

Theory of the Shubnikov–de Haas effect in quasi-two-dimensional metals

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The Shubnikov–de Haas effect in quasi-two-dimensional normal metals is studied. The interlayer conductivity is calculated using the Kubo formula. The electron scattering on short-range impurities is considered in the self-consistent Born approximation. The result obtained is given in the analytical form, that allows an easy comparison with experimental data. It differs from the result derived using the Boltzmann transport equation. This difference is shown to be a general feature of conductivity in magnetic field. A detailed description of the field-dependent phase shift of beats and of the slow oscillations of conductivity is provided. The obtained results are applicable to strongly anisotropic organic metals and to other quasi-two-dimensional compounds.

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I. INTRODUCTION

Magnetic quantum oscillations were discovered long ago, and were frequently used as a powerful tool for studying the geometry of Fermi surfaces and other electronic properties of various metals.¹ In recent years, quasi-two-dimensional (quasi-2D) materials (as, e.g. organic metals,² heterostructures, intercalated compounds, high T_C superconductors) have attracted a great deal of interest. Magnetic quantum oscillations in quasi-2D organic metals were reviewed, for example, in Ref. 3.

A theory of quantum magnetization oscillations in quasi-2D compounds was recently provided in a number of theoretical papers.^{4–6} It gives a rather good agreement with experiment. Attempts to make a theoretical description of the quasi-2D Shubnikov-de Haas (SdH) effect were not as successful, although some work in this direction appeared.^{5,7–10} The existing theory of the de Haas–van Alphen effect reliably allows us to determine the Fermi surface structure from the experimental data on different quasi-2D compounds (see, e.g., Refs. 11, 12, and Ref. 3). However, two qualitative effects peculiar to the quasi-2D magnetotransport (namely, the phase shift of beats and the slow oscillations of magnetoresistance) were observed in a number of quasi-2D organic metals.^{14–19} An explanation for and a brief qualitative description of the phase shift of beats (based on the Boltzmann transport equation) were proposed only very recently²⁰ together with a comparative experimental study of this effect. However, a quantitative agreement between theory and experiment has not been achieved in this paper. The idea that slow oscillations may arise as an entanglement of different rapidly oscillating contributing factors in conductivity which have slowly oscillating amplitudes due to beats was also recently suggested in Ref. 21, and proved by presenting experimental results on temperature and angular dependence of slow oscillations. The theoretical description of the slow oscillations was also based on the Boltzmann equation, that can be used only for a qualitative description. In this paper we give a more accurate quantitative description of the quasi-2D SdH effect, based on the Kubo formalism.

In Sec. II the general formula for the interlayer conductivity [Eq. (10)] is derived. A simple explicit formula for

interlayer conductivity is obtained in the self-consistent Born approximation in Sec. III. A discussion of the results obtained and the comparison with experimental data are given in Sec. IV. In Sec. V the results are briefly summarized.

II. GENERAL FORMULA FOR INTERLAYER CONDUCTIVITY

We consider a quasi-2D metal in a magnetic field perpendicular to the conducting layers: $\vec{B} \parallel \vec{z}$ (a generalization for arbitrary tilt angle of magnetic field is discussed in Sec. IV). The electron spectrum of a quasi-2D electron gas in a magnetic field is then given by

$$\epsilon(n, k_z) = \hbar \omega_c (n + 1/2) - 2t \cos(k_z d), \quad (1)$$

where t is the interlayer transfer integral, k_z is the wave vector perpendicular to the layers, d is the interlayer distance, and $\omega_c = eB/m^*c$ is the cyclotron frequency. Both $\hbar \omega_c$ and t are assumed to be much smaller than the Fermi energy.

To calculate the conductivity we use the Kubo formula.²² The procedure is similar to that in three-dimensional metals without a magnetic field (Ref. 22, Sec. 7.1.2). In a magnetic field only the set of quantum numbers $m \equiv \{n, k_z, k_y\}$ should be used instead of the momentum \vec{p} and the alternative dispersion relation [Eq. (1)]. We consider only the perpendicular layer component σ_{zz} of the electric conductivity, since this component is simpler both for measurements and for a theoretical description. An evaluation of the Kubo formula without vertex corrections gives

$$\sigma_{zz} = \frac{e^2 \hbar}{V} \sum_m v_z^2(m) \int \frac{d\epsilon}{2\pi} [2 \operatorname{Im} G_R(m, \epsilon)]^2 [-n'_F(\epsilon)], \quad (2)$$

where the volume V normalizes the sum over quantum numbers m , e is the electron charge, v_z is the electron velocity, the limits of the integration over ϵ are $(-\infty; \infty)$, $n'_F(\epsilon)$ is the derivative of the Fermi distribution function,

$$-n'_F(\epsilon) = 1/\{4T \cosh^2[(\epsilon - \mu)/2T]\}, \quad (3)$$

and the electron Green's function $G_R(m, \epsilon)$ is related to the retarded self-energy part $\Sigma^R(m, \epsilon)$ by

$$\text{Im } G_R(m, \epsilon) = \frac{\text{Im } \Sigma^R(m, \epsilon)}{[\epsilon - \epsilon(m) - \text{Re } \Sigma^R(m, \epsilon)]^2 + [\text{Im } \Sigma^R(m, \epsilon)]^2}. \quad (4)$$

The self-energy part $\Sigma^R(m, \epsilon)$ arises from the electron scattering. The main contribution to the resistance comes from the short-range impurity scattering. We approximate the short-range impurities by pointlike ones. We also disregard the diagrams with intersections of impurity lines in the self-energy (the contribution of these diagrams in the 3D case is negligible, and if we consider the case $t \gg T_D$ this contribution is also negligibly small). Then the electron self-energy part depends only on the electron energy and not on the electron quantum numbers: $\Sigma^R(m, \epsilon) = \Sigma^R(\epsilon)$. This fact greatly simplifies the calculations because the sum over the quantum numbers m in formula (2) can be now computed analytically.

