Interplay between angular and quantum magnetoresistance oscillations

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Abstract. We investigate the mutual influence of angular (AMRO) and quantum oscillations (MQO) of interlayer magnetoresistance $R_{zz}(\theta)$ in quasi-two-dimensional (quasi-2D) layered metals. The MQO and the shape of Landau levels (LL) affects the AMRO amplitude. The influence of AMRO on MQO leads to the new qualitative effect: the angular oscillations of the amplitude of MQO, called "false spin zeros", that could lead to a wrong determination of electron g-factor from experiment.

1. Introduction

Determination of the electronic structure of strongly-correlated electronic conductors is a fundamental problem of modern condensed state physics. Most actively studied conductive materials, such as high-temperature cuprate and iron-based superconductors, organic metals and other strongly correlated electron systems, are usually characterized by high quasi-2D anisotropy. Angular and field dependences of magnetoresistance (MR) and magnetization, in particular quantum magnetic oscillations, make it possible to reveal even subtle details of the electronic dispersion and the geometry of the Fermi surface.

The Fermi surface in quasi-2D system under study is a slightly corrugated cylinder with strongly anisotropic spectrum, approximately given by:

$$\epsilon_{3D}(\mathbf{k}) \approx \epsilon_{2D}(k_x, k_y) - 2t_z \cos (k_z d),$$

where $\epsilon_{2D}(k_x, k_y) = \hbar^2 (k_x^2 + k_y^2)/(2m^*)$ represents an isotropic in-plane dispersion with effective mass $m^*$, $t_z$ is the interlayer transfer integral, which is much less than the Fermi energy $E_F$ and is assumed to be independent on in-plane momentum, and $d$ is the interlayer distance.

The angular magnetoresistance oscillations in quasi-2D metals were discovered in [1], and explained in [2] and [3]. The first expression for interlayer conductivity as a function of tilt angle $\theta$ of magnetic field was obtained in tau-approximation from the semiclassical equations of electron motion [3]:

$$\frac{\sigma_{zz}(\theta)}{\sigma_{zz}^0} = J_0^2(\kappa) + 2 \sum_{p=1}^{+\infty} \frac{J_p^2(\kappa)}{1 + (p\omega_c\tau)^2},$$

where $\sigma_{zz}(\theta)$ is the interlayer conductivity as a function of tilt angle $\theta$, $\sigma_{zz}^0$ is the interlayer conductivity in the absence of an oscillating magnetic field, $J_n(\kappa)$ are Bessel functions of the first kind, $\kappa = \sqrt{\epsilon_{2D}(k_x, k_y) - \epsilon_{3D}(k_z, \theta)}$, $\omega_c = eB/m^*$ is the cyclotron frequency, and $\tau$ is the electron scattering time.
where $\sigma_z^0 = 2e^2m^*t_z^2\tau d/(\pi \hbar^4)$ is the Drude conductivity along the z-direction in zero magnetic field, $J_0(\kappa)$ is the Bessel’s function, $\tau$ is the electron mean free time, the cyclotron frequency $\omega_c$ in quasi-2D metal depends on the tilt angle $\theta$ of magnetic field as $\omega_c \equiv eB_z/(m^*c) = \omega_{e0}\cos(\theta)$, where $B_z$ is component of magnetic field perpendicular to the conducting layers, $c$ is light velocity, $\kappa \equiv k_Fd\tan\theta$, and $k_F$ is the in-plane Fermi momentum.

Eq. (2) predicts sharp minima of interlayer magnetoconductivity $\sigma_{zz}(\theta)$ at the so-called Yamaji angles, corresponding to the zeros of the Bessel function $J_0(\kappa)$. These Yamaji angles have been observed in many experiments [4] and used to extract the value of $k_Fd$. At the Yamaji angles the first term of (2) is zero, and the second one predicts the quadratic field dependence of interlayer conductivity. Nevertheless, there are experimental data in organic metals, that can not be described with quadratic field dependence.

