives \( \eta = \sqrt{\pi}/4 \) (see below). In Ref. [18] the calculation of \( \bar{R}_{zz} (B_z) \) was generalized to a finite \( t_z \geq \Gamma_0 \) but still in the high-field limit \( \hbar \omega_c > 4t_z \). The behavior at \( \hbar \omega_c \sim \Gamma \) is still unknown. The smooth dependence

\[
\bar{R}_{zz} (B_z) \propto \left( (\hbar \omega_c / \Gamma_0)^2 + 1 \right)^{1/4},
\]

assumed in Refs. [18, 44], to compare with experimental data, does not have a theoretical substantiation. The aim of this paper is to calculate longitudinal interlayer magnetoresistance at \( \hbar \omega_c \lesssim \Gamma \).

II. ANALYTICAL CALCULATIONS

We apply the same "weakly incoherent" [32] model as in Refs. [18, 44], 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 [19] in the second order in the interlayer tunneling \( t_z \), taking into account only two adjacent conducting layers. As was shown in Ref. [44], 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 \( \langle G_R (r, j, \varepsilon) \rangle = \langle G_R (r_1 - r_2, j, \varepsilon) \rangle \) on 2D conduct-
ing layer with number \( j \) (see Eq. (12) of Ref. [43]):

\[
\sigma_{zz} = \frac{2\sigma_0 \Gamma_0}{\pi \nu_{2D}} \int d^2 r \int d\varepsilon \left[ -n'_{F}(\varepsilon) \right] \times \langle \text{Im} G_R(r, j, \varepsilon) \rangle \langle \text{Im} G_R(r, j + 1, \varepsilon) \rangle,
\]

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

\[
\sigma_0 = \epsilon^2 e^2 \nu_{2D} d / \hbar \Gamma_0
\]
is the interlayer conductivity without magnetic field, \( \nu_{2D} = 2g_{LL}/\hbar \omega_c = m^*/\hbar^2 = \nu_{SD} d \) 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

\[
G(r_1, r_2, \varepsilon) = \sum_{n, k_y} \Psi_{n, k_y}^\dagger (r_2) \Psi_{n, k_y}^0 (r_1) G(\varepsilon, n),
\]

where \( \Psi_{n, k_y}^0 (r_1) \) 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 \( k_y \):

\[
G(\varepsilon, n) = \frac{1}{\varepsilon - \hbar \omega_c (n + 1/2) - \Sigma(\varepsilon)},
\]

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\[55\] reduces to the normalization of the wave functions and gives (see Eq. (14) of Ref. [43]):

\[
\sigma_{zz} = \frac{\sigma_0 \Gamma_0 \hbar \omega_c}{\pi} \int d\varepsilon \left[ -n'_{F}(\varepsilon) \right] \sum_n |\text{Im} G(\varepsilon, n)|^2
\]

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

\[
\alpha = 2\pi (\varepsilon - \text{Re} \Sigma(\varepsilon)) / \hbar \omega_c, \quad \gamma \equiv 2\pi |\text{Im} \Sigma(\varepsilon)| / \hbar \omega_c,
\]

the sum over \( n \) in Eq. (7) gives

\[
\sigma_{zz} = \frac{\sigma_0 \Gamma_0 \hbar \omega_c}{\pi} \int d\varepsilon \left[ -n'_{F}(\varepsilon) \right] \left[ \frac{\sinh \gamma}{\cosh \gamma + \cos \alpha} \right. - \left. \gamma \frac{\cos \alpha \cosh \gamma + 1}{(\cosh \gamma + \cos \alpha)^2} \right]
\]
in agreement with Eqs. (19)-(21) of Ref. [37] or with Eq. (C3) of Ref. [56].

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

\[
V_i (r) = U \sum_i \delta^3 (r - r_i).
\]

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:\[44\]

\[
\Sigma(\varepsilon) = \frac{n_i U}{1 - U G(\varepsilon)},
\]

where the Green’s function

\[
G(\varepsilon) = \sum_{n, k_y, k_z} G(\varepsilon, n) = \frac{g_{LL}}{d} \sum_n G(\varepsilon, n)
\]

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

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

\[
g(\varepsilon) \equiv G(\varepsilon) \hbar \omega_c d / \pi g_{LL}.
\]

To obtain the monotonic growth of longitudinal interlayer magnetoresistance, the self-consistent Born approximation (SCBA) is sufficient, which gives instead of Eq. (11)

\[
\Sigma(\varepsilon) - n_i U = n_i U^2 \Sigma(\varepsilon) = \Gamma_0 g(\varepsilon).
\]

Here we used that the zero-field level broadening is \( \Gamma_0 = \pi n_i U^2 \nu_{2D} = \pi n_i U^2 g_{LL} / \pi \hbar \omega_c \). Below we also neglect the constant energy shift \( n_i U \) in Eq. (15), which does not affect physical quantities as conductivity.