In the real part $\text{Re } \Sigma^R(\epsilon)$ of the electron self-energy one can only keep a small oscillating part $\text{Re } \tilde{\Sigma}^R(\epsilon)$. The remaining weakly dependent term of $\text{Re } \Sigma^R(\epsilon)$ produces only a constant shift of the chemical potential. This does not influence the physical effects and, hence, is omitted in the subsequent calculations. The small oscillating part $\text{Re } \tilde{\Sigma}^R(\epsilon)$ always come in the combination $\epsilon^* \equiv \epsilon - \text{Re } \tilde{\Sigma}^R(\epsilon)$. The imaginary part of the self-energy $\text{Im } \Sigma^R(\epsilon)$ describes the momentum relaxation of electrons and, therefore, is very important for conductivity.

Performing the summation over k_y in Eq. (2) and changing the integration over k_z by an integration over energy $\epsilon' \equiv \epsilon(n, k_z)$ we obtain

$$\sigma_{zz} = e^2 N_{LL} d \int \frac{d\epsilon'}{\pi} \sum_n |v_z(\epsilon', n)| \int \frac{d\epsilon}{2\pi} 4[\text{Im } G_R(\epsilon', \epsilon)]^2 \times [-n'_F(\epsilon)], \quad (5)$$

where $N_{LL} \equiv B/\Phi_0 d$ is the electron density on one Landau level, $\Phi_0 = 2\pi\hbar c/e$ is the magnetic flux quantum, and the electron velocity $v_z(\epsilon, n)$ is given by Eq. (A2). To go further we have to transform the sum over Landau levels (LLs) to a sum over harmonics. This can be done using the Poisson summation formula (Appendix A). Substituting Eq. (A3) into Eq. (5), we obtain

$$\sigma_{zz} = e^2 N_{LL} \sum_{k=-\infty}^{\infty} (-1)^k \frac{2td^2}{\hbar k} J_1\left(\frac{4\pi kt}{\hbar\omega_c}\right) \int \frac{d\epsilon}{2\pi} \times (-n'_F(\epsilon)) I_z(\epsilon, k), \quad (6)$$

where one should use the expansion $J_1(kx)/k = x/2$ for the zeroth harmonic $k=0$, and the integral $I_z(\epsilon, k)$ over ϵ' can be easily evaluated with Green's function (4),

$$I_z(\epsilon, k) \equiv \int \frac{d\epsilon'}{2\pi} 4[\text{Im } G_R(\epsilon', \epsilon)]^2 \exp\left(\frac{2\pi i k \epsilon'}{\hbar\omega_c}\right) \quad (7)$$

$$= \exp\left(\frac{2\pi i k \epsilon^*}{\hbar\omega_c}\right) \left(\frac{1}{|\text{Im } \Sigma^R(\epsilon)|} + \frac{2\pi k}{\hbar\omega_c} \right) R_D(k, \epsilon), \quad (8)$$

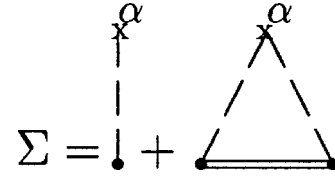


FIG. 1. The Dyson equation for the irreducible self-energy in the self-consistent Born approximation. The double solid line symbolizes the exact electron Green's function.

where $\epsilon^* \equiv \epsilon - \text{Re } \tilde{\Sigma}^R(\epsilon)$, and

$$R_D(k, \epsilon) = \exp(-2\pi|k| |\text{Im } \Sigma^R(\epsilon)| / \hbar\omega_c) \quad (9)$$

has a form similar to that of the usual Dingle factor $R_D(k) = \exp(-2\pi^2 k k_B T_D / \hbar\omega_c)$. Collecting formulas (6) and (8) we obtain

$$\sigma_{zz} = e^2 N_{LL} \int \frac{d\epsilon}{2\pi} (-n'_F(\epsilon)) \sum_{k=-\infty}^{\infty} \frac{(-1)^k 2td^2}{\hbar k} J_1\left(\frac{4\pi kt}{\hbar\omega_c}\right) \times \exp\left(\frac{2\pi i k \epsilon^*}{\hbar\omega_c}\right) \left(\frac{1}{|\text{Im } \Sigma^R(\epsilon)|} + \frac{2\pi k}{\hbar\omega_c} \right) R_D(k, \epsilon). \quad (10)$$

Note that this expression has an additional term $2\pi k / \hbar\omega_c$ near the standard $1/|\text{Im } \Sigma^R(\epsilon)|$ term in round brackets in the second line. This term cannot be obtained from the Boltzmann transport equation (compare, for example, with the results of Refs. 20 and 21). Let us reveal the origin of this term. The function $[2 \text{Im } G_R(\epsilon', \epsilon)]^2 = G_A^2 + G_R^2 - 2G_A G_R$ in Eq. (7) has one first-order pole and one second-order pole in each complex half-plane. The first-order poles appears from the last term $-2G_A G_R$ while the second order poles come from $G_A^2 + G_R^2$. In the standard theory only the first-order poles are taken into account. In the 3D case the contribution from the second-order poles is small by a factor of $\hbar\omega_c/2t \approx \hbar\omega_c/\epsilon_F \ll 1$, and can be neglected. However, in the quasi-2D case (where $\hbar\omega_c/2t \sim 1$) the contribution of second-order poles becomes important. As one can see from formula (18) this contribution $\sim \pi T_D/t$ and is, probably, only a first-order term in the expansion over $\pi T_D/t$. The case $\pi T_D/t > 1$ corresponds to the so-called incoherent limit,⁸ which we do not consider here. To go further, we need an explicit form of the electron self-energy which enters formula (10). It is calculated in the next section.