Beforementioned Eq. (2) was confirmed in Ref. [5] with the help of Kubo formula in the two-layer model in the limit $\Gamma_0 \gg \tau_z$ ($\Gamma_0 = \hbar/(2\pi n)$ is the electron-level width due to scattering on impurities in zero-magnetic field), where electrons on average scatter on impurities many times before tunneling on the adjacent conducting layer. Therefore, this limit was called “weakly incoherent” in Ref. [5]. However, since the obtained formulas for conductivity turned out to be the same as in the coherent limit, in Ref. [6] this limit was named as “weakly coherent”. Also, in Ref. [6, 7] it was suggested that in the limit $t_z \ll \hbar\omega_c$ a crossover between two qualitatively different regimes is driven by another parameter $\hbar\omega_z/\Gamma_0$. At $\hbar\omega_z/\Gamma_0 > \pi$ the LLs become isolated, because the growth of the LL broadening [8, 9] $\Gamma(B_z) \propto \sqrt{B_z}$ is slower than that of the LL separation $\hbar\omega_c \propto B_z$. This leads, e.g., to longitudinal interlayer magnetoconductivity [13]–[17] contradicting the prediction of tau-approximation. Within the two-layer model it was shown that at $\hbar\omega_z/\Gamma_0 \gg 1$ MQO generate this monotonic growth [13]–[16] of the interlayer magnetoconductance $R_{zz}(B_z) = 1/\sigma_{zz}$. This result was confirmed within the anisotropic 3D model [17]. In Ref. [17] it was also shown that the two-layer model is applicable in the limit $t_z \ll \sqrt{\hbar\omega_z/\Gamma_0}$.

The effect of MQOs on AMROs was explored in Ref. [18]. It was shown that the shape of LLs influences AMRO. The amplitude is stronger for the Gaussian or dome-like LL shapes, suitable for the microscopic models at $t_z \ll \Gamma_0 \ll \hbar\omega_c$, than for commonly used Lorentzian LL shape. The effect of AMROs on MQOs was investigated in Ref. [19], where it was shown that factorization of magnetoconductivity by purely angle $\Phi_{AMRO}(\theta)$ and field factors $\sigma_{zz}^{MQO}(B_z)$ is not generally valid: $\sigma_{zz}(B) \neq \Phi_{AMRO}(\theta)\sigma_{zz}^{MQO}(B_z)$. Especially it fails at large $\omega_\tau$ and near Yamaji angles. This leads to the appearance of “false spin zeros” on the angular dependence of MR, which may be confused with the true spin zeros used to extract the electron g-factor.

In spite of this extensive investigation, a number of important problems remained. In particular, a detailed theoretical study of the behavior at the Yamaji angles is required to describe the experimental data in organic metals and in other quasi-two-dimensional structures.

In this work, we derive a more convenient expression for the angular dependence of interlayer conductivity and with its help we calculate the field dependence of MR at the Yamaji angles. In doing so, we consider various cases. In particular, the presence of a reservoir is necessary to describe the experimental data in some layered compounds, where the reservoir may come from quasi-one-dimensional parts of the Fermi surface. It is interesting to see how the reservoir states affect conductivity. Since Eq. (2) was obtained within the framework of the approximate model, namely, in the $\tau$-approximation [3] or neglecting the MQO [5], in our calculations we use a more rigorous two-layer model that takes into account MQO in the limit $t_z \ll \sqrt{\hbar\omega_z/\Gamma_0}$.

2. General formulas

In Ref. [19] with the two-layer model, applicable at $t_z \ll \sqrt{\hbar\omega_z/\Gamma_0}$, for the case of coherent (i.e., conserving the in-plane momentum) interlayer tunneling and neglecting the electron-electron interaction (approximately valid when many LL are filled) the following formula for interlayer
conductivity in tilted magnetic field was derived:

\[
\frac{\sigma_{zz}(\epsilon)}{\sigma_{0}^{zz}} = \frac{\Gamma_{0}}{\Gamma(\epsilon)} \sum_{p=-\infty}^{+\infty} S_{p} |J_{p}(\kappa)|^{2},
\]

where \( \epsilon^{*} = \epsilon - Re\Sigma^{R}(\epsilon), \gamma \equiv -2\pi Im\Sigma^{R}(\epsilon)/\hbar\omega_{c}, \alpha \equiv 2\pi \epsilon^{*}/\hbar\omega_{c}, \) the function

\[
S_{0} \equiv \sum_{n \in \mathbb{Z}} \frac{(2/\pi)\hbar\omega_{c}\Gamma_{0}^{3}}{\left[(\epsilon^{*} - \hbar\omega_{c}(n + 1/2))^{2} + \Gamma^{2}\right]} = \frac{\sinh(\gamma)}{(\cos(\alpha) + \cosh(\gamma))^{2}} - \frac{1}{\gamma^{2} \left(\cos(\alpha) + \cosh(\gamma)\right)}(1 + \cos(\alpha) \cosh(\gamma))
\]