Eqs. (13)-15 give the following equations on \( g \equiv g(\varepsilon) \):

\[
\text{Im} = \frac{\sinh (2\pi \Gamma_0 \text{Im} \omega_c / \hbar \omega_c)}{\cosh (2\pi \Gamma_0 \text{Im} \omega_c / \hbar \omega_c) + \cos (2\pi \varepsilon / \omega_c)},
\]

\[
\text{Reg} = \frac{-\sin (2\pi \varepsilon / \hbar \omega_c)}{\cosh (2\pi \Gamma_0 \text{Im} \omega_c / \hbar \omega_c) + \cos (2\pi \varepsilon / \omega_c)}.
\]

where

\[
\varepsilon^* \equiv \varepsilon - \text{Re} \Sigma^R(\varepsilon) = \varepsilon - \Gamma_0 \text{Reg}(\varepsilon).
\]

These equations can be written also for \( \Sigma^R(\varepsilon) \). With notations \( \gamma_0 = 2\pi \Gamma_0 / \hbar \omega_c, \quad \gamma = 2\pi \text{Im} \Sigma^R(\varepsilon) / \hbar \omega_c, \quad \alpha = \)
\[
2\pi \varepsilon^*/\hbar\omega_c, \quad \delta \equiv -2\pi \text{Re} \Sigma^R(\varepsilon)/\hbar\omega_c = 2\pi (\varepsilon^* - \varepsilon)/\hbar\omega_c,
\]
Eqs. (15) and (16) give
\[
\gamma_0 = \frac{\sinh (\gamma)}{\cosh (\gamma) + \cos (\alpha)}.
\]
\[
\delta \equiv \alpha \frac{2\pi \varepsilon}{\hbar\omega_c} = \frac{\gamma_0 \sin (\alpha)}{\cosh (\gamma) + \cos (\alpha)}.
\]

The solution of Eq. (19) gives \(\text{Im} \Sigma(\alpha)\), while Eq. (20) allows to find \(\alpha(\varepsilon)\) and \(\text{Re} \Sigma(\varepsilon)\). The system of Eqs. (19) and (20) differs from Eq. (30) of Ref. [37] even in the absence of electron reservoir (at \(R = 0\)), because in Eq. (30) of Ref. [37] the oscillating real part of the electron self energy is neglected, which leads to a different dependence of \(\sigma_{zz}(B_z)\). Eqs. (19) (19) and (20) will be used for numerical calculations in the next section.

**A. High-field limit**

In the high-field limit, the monotonic growth of longitudinal interlayer MR \(R_{zz}(B_z)\), given by Eq. (11), was calculated for the Lorentzian LL shape in Refs. [41] [42]. In Ref. [43] \(R_{zz}(B_z)\) was calculated in the non-crossing approximation, but the coefficient \(\eta\) in Eq. (24) of Ref. [43] is greater than the correct value by a factor 4/3 [43]. 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. III. At \(\hbar\omega_c > \Gamma_0\) the summation over \(n\) in Eq. (12) restricts to only one LL \(n = n_F\) on the Fermi level and gives the equation for \(G(\Delta \varepsilon) = (g_{LL}/d)G(\varepsilon, n_F)\):
\[
G(\Delta \varepsilon) = g_{LL}/d/ \left[\Delta \varepsilon - n_i U^2 G(\Delta \varepsilon)\right],
\]
where we have used Eq. (15) and the notation \(\Delta \varepsilon = \varepsilon - h\omega_c (n_F + 1/2) - n_i U\). This equation yields
\[
\text{Im} G(\Delta \varepsilon, n_F) = \frac{\pi}{2\Gamma_0 \hbar\omega_c} \sqrt{4\hbar\omega_c \Gamma_0/\pi - (\Delta \varepsilon)^2},
\]
which is nonzero only at \(|\Delta \varepsilon| < E_1 \equiv \sqrt{4\hbar\omega_c \Gamma_0/\pi}\). Substituting Eq. (22) to Eq. (7), keeping only one LL at the Fermi level and averaging over MQO period, we get
\[
\sigma_{zz} = \frac{\sigma_0 \Gamma_0}{\pi} \left(\frac{\pi}{2\Gamma_0 \hbar\omega_c}\right)^2 \int_{-E_1}^{E_1} d\varepsilon \left[\varepsilon_1^2 - (\Delta \varepsilon)^2\right] = \frac{\sigma_0 \Gamma_0}{\pi} \left(\frac{\pi}{2\Gamma_0 \hbar\omega_c}\right)^2 \frac{4E_1^3}{3} = \frac{\sigma_0 \Gamma_0}{\pi \hbar\omega_c},
\]
corresponding to \(\eta = \sqrt{\pi/4}\) in Eq. (11).

**III. NUMERICAL RESULTS AND DISCUSSION**

Substituting the solutions of Eqs. (19) and (20) into Eq. (9) one can calculate interlayer conductivity \(\sigma_{zz}\) 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. [37] [43]. 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 \(2\Gamma\) (see Fig. 9). Below this
field, at $B < B_c$, $\sigma_z (B_c)$ flat within the accuracy of our calculation. This means, that the field dependence of the monotonic part of longitudinal MR $R_{zz} (B)$ is not a simple analytic function, as was assumed in Refs. [34, 41] [see Eq. (22)]: within SCBA it is constant at $B < B_c$ and starts to grow at $B > B_c$, reaching the dependence $R_{zz} (B_c) \propto B_c^{3/2}$ at $\hbar \omega_c \gg \Gamma_0$. Such a crossover from low-field flat to the high-field increasing MR $R_{zz} (B_c)$ was observed in the strongly anisotropic quasi-2D organic metal $\beta^\prime$-(BEDT-TTF)$_2$SF$_6$CH$_2$CF$_2$SO$_4$ 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 $R_{zz} (B) \propto B_c^{3/2}$ in strong field. However, more elaborated theories predict exponential tails of the electronic DoS for each LL, [19–24, 44, 48, 52] which may lead to the small deviations from the flat average MR $\bar{R}_{zz} (B_c)$ at $B < B_c$.

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