III. CONDUCTIVITY IN THE SELF-CONSISTENT BORN APPROXIMATION

We consider electron scattering only by short-range impurities because these impurities make the main contribution to the relaxation of electron momentum. To calculate the electron self-energy we use the self-consistent Born approximation. A graphical representation of the Dyson equation for the irreducible self-energy part in the self-consistent Born approximation is shown in Fig. 1. By such an approximation we neglect the multiple scattering of an electron on one impurity (no more than two dashed lines go to one impurity, denoted by a cross in Fig. 1). The single dashed line in Fig.

1 corresponding to the first-order term leads only to a constant shift of the chemical potential and, hence, can be omitted.

The corresponding analytical expression is

$$\Sigma^R(m, \epsilon) = \left\langle \sum_i U^2 G(r_i, r_i, E) \right\rangle = C_i U^2 \int d^3r G(r, r, E), \quad (11)$$

where Σ_i is a sum over all impurities and the brackets $\langle \dots \rangle$ denote an averaging over impurity positions; C_i is the concentration of impurities which are assumed to be uniformly distributed.²⁴ The electron Green's function $G(r, r, E)$ in formula (11) contains the self-energy determined by the same formula (11). The Green's function is uniform along the conducting planes. Hence one can write

$$G(r, r, E) = |\phi(z)|^2 G(E). \quad (12)$$

The electron wave function $\phi(z)$ along z axis does not enter the final result because it disappears after integration over z in Eq. (11), and

$$G(E) = \frac{-N_{LL}}{\hbar \omega_c} \left\{ A(E) + i\pi \left[1 + 2 \sum_{k=1}^{\infty} (-1)^k J_0 \left(\frac{4\pi k t}{\hbar \omega_c} \right) \exp \left(2\pi i k \frac{E - \Sigma(E)}{\hbar \omega_c} \right) \right] \right\}. \quad (13)$$

$A(E)$ is a slowly varying function of energy which can be taken at the Fermi energy: $A(E) \approx A(E_F)$. The value of $A(E_F)$ is not important for conductivity in the Born approximation.

Formulas (12) and (13) can be derived by performing a summation over the electron quantum numbers $m \equiv \{n, k_z, k_x\}$ in the definition of the Green's function:

$$G(r, r, E) = \sum_{n, k_z, k_x} \frac{\Psi_{n, k_z, k_x}^*(r) \Psi_{n, k_z, k_x}(r)}{E - \epsilon(n, k_z) - \Sigma(E)}. \quad (14)$$

The electron wave function $\Psi_{n, k_z, k_x}(r)$ in the Landau gauge is approximately given by

$$\Psi_{n, k_z, k_x}(r) = \frac{e^{i(k_x x + k_z z)}}{\sqrt{L_x L_z}} \chi_n(y - y_0) \phi(z),$$

where $y_0 = -c\hbar k_x / eB$, and the normalization condition $\int_{-\infty}^{\infty} |\chi_n(y)|^2 dy = 1$ should be used to perform the integration over k_x in Eq. (14). The further calculation of the sum in Eq. (14) is similar to that in Eq. (2).

The Born approximation [formula (11)] takes into account only the first term of the expansion in the small parameter $\pi U N_{LL} / \hbar \omega_c = \pi f / d$, where f is the scattering amplitude on impurities. The imaginary part of the self-energy in the Born approximation is proportional to the density of states.²⁵ The mean value of the imaginary part of the self-energy is simply

related to the average Dingle temperature T_D : $\langle |\text{Im} \Sigma^R(m, \epsilon)| \rangle = \pi k_B T_D$. From formulas (11)–(13) we obtain

$$|\text{Im} \Sigma^R(m, \epsilon)| = \pi k_B T_D \left[1 + 2 \sum_{k=1}^{\infty} (-1)^k J_0 \left(\frac{4\pi k t}{\hbar \omega_c} \right) \times \cos \left(\frac{2\pi k \epsilon^*}{\hbar \omega_c} \right) R_D(k, \epsilon) \right]. \quad (15)$$

Together with Eq. (9) this gives a nonlinear equation for $\text{Im} \Sigma^R(m, \epsilon)$. We can solve it in the strong harmonic damping limit by making an expansion in the small parameter $R_D \sqrt{\hbar \omega_c} / 2\pi^2 t$ (that is the ratio of oscillating and constant parts of the density of states). To treat the slow oscillation accurately one also has to pick up all second-order slowly oscillating terms. We obtain

$$|\text{Im} \Sigma^R(\epsilon)| \approx \pi k_B T_D \left\{ 1 - 2J_0 \left(\frac{4\pi t}{\hbar \omega_c} \right) \cos \left(\frac{2\pi \epsilon}{\hbar \omega_c} \right) R_{0D} \right\}, \quad (16)$$

where $R_{0D} = \exp(-2\pi^2 k_B T_D / \hbar \omega_c)$. There is no slowly oscillating second-order term in the self-energy in the Born approximation. At this point the real part of the electron self-energy is important because it cancels the contribution from the entanglement with the oscillations of the Dingle factor [Eq. (9)]. Disregard of the real part of the self-energy may incorrectly lead to an additional slowly oscillating term in conductivity.²⁶ In the second order in damping factors any combination of the form

$$\begin{aligned} & \cos \left(\frac{2\pi(\epsilon - \text{Re} \Sigma^R(\epsilon))}{\hbar \omega_c} \right) \exp \left(\frac{-2\pi |\text{Im} \Sigma^R(\epsilon)|}{\hbar \omega_c} \right) \\ &= \cos \left(\frac{2\pi \epsilon}{\hbar \omega_c} \right) R_{0D} \end{aligned} \quad (17)$$

does not produce a slowly oscillating term. This statement can be easily checked by substituting Eq. (11) with Eq. (13) into Eq. (17).

