Magnetic quantum oscillations of the conductivity in layered conductors

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The Shubnikov-de Haas conductivity across the layers σ_{zz} in layered conductors in a perpendicular magnetic field B is calculated for coherent and weakly incoherent interlayer electron hopping. In the strong two-dimensional regime $(2\pi t \ll \hbar/\tau_0 \ll \hbar\Omega)$ σ_{zz} is a set of sharp peaks periodic in $1/B$ due to the quantum (non-Boltzmann) transport only (Ω is the cyclotron frequency, t is the interlayer hopping integral, τ_0 is the intralayer scattering time). The peaks are split if the chemical potential $\mu(B)$ has an inverse sawtooth shape. The σ_{zz} minima display a thermally activated behavior, and the σ_{zz} oscillations are proportional to the derivative of the magnetization on B as in experiments on ET salts.

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I. INTRODUCTION

The layered organic quasi-two-dimensional conductor family $(\mathrm{BEDT\text{-}TTF})_2X$, or ET salts, attract much interest because many of their electronic properties are unusual and similar to those of high-T_c cuprates.[1] De Haas-van Alphen (dHvA) and Shubnikov-de Haas (SdH) studies of the electronic spectrum in ET salts have shown numerous deviations from the Lifshitz-Kosevich theory.[2] The Fermi surfaces (FS) within the planes in the ET salts consist of two open one-dimensional (1D) sheets and closed orbits between them.[3,4] In some ET salts the oscillations are much more complex due to the so-called "forbidden frequencies" in the spectrum of the SdH and dHvA[5] signals caused by magnetic breakdown.

Contrary to the consensus on the shape of the FS within the planes, there is no agreement about the type of interlayer electronic transport in some ET salts.[6,7] The beats of the quantum magnetic oscillations observed in $\beta-(\mathrm{ET})_2\mathrm{I}_3$, $\beta-(\mathrm{ET})_2\mathrm{IBr}_2$ and some other organic conductors[8,9] testify in favor of coherent (dispersive) transport across the layers, which implies a warped cylindrical 3D FS due to the interlayer dispersion $\varepsilon(p_z)$. The absence of beats as well can be attributed to the smallness of the warping. There is an alternative view that in some ET salts the interlayer transport is incoherent and there is no 3D FS.[10] Experimental tests of this point within the standard fermiology picture were done in Refs. 6 and 7. The results have shown that most organic conductors have a 3D FS but $\beta''-(\mathrm{BEDT\text{-}TTF})_2\mathrm{SF}_5\mathrm{CH}_2\mathrm{CF}_2\mathrm{SO}_3$ (β'' salt) presumably does not. It displays an incoherent interlayer transport[7] for which the dispersion $\varepsilon(p_z)$ and 3D FS have no meaning, since the interlayer tunneling does not preserve the energy of interlayer hopping ε. This is a generalization to the case $B \neq 0$ of the definition, adopted in Ref. 11, that incoherent tunneling does not preserve the momentum. We assume below that ε is distributed with the density of states (DOS) $g(\varepsilon)$. In terms of the $g(\varepsilon)$ both cases of the coherent and incoherent electron motion across the layers can be described within the unified theoretical approach, as will be shown below. In the coherent case the DOS $g(\varepsilon)$ can be calculated exactly. In the incoherent case the shape of this function is basically unknown, but its width is of the order of the interlayer hopping integral t. The uniquely small value of the tunneling amplitude t in the β'' compound may be related to the very large size of the anion $\mathrm{SF}_5\mathrm{CH}_2\mathrm{CF}_2\mathrm{SO}_3$.