in agreement with Eq. (23) of Ref. [20], and for \( p \neq 0 \)

\[
S_{p} \equiv \sum_{n \in \mathbb{Z}} \frac{(2/\pi)\hbar\omega_{c}\Gamma_{0}^{3}}{\left[(\epsilon^{*} - \hbar\omega_{c}(n + 1/2))^{2} + \Gamma^{2}\right]} \left[\left(\epsilon^{*} - \hbar\omega_{c}(n + p + 1/2)\right)^{2} + \Gamma^{2}\right] = \frac{1}{\sinh(\gamma)} \frac{\sinh(\gamma)}{(1 + (p\pi/\gamma)^{2})}.
\]

In [21] one can find the following relation:

\[
\sum_{k=1}^{+\infty} \frac{J_{k}^{2}(z)}{(k^{2} - a^{2})} = \frac{J_{0}^{2}(z)}{2a^{2}} - \frac{\pi J_{a}(z)J_{-a}(z)}{2a \sin(\pi a)}.
\]

Replacement \( a \rightarrow ia \) gives us the following formula:

\[
\sum_{k=1}^{+\infty} \frac{J_{k}^{2}(z)}{(k^{2} + a^{2})} = -\frac{J_{0}^{2}(z)}{2a^{2}} + \frac{\pi J_{ai}(z)J_{-ai}(z)}{2a \sinh(\pi a)}.
\]

Using the property \( J_{ai}(z) = J_{-ai}(z) \) and relation (7) one can deduce from (3):

\[
\frac{\sigma_{zz}}{\sigma_{0}^{zz}} = \gamma_{0} \left(\frac{|J_{\gamma i/\pi}(\kappa)|^{2}}{(\cos(\alpha) + \cosh(\gamma))} - \frac{1}{\gamma_{0}^{2}} \frac{1 + \cos(\alpha) \cosh(\gamma)}{(\cos(\alpha) + \cosh(\gamma))^{2}}\right),
\]

where \( \gamma_{0} \equiv 2\pi \Gamma_{0}/(\hbar\omega_{c}). \) In Eq. (8) \( \cos(\alpha) = 1 \) corresponds to the minimum of interlayer conductivity or maximum of resistivity, and \( \cos(\alpha) = -1 \) vice versa.

This formula is quite general and convenient for numerical calculations. It differs from Eq. (2) in two aspects. First, it contains field-dependent self-energy part \( \gamma \), which leads to qualitatively different behavior in the high-field limit \( \omega_{c}\tau \gg 1 \). Second, it does not contain infinite series, which is especially helpful in the low-field limit \( \omega_{c}\tau \ll 1 \).

3. Influence of quantum on angular oscillations of magnetoresistance

The LL quantization leads to the MQO of the electron DoS on the Fermi level. While the period of the DoS oscillations is determined by the Fermi-surface geometry, the shape of DoS oscillations depend on the compound, on type of disorder, on the strength of magnetic field, etc. Below we analyze how the shape of LLs influences AMRO.

The case of Lorentzian LL shape is simple: the electron self-energy \( Im\Sigma = \Gamma \) is independent of energy and \( |ImG(\epsilon, n)| = \Gamma/((\epsilon - \epsilon_{n})^{2} + \Gamma^{2}). \) The Gaussian LL shape is given by

\[
|ImG(\epsilon, n)| = \sqrt{2\pi}/\Gamma \exp[-2(\epsilon - \epsilon_{n})^{2}/\Gamma^{2}] .
\]
Now, to find $\gamma(\epsilon)$ we assume that the following identity is approximately valid even in the case of Gaussian LL shape, as it takes place in the self-consistent Born approximation (SCBA):

$$Im\Sigma(\epsilon) \approx n_i\epsilon^2(0) \sum_n ImG(\epsilon, n), \quad (10)$$

where $n_i$ is volume concentration of short-range and randomly distributed impurities. Unfortunately, we do not have the strict proof of (10), but the inclusion of diagrams with the intersection of impurity lines in addition to SCBA gives $|ImG(\epsilon, n)|$ close to Gaussian [22]. In the case of SCBA the imaginary part of self-energy function is [7]:

$$\frac{\gamma}{\gamma_0} = \frac{\sinh (\gamma)}{\cosh (\gamma) + \cos (\alpha)}, \quad (11)$$

while the real part of self-energy function is (influence of magnetostriction is neglected):

$$\delta \equiv \alpha - \frac{2\pi \epsilon}{\hbar \omega_c} = \frac{\gamma_0 \sin (\alpha)}{\cosh (\gamma) + \cos (\alpha)} . \quad (12)$$