Substituting Eqs. (16) and (17) into Eq. (10), we obtain the following expression for the conductivity:

$$\begin{aligned} \sigma_{zz} = \sigma_0 \int d\epsilon [-n'_F(\epsilon)] & \\ & \times \left\{ \frac{1 - \frac{\hbar \omega_c}{\pi t} J_1 \left(\frac{4\pi t}{\hbar \omega_c} \right) \cos \left(\frac{2\pi \epsilon^*}{\hbar \omega_c} \right) R_D(\epsilon)}{\left[1 - 2J_0 \left(\frac{4\pi t}{\hbar \omega_c} \right) \cos \left(\frac{2\pi \epsilon^*}{\hbar \omega_c} \right) R_D(\epsilon) \right]} \right. \\ & \left. - \frac{2\pi k_B T_D}{t} J_1 \left(\frac{4\pi t}{\hbar \omega_c} \right) \cos \left(\frac{2\pi \epsilon^*}{\hbar \omega_c} \right) R_D(\epsilon) \right\}, \quad (18) \end{aligned}$$

where the nonoscillating part of the conductivity is $\sigma_0 \approx (e^2 N_{LL} 2t^2 d^2) / (\hbar^2 \omega_c \pi k_B T_D)$.

If the transfer integral is large enough ($4\pi t > \hbar\omega_c$) one can use an expansions of the Bessel function at a large value of the argument:

$$J_0(x) \approx \sqrt{2/\pi x} \cos(x - \pi/4), \quad x \gg 1,$$

$$J_1(x) \approx \sqrt{2/\pi x} \sin(x - \pi/4), \quad x \gg 1.$$

Then, again performing an expansion in the small parameter ($R_D \sqrt{\hbar\omega_c/2\pi^2 t}$) and making use of the standard trigonometric formulas we obtain

$$\begin{aligned} \sigma_{zz} = \sigma_0 & \left\{ 1 + 2 \sqrt{\frac{\hbar\omega_c(1+a^2)}{2\pi^2 t}} \cos\left(\frac{2\pi\mu}{\hbar\omega_c}\right) \right. \\ & \times \cos\left(\frac{4\pi t}{\hbar\omega_c} - \frac{\pi}{4} + \phi_b\right) R_D^{tot} R_T \\ & \left. + \frac{\hbar\omega_c}{2\pi^2 t} R_D^2 \sqrt{1+a_S^2} \cos\left[2\left(\frac{4\pi t}{\hbar\omega_c} - \frac{\pi}{4} + \phi_S\right)\right] \right\}, \end{aligned} \quad (19)$$

where the phase shift of the beats is

$$\phi_b = \arctan(a), \quad a = \frac{\hbar\omega_c}{2\pi t} \left(1 + \frac{2\pi^2 k_B T_D}{\hbar\omega_c}\right), \quad (20)$$

and the phase of slow oscillations is

$$\phi_S = \arctan(a_S)/2 \quad \text{where} \quad a_S = \hbar\omega_c/2\pi t. \quad (21)$$

The temperature smearing factor is given by the usual Lifshitz–Kosevich (LK) expression:

$$R_T = \frac{2\pi^2 k_B T / \hbar\omega_c}{\sinh(2\pi^2 k_B T / \hbar\omega_c)}.$$

It appears in the fast Shubnikov oscillations after the integration of a rapidly oscillating function of energy with the Fermi distribution function. The slowly oscillating term depends only on the transfer integral t and is independent of energy. Hence it does not acquire any temperature smearing.²⁷

The superscript “*tot*” after the Dingle-type damping factor R_D^{tot} of the fast quantum oscillations means that this damping factor comes not only from the short-range impurities (like R_D of slow oscillations²¹) but from all crystal imperfections such as macroscopic sample inhomogeneities and other long-range defects.

Phase shift (20) obtained from the Kubo formula is larger than that of Ref. 20, formula (9), obtained using the Boltzmann transport equation by a factor $(1 + 2\pi^2 k_B T_D / \hbar\omega_c)$. This difference originates from the additional term $2\pi k / \hbar\omega_c$ near $1/\text{Im}\Sigma^R(\epsilon)$ in round brackets in the second line of Eq. (10) that comes from the fast energy dependence of the electron mean square velocity [see the discussion after formula (10)]. The slowly oscillating term in Eq. (19) does not differ from that in [Ref. 21, formula (4)], though the present derivation is more rigorous.

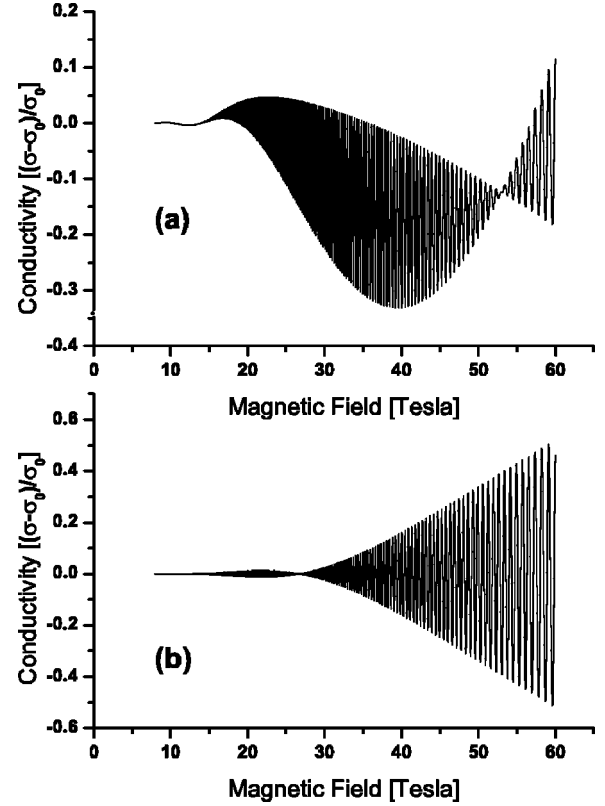


FIG. 2. Interlayer conductivity given by formula (19) (a) and by the standard LK formula (b) at the same parameters. The difference between the L-K formula and the new formula is very pronounced. The parameters are taken to be relevant to the SdH effect in β -(BEDT-TTF)₂IBr₂ in a tilted magnetic field. The parameters are $T_D = 0.4$ K, $T_D^{tot} = 1.0$ K, $T = 1.2$ K, and $F_b = 10$ T, that correspond to the tilt angle $\theta \approx 26^\circ$ or -12° .

IV. DISCUSSION OF THE RESULTS

Above we performed a detailed calculation of the interlayer magnetotransport in quasi-2D normal metals. The specific features of quasi-two-dimensionality and strong magnetic field result in several qualitative effects. The standard formula for conductivity (derived for 3D metals but traditionally used also for quasi-2D compounds)

$$\sigma_{zz}^{3D} = \sigma_0 \left\{ 1 + 2 \sqrt{\frac{\hbar\omega_c}{2\pi^2 t}} \cos\left(\frac{4\pi t}{\hbar\omega_c} - \frac{\pi}{4}\right) R_D^{tot} R_T \cos\left(\frac{2\pi\mu}{\hbar\omega_c}\right) \right\} \quad (22)$$

describes neither the phase shift of beats nor the slow oscillations.

In Fig. 2 I plot a general view of the conductivity as a function of the magnetic field using the formula (19) (a) and the standard 3D formula [Eq. (22)] (b). The difference between the LK prediction and the new formula is clearly visible. For example, the outer beat node is shifted from $B_{node}^{LK} = 26.7$ T to $B_{node} = 53$ T. Practically, this means that the outer beat node (expected at 26.7 T) may disappear because the field of 53 T is reachable only in pulsed magnets at the present time. The parameters in Fig. 2 are taken to be close to that of real experiments on β -(BEDT-TTF)₂IBr₂; in other

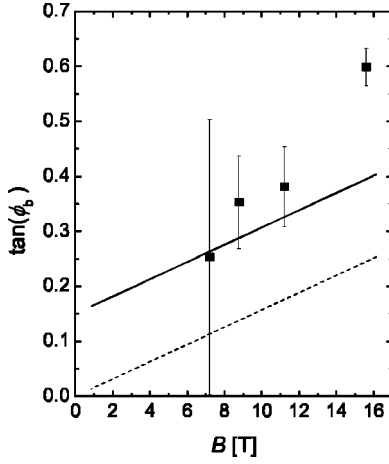


FIG. 3. A comparison of the results of different theoretical models with the experimental data from Ref. 20 on the field dependence of the phase shift of beats. The standard 3D theory gives $\phi_b=0$. The dashed line is the prediction of the Boltzmann transport equation while the solid line is the result of the present theory (see the text).

compounds or at higher tilt angle (where the interlayer transfer integral is less several times) Fig. 2 is scaled along the x-axis by the same factor. The next node at lower fields is shifted much weaker: from 11.5 to 13.5 T. If one uses these two node positions to determine the beat frequency F_b according to the LK formula [Eq. (22)], which gives

$$B_{node}^{LK}/2F_b = 4/(4n-1), \quad n=1,2,3 \dots, \quad (23)$$

one obtains $F_b=9$ T instead of the correct answer $F_b=10$ T. One will obtain a much larger error if one tries to determine the beat frequency using only one beat node and formula (23). For example, for the outer node ($n=1$) at $B=53$ T one would get $F_b \approx 20$ T instead of $F_b=10$ T. The beats of magnetoresistance oscillations in layered compounds are used for estimating the interlayer transfer integral $2t=F_b(\hbar\omega_c/B)$ that determines the electronic properties of strongly anisotropic compounds. The field-dependent phase shift of beats may lead to the errors in this estimate. The modification of formula (23) is

$$B_{node}/2F_b = 4/(4n-1-4\phi_b/\pi), \quad n=1,2,3 \dots, \quad (24)$$

where ϕ_b is given by Eq. (20).

The field dependence of the phase shift ϕ_b was studied experimentally in Ref. 20, and the result was compared with the prediction of the Boltzmann transport equation (Fig. 4 of Ref. 20). It was noted there that the slope of the fit line to the experimental points according to the Boltzmann equation corresponds to the value of the transfer integral $t \approx 0.48$ meV or the ratio $\Delta F/F \approx 1/230$, which is 2.3 times less than the value $\Delta F/F=1/96$ obtained directly from the ratio between the beat and the fundamental frequencies. This discrepancy was attributed to the approximate character of the theoretical model, based on the Boltzmann transport equation. The present theoretical model is more rigorous.

In Fig. 3 a comparison of the different theoretical models

with the experimental data on the field dependence of the phase shift of beats $\phi_b(B)$ is shown. The experimental points are taken from Ref. 20. The standard 3D magnetotransport theory gives $\phi_b=0$. The dashed line is the prediction of the Boltzmann transport equation with the value of t taken from the beat frequency. This line cannot fit the experimental points properly. The solid line is the result of the present theory, based on the Kubo formula. It gives a much better agreement with the experimental points. However, the last experimental point at the highest field $B=15.7$ T is not in accord with the theoretical line. This is because at rather high magnetic field the Born approximation fails (due to a strong degeneracy of the LLs) and result (20) becomes only a first-order term in the expansion over $\pi k_B T_D/t$ and $\hbar\omega_c/t$.

The slopes of the solid and dashed lines in Fig. 3 are the same (they are determined by the ratio $\hbar\omega_c/2\pi t$). The phase shift in our approach increases by a constant $\pi k_B T_D/t$. This augmentation contains T_D , which is the part of the Dingle temperature arising only from the short-range impurities. Approximately the same Dingle temperature enters the slow oscillations. In Fig. 3 the value of $T_D \approx 0.15$ K is taken from the Dingle plot of the slow oscillations²¹ (the measurements in Ref. 21 were done on the same sample as in Ref. 20).