Also we took into account semi-phenomenological amendment to $\gamma$ in magnetic field: $\Gamma \rightarrow \Gamma(B_z) \approx \Gamma_0[1 + (2\hbar \omega_c/(\sqrt{\pi} \Gamma_0))^4]^{1/8}$. This approximate formula describes the width of LLs in both limits and during the crossover [7] from the weak to strong-field behavior.

In Figs. 1 and 2 one can see that the maximum of conductivity is not at $\theta = 0$, which clearly demonstrates how quantum oscillations affect on AMRO. This happens because for taken parameters Fermi-level stays in the middle between two closest LLs at $\theta = 0$, where density of electron states is minimal. Surprisingly, on Fig. 2 oscillations for all three shapes of LLs are close to each other.

![Figure 1](image)

**Figure 1.** The angular dependence of normalized interlayer conductivity for the Lorentzian LL shape (thin solid green curve), Gaussian LL shape (dashed red curve), SCBA shape (dotted blue curve) with $\Gamma_0 = 4 K$. The other parameters are $kFd = 4$, $\mu = 500 K$, $T = 2 K$, and $B_0 = 17.4 T$, which for cyclotron mass $m^* = m_e$ and for $\theta = 0$ corresponds to $\hbar \omega_c = 15 K$. 
Figure 2. The angular dependence of normalized interlayer conductivity for the Lorentzian LL shape (thin solid green curve), Gaussian LL shape (dashed red curve), SCBA shape (dotted blue curve) with $\Gamma_0 = 0.1\,K$. The other parameters are the same as in Fig. 1.

4. Effect of angular on quantum magnetoresistance oscillations. False spin zeros
If in SCBA we take into account reservoir states that do not give addition to quantum oscillations, we find the imaginary part of self-energy function [20]:

$$\frac{\gamma}{\gamma_0} = \frac{R}{R + 1} + \frac{1}{R + 1} \frac{\sinh(\gamma)}{\cosh(\gamma) + \cos(\alpha)},$$  
(13)

where $R$ is relation of density of states of the reservoir to the density of states of the rest of the system in zero magnetic field. If we neglect the effect of magnetostriction, we find the following expression for the real part of self-energy function (new result):

$$\delta \equiv \alpha - \frac{2\pi\varepsilon}{\hbar\omega_c} = Const + \frac{1}{R + 1} \frac{\gamma_0\sin(\alpha)}{\cosh(\gamma) + \cos(\alpha)},$$  
(14)

where $Const$ depends on the model of reservoir. We consider the case in which the conductivity of reservoir states $\sigma_{zz}^r$ is much smaller than $\sigma_{zz}^0$. This is true if the reservoir states are localized or conductivity is suppressed by magnetic field. The total conductivity is a sum of the coherent and incoherent conductivity channels: $\sigma_{zz}^{tot} = \sigma_{zz} + \sigma_{zz}^r$. Fig. 3 shows the angular dependence of the amplitude of resistivity quantum oscillations for different strengths of reservoir $R$. One can see strong angular oscillations of the MQO amplitude, which are somewhat similar to the effect of spin-zeros, originating from Zeeman splitting. However, the proposed "false spin zeros" have completely different origin. They come from the interplay of AMRO and MQO, and the minima of MQO amplitude approximately correspond to the Yamaji angles.

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Figure 3. The angular dependence of amplitude of oscillations normalized interlayer resistivity $1/\sigma_{zz}^{\text{tot}}$, calculated in SCBA for $R = 0.01$ (green curve), $R = 1$ (dashed red curve) and $R = 100$ (dashed blue curve) with $\Gamma_0 = 0.5 K$, $\sigma_{zz}^i = 0.05 \sigma_{zz}^0$, $R_{zz}^0 = 1/\sigma_{zz}^0$. The other parameters are the same as in Fig. 1.

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