The slow oscillations in formula (19) do not have a temperature damping factor. Hence, although the amplitude of the slow oscillations contains the square of the Dingle factor (they are a second-order effect), it can be larger than the amplitude of the fast SdH oscillations at $T \sim T_D$. The amplitude of slow oscillations diminishes only at much higher temperatures because the oscillations of the density of electron states (DoS) are damped by the electron-phonon and electron-electron interactions. In normal 3D metals¹³ the electron-electron ($e-e$) scattering rate $1/\tau_{ee} \sim (k_B T)^2/\hbar\mu$ while the electron-phonon scattering rate $1/\tau_{ph} \sim (k_B T/\hbar)(k_B T/\hbar\omega_D)^2$. One can estimate the effect of these scattering processes on the DoS oscillations by introducing the additional damping factor

$$R_{TD} \approx \exp[-\pi(1/\omega_c\tau_{ee} + 1/\omega_c\tau_{ph})], \quad (25)$$

analogous to the usual Dingle factor. This factor enters squared in the amplitude of slow oscillations. The temperature T_{SO} at which the slow oscillations become damped by this factor is much higher than the characteristic temperature of the damping of fast quantum oscillations. It is approximately given by $\pi[1/\omega_c\tau_{ee}(T_{SO}) + 1/\omega_c\tau_{ph}(T_{SO})] \approx 1$. In the experiment²¹ the slow oscillations were damped at temperature ≈ 9 K.

The present analysis is made when the magnetic field is perpendicular to the conducting layers. A finite tilt angle θ of the magnetic field with respect to the normal to the conducting planes may approximately be taken into account by a rescaling of the Landau level separation, $\omega_c \rightarrow \omega_c \cos \theta$, and of the warping of the Fermi surface,²⁸ $t(\theta) = t(0)J_0(k_F d \tan \theta)$, where k_F is the in-plane Fermi momentum. This result is based on the semiclassical approximation, and the assumption that the Fermi surface remains the same. The quantum mechanical calculation of the dispersion rela-

tion in a tilted magnetic field in the first order of the transfer integral gives²⁹ $t(\theta)/t(0) = \exp(-g^2/4)L_n^0(g^2/2)$, where $g \equiv d \tan \theta/a_H$, $a_H = \sqrt{\hbar c/eB_z}$ is the magnetic length, and $L_n^0(x)$ is Laguerre polynomial. In the limit $n \rightarrow \infty$ the above two results coincide.

In the above calculations we omit the spin splitting. Since the impurity scattering is spin independent, one can take the spin splitting into account by the replacement in the final answer, $\sigma_{zz}(\mu) \rightarrow [\sigma_{zz}(\mu - \Delta_B) + \sigma_{zz}(\mu + \Delta_B)]/2$, where $\Delta_B = e\hbar B/m_e c$ is the shift of the Fermi level due to the spin splitting [the conductivity given by formulas (2) and (19) already has a factor 2 due to two spin orientation].

The entanglement with the oscillations of chemical potential contributes an additional temperature-dependent term to the slow oscillations of conductivity. This term can be easily obtained by substituting Eq. (B2) into Eq. (19). However, this term has additional small factors R_T^2 and $(R_D^{tot}/R_D)^2$ compared to the main slowly oscillating term.

Slow oscillations do not appear in the magnetization because there is no suitable entanglement of different oscillating quantities in the magnetization. The magnetization, being a thermodynamic quantity, is completely determined by the electron density of states that does not have slowly oscillating terms. The mixing with the oscillations of the chemical potential, or with those of the Dingle factor and of $\text{Re} \Sigma^R(\epsilon)$, also does not lead to slow oscillations of magnetization (see Appendix B).

The above analysis does not take into account the vertex corrections. In our case (of pointlike impurity scattering) this is justified because, according to the Ward identity, the vertex $\vec{\Gamma}(m, E) = \vec{p} + m_e \vec{\nabla}_p \Sigma^R(m, E)$. Hence, if the retarded self-energy depends only on the energy, the vertex corrections are zero. The fact that $\Sigma^R(m, \epsilon)$ is approximately a function of energy ϵ only is a consequence of the short-range (or pointlike) impurity potential. In the three-dimensional case without a magnetic field the vertex corrections produce an additional factor $(1 - \cos \alpha)$ in the transport scattering relaxation time (α is the scattering angle). But the scattering probability is independent of the scattering angle in the case of pointlike impurities, and the additional term $\propto \cos \alpha$ vanishes after the integration over angles. Hence the vertex corrections vanish.

V. SUMMARY

In this paper a quantitative theory of the Shubnikov–de Haas effect in quasi-2D metals is developed. The calculation is based on a Kubo formula that is more accurate than the calculation based on the Boltzmann transport equation, and gives a much better agreement with experiment (see Fig. 3). The final result is given in analytical form, that allows a convenient comparison with any experimental data. Formulas (19)–(21) and (24) describe the general features of quasi-2D magnetoresistance and are applicable not only to organic metals, but also to heterostructures, intercalated compounds, and other layered or quasi-2D metals. The property of the slow oscillations to remain at much higher temperatures than that of the usual quantum oscillations may be useful for studying the layered high-temperature superconductors.

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APPENDIX A: TRANSFORMATION OF SUMS OVER LLS TO SUMS OVER HARMONICS

To transform the sums over the LL number into harmonic sums we shall apply the Poisson summation formula²³

$$\sum_{n=n_0}^{\infty} f(n) = \sum_{k=-\infty}^{\infty} \int_a^{\infty} e^{2\pi i k n} f(n) dn, \quad (\text{A1})$$

where $a \in (n_0 - 1; n_0)$. This formula is valid for arbitrary function $f(n)$. The electron velocity is determined from dispersion relation (1) as

$$\begin{aligned} v_z(\epsilon, n) &\equiv \frac{\partial \epsilon(n, k_z)}{\hbar \partial k_z} = -\frac{2td}{\hbar} \sin(k_z d) \\ &= \frac{d}{\hbar} \sqrt{4t^2 - [\epsilon - \hbar \omega_c(n + 1/2)]^2}. \end{aligned} \quad (\text{A2})$$

The sum in Eq. (5) now becomes

$$\begin{aligned} \sum_n |v_z(\epsilon, n)| &= \sum_{n=0}^{\infty} \frac{d}{\hbar} \sqrt{4t^2 - \left[\epsilon - \hbar \omega_c \left(n + \frac{1}{2} \right) \right]^2} \\ &= \frac{d}{\hbar} \hbar \omega_c \sum_{k=-\infty}^{\infty} \int_0^{\infty} dn e^{2\pi i k (n - \frac{1}{2})} \\ &\quad \times \sqrt{\left(\frac{2t}{\hbar \omega_c} \right)^2 - \left(\frac{\epsilon}{\hbar \omega_c} - n \right)^2} \\ &= \frac{d}{\hbar} \hbar \omega_c \sum_{k=-\infty}^{\infty} (-1)^k \exp\left(\frac{2\pi i k \epsilon}{\hbar \omega_c} \right) \\ &\quad \times \int_{-\infty}^{\infty} dx e^{2\pi i k x} \sqrt{\left(\frac{2t}{\hbar \omega_c} \right)^2 - x^2} \\ &= \sum_{k=-\infty}^{\infty} \frac{dt}{\hbar} \frac{(-1)^k}{k} \exp\left(\frac{2\pi i k \epsilon}{\hbar \omega_c} \right) J_1\left(\frac{4\pi k t}{\hbar \omega_c} \right). \end{aligned} \quad (\text{A3})$$

In this formula for the zeroth harmonic $k=0$, one should use the expansion $J_1(kx)/k = x/2$.

APPENDIX B: MAGNETIZATION

The first harmonic of the oscillating part of magnetization is given by (see Ref. 6, formula 6)

$$\tilde{M}(B) = \frac{2N_{LL}\varepsilon_F}{\pi B} \sin\left(\frac{2\pi[\varepsilon_F + \tilde{\mu}(B)]}{\hbar\omega_c}\right) \times J_0\left(\frac{4\pi t}{\hbar\omega_c}\right) R_T R_S R_D(\varepsilon_F). \quad (\text{B1})$$

where the oscillating part of the chemical potential is (Ref. 6, formula 5)

$$\tilde{\mu}(B) = \frac{\hbar\omega_c}{\pi[1 + n_R(\varepsilon_F)]} \times \sin\left(\frac{2\pi[\varepsilon_F + \tilde{\mu}(B)]}{\hbar\omega_c}\right) J_0\left(\frac{4\pi t}{\hbar\omega_c}\right) R_T R_S R_D. \quad (\text{B2})$$

The entanglement of magnetization oscillations with the oscillations of the Dingle factor [Eq. (9)] produces an additional term

$$\propto \sin\left(\frac{2\pi\varepsilon_F}{\hbar\omega_c}\right) J_0\left(\frac{4\pi t}{\hbar\omega_c}\right) \times \cos\left(\frac{2\pi\varepsilon_F}{\hbar\omega_c}\right) J_0\left(\frac{4\pi t}{\hbar\omega_c}\right) = \frac{1}{2} \sin\left(\frac{4\pi\varepsilon_F}{\hbar\omega_c}\right) J_0^2\left(\frac{4\pi t}{\hbar\omega_c}\right),$$

which gives rise to the second harmonic but makes zero contribution to the slow oscillations of magnetization.

The entanglement with the oscillations of the chemical potential [Eq. (B2)] produces the term

$$\propto \sin\left(\frac{2\pi[\varepsilon_F + \tilde{\mu}(B)]}{\hbar\omega_c}\right) - \sin\left(\frac{2\pi\varepsilon_F}{\hbar\omega_c}\right) = \sin\left(\frac{2\pi\varepsilon_F}{\hbar\omega_c}\right) \times \left[\cos\left(\frac{2\pi\tilde{\mu}(B)}{\hbar\omega_c}\right) - 1 \right] + \cos\left(\frac{2\pi\varepsilon_F}{\hbar\omega_c}\right) \sin\left(\frac{2\pi\varepsilon_F}{\hbar\omega_c}\right) J_0\left(\frac{4\pi t}{\hbar\omega_c}\right) \frac{2R_T R_D}{1 + n_R},$$

which also contributes only to the second harmonics (or higher harmonics) but not to slow oscillations.

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- ¹D. Shoenberg, *Magnetic Oscillations in Metals* (Cambridge University Press, Cambridge, 1984).
- ²T. Ishiguro, K. Yamaji, and G. Saito, *Organic Superconductors*, 2nd ed. (Springer-Verlag, Berlin, 1998).
- ³J. Wosnitzer, *Fermi Surfaces of Low-Dimensional Organic Metals and Superconductors* (Springer-Verlag, Berlin, 1996); M. V. Kartsovnik and V. N. Laukhin, *J. Phys. I* **6**, 1753 (1996); J. Singleton, *Rep. Prog. Phys.* **63**, 1111 (2000).
- ⁴V. M. Gvozdkov, *Fiz. Tverd. Tela (Leningrad)* **26**, 2574 (1984) [*Sov. Phys. Solid State* **26**, 1560 (1984)]; K. Jauregui, V. I. Marchenko, and I. D. Vagner, *Phys. Rev. B* **41**, 12 922 (1990); M. A. Itskovsky, T. Maniv, and I. D. Vagner, *ibid.* **61**, 14 616 (2000); P. Grigoriev and I. Vagner, *Pis'ma Zh. Éksp. Teor. Fiz.* **69**, 139 (1999) [*JETP Lett.* **69**, 156 (1999)]; T. Champel and V. P. Mineev, *Philos. Mag. B* **81**, 55 (2001); T. Champel, *Phys. Rev. B* **64**, 054407 (2001).
- ⁵N. Harrison *et al.*, *Phys. Rev. B* **54**, 9977 (1996).
- ⁶P. Grigoriev, *Zh. Éksp. Teor. Fiz.* **119**, 1257 (2001) [*JETP* **92**, 1090 (2001)].
- ⁷A. E. Datars and J. E. Sipe, *Phys. Rev. B* **51**, 4312 (1995).
- ⁸P. Moses and R. H. McKenzie, *Phys. Rev. B* **60**, 7998 (1999).
- ⁹V. M. Gvozdkov, *Fiz. Nizk. Temp.* **27**, 956 (2001) [*J. Low Temp. Phys.* **27**, 704 (2001)].
- ¹⁰N. S. Averkiev, L. E. Golub, S. A. Tarasenko, and M. Willander, *J. Phys.: Condens. Matter* **13**, 2517 (2001).
- ¹¹A. P. Mackenzie *et al.*, *Phys. Rev. Lett.* **76**, 3786 (1996); C. Bergemann, S. R. Julian, A. P. Mackenzie, S. NishiZaki, and Y. Maeno, *ibid.* **84**, 2662 (2000).
- ¹²J. Wosnitzer, G. W. Crabtree, K. D. Carlson, H. H. Wang, and J. M. Williams, *Physica B* **194-196**, 2007 (1994); J. Wosnitzer, G. Goll, D. Beckmann, S. Wanka, D. Schweitzer, and W. Strunz, *J. Phys. I* **6**, 1597 (1996).
- ¹³A. A. Abrikosov, *Fundamentals of the Theory of Metals* (North-Holland, Amsterdam, 1988).
- ¹⁴H. Weiss, M. V. Kartsovnik, W. Biberacher, E. Balthes, A. G. M. Jansen, and N. D. Kushch, *Phys. Rev. B* **60**, R16 259 (1999).
- ¹⁵M. Schiller *et al.*, *Europhys. Lett.* **51**, 82 (2000).
- ¹⁶M. Kartsovnik, V. Laukhin, V. Nizhankovskii, and A. Ignat'ev, *Pis'ma Zh. Éksp. Teor. Fiz.* **47**, 302 (1988) [*JETP Lett.* **47**, 363 (1988)]; M. Kartsovnik, P. Kononovich, V. Laukhin, and I. Schegolev, *ibid.* **48**, 498 (1988) [**48**, 541 (1988)]; M. Kartsovnik, P. Kononovich, V. Laukhin, S. Pesotskii, and I. F. Schegolev, *ibid.* **49**, 453 (1989) [**49**, 519 (1989)]; M. Kartsovnik, V. Laukhin, and S. Pesotskii, *Fiz. Nizk. Temp.* **18**, 22 (1992) [*Sov. J. Nucl. Phys.* **18**, 13 (1992)].
- ¹⁷T. Terashima, S. Uji, H. Aoki, M. Tamura, M. Kinoshita, and M. Tokumoto, *Solid State Commun.* **91**, 595 (1994); E. Ohmichi, H. Ito, T. Ishiguro, G. Saito, and T. Komatsu, *Phys. Rev. B* **57**, 7481 (1998).
- ¹⁸B. Narymbetov *et al.*, *Eur. Phys. J. B* **5**, 179 (1998); T. Togonidze, M. Kartsovnik, J. Perenboom, N. Kushch, and H. Kobayashi, *Physica B* **294-295**, 435 (2001).
- ¹⁹L. Balicas, J. Brooks, K. Storr, D. Graf, S. Uji, H. Shinagawa, E. Ojima, H. Fujiwara, H. Kobayashi, A. Kobayashi, and M. Tokumoto, cond-mat/0008287 (unpublished).
- ²⁰P. D. Grigoriev, M. V. Kartsovnik, W. Biberacher, N. D. Kushch, and P. Wyder, *Phys. Rev. B* **65**, 060403(R) (2002).
- ²¹M. V. Kartsovnik, P. D. Grigoriev, W. Biberacher, N. D. Kushch, and P. Wyder, *Phys. Rev. Lett.* **89**, 126802 (2002).
- ²²G. Mahan, *Many-Particle Physics*, 2nd ed. (Plenum Press, New York, 1990), Sec. 7.1.
- ²³Standard Mathematical Tables and Formulae (CRC Press, Boca Raton, FL, 1996) (or another similar book).
- ²⁴In the real layered compounds the impurity distribution may have a periodic modulation in the direction perpendicular to the layers, and with a period equal to the interlayer distance. However, in the Born approximation this modulation leads only to a con-

stant factor in (11) that renormalizes the Dingle temperature.

- ²⁵This fact has an evident physical meaning. The matrix element of the electron scattering by a point-like impurity U is the same for all transitions that do not change the electron energy. Hence the scattering rate $1/\tau(\epsilon) = -2 \text{Im} \Sigma^R/\hbar$ is proportional to the number of states to which an electron may scatter, that is, to the density of states at a given energy.

²⁶P. D. Grigoriev, M. V. Kartsovnik, W. Biberacher, and P. Wyder,

cond-mat/0108352 (unpublished).

- ²⁷This fact can be understood in a different way: slow oscillations originate from local electron motion and are not sensitive to global variations of the position of the chemical potential with respect to the bottom of the conducting band.

²⁸K. Yamaji, J. Phys. Soc. Jpn. **58**, 1520 (1989).

²⁹Yasunari Kurihara, J. Phys. Soc. Jpn. **61**, 975 (1992).