It was found in Ref. 12 that the SdH signal in the β'' salt is proportional to the magnetization derivative $B^2 dM/dB$ and the magnetization pattern has an inverse sawtooth profile. The SdH conductivity minima in the β'' salt exhibit a thermally activated behavior $\sigma_{zz} \propto \exp[-(\hbar\Omega - E_0)/T]$ where $\hbar\Omega$ is the Landau levels (LL) separation and E_0 is a constant.[13] The Boltzmann-equation (BE) approach is a firm basis for the electron theory of metals.[14] Recently the importance of quantum corrections to the SdH effect in ET salts was discussed in Refs. 15 and 16. We show below that in the strong 2D regime the BE contribution to σ_{zz} does not oscillate at all, because oscillations in the self-energy and the DOS compensate each other. This surprising result holds even if there is no 3D FS. Small oscillations of $\mu(B)$ (of the order of $\hbar\Omega$) strongly affect the shape of $\sigma_{zz}(B)$ and amazingly split the peaks only if $\mu(B)$ has an inverse sawtooth profile. This is in sharp contrast to the case of 3D conductors, where $\mu(B)$ is fixed at the Fermi level E_f. More precisely, in this paper we prove analytically that (1) the BE term in σ_{zz} does not oscillate in the strong 2D regime, and the oscillations are solely due to quantum transport, both for coherent and weakly incoherent interlayer electron hopping, (2) we explain the experimental observations in the β'' salt that the SdH oscillations are (i) proportional to the magnetization derivative $B^2 dM/dB$,[12] and (ii) display thermally activated behavior.[13] (3) We found a strong effect of the chemical potential oscillations on σ_{zz}, and predict the peak-splitting effect in the case $\mu(B)$ has an inverse sawtooth shape. These results are obtained on the basis of Eq. (10) for the SdH conductivity across the layers valid, as it is shown in Appendix A, both for the coherent and weakly incoherent interlayer hopping.

II. BASIC EQUATIONS FOR THE COHERENT AND WEAKLY INCOHERENT INTERLAYER CONDUCTIVITY

The calculation of the conductivity across the layers differs for coherent and incoherent cases.[10] The coherent case implies a 3D FS with the dispersion across the layers $\varepsilon(p_z)$. The corresponding velocity is $v_z(p_z)=\partial\varepsilon(p_z)/\partial p_z$, and the conductivity σ_{zz} is given by the standard Kubo formula. Written in terms of the Green function $G_\eta(E)=[E-E_\eta-\Sigma(E,\eta)]^{-1}$ it yields[15]

$$\sigma_{zz}=\frac{2\hbar e^2}{V}\sum_\eta v_z^2(\eta)\int\frac{dE}{\pi}[\mathrm{Im}\,G_\eta(E)]^2\left(-\frac{\partial f}{\partial E}\right),\qquad(1)$$

where $\eta=n$, p_z is the Landau state and E_η is the Landau energy spectrum

$$E_\eta=\hbar\Omega(n+1/2)+\varepsilon(p_z),\qquad(2)$$

V is the volume, $f(E)$ is the Fermi function, and $\Sigma(E,\eta)$ is the self-energy. In the incoherent case the momentum p_z is not preserved and the Kubo Eq. (1) is inappropriate since the energy of the interlayer hopping ε is itself a quantum number distributed with the DOS $g(\varepsilon)$. The conductivity σ_{zz} in that case is proportional to the tunneling rate between the adjacent layers.[10,11]

To calculate it, we take the single particle tunneling Hamiltonian H_t between the adjacent layers in the form

$$H_t=\sum_{\eta,\eta'}t_{\eta\eta'}\psi_u^+(\eta)\psi_l(\eta').\qquad(3)$$

Here $\psi_u^+(\eta)$ and $\psi_l(\eta')$ stand for the creation and annihilation electron operators in the upper (u) and lower (l) layers in the Landau state η. The tunneling matrix elements satisfy the condition $t_{\eta\eta'}=t^*_{\eta'\eta}$ and the current between the layers can be written as follows:[11]

$$I=\frac{e}{\hbar}\sum_{\eta,\eta'}|t_{\eta\eta'}|^2\int[f(E-eU)-f(E)]\mathrm{Im}\,G_\eta(E)\times\mathrm{Im}\,G_{\eta'}(E-eU)dE,\qquad(4)$$

U is the voltage between the layers. The conductivity σ_{zz} is given by the derivative[10]

$$\sigma_{zz}=\frac{a}{A}\left(\frac{dI}{dU}\right)_{U=0}\qquad(5)$$

and takes the form

$$\sigma_{zz}=\frac{e^2a}{\hbar A}\sum_{\eta,\eta'}|t_{\eta\eta'}|^2\int\left(-\frac{\partial f}{\partial E}\right)\mathrm{Im}\,G_\eta(E)\mathrm{Im}\,G_{\eta'}(E)dE.\qquad(6)$$

A is the area of the layers and a is the distance between them. Comparing this equation with the Kubo Eq. (1) we see a similarity with the principal difference in that in Eq. (6) there is a double summation over the Landau quantum numbers η. Another difference is that in the coherent case $\eta=n$, p_z and the spectrum is given by Eq. (2). In the incoherent case $\eta=n$, ε and

$$E_\eta=\hbar\Omega(n+1/2)+\varepsilon.\qquad(7)$$

In the coherent case for the model taking account of only nearest layer hopping the dispersion across the layers is $\varepsilon(p_z)=t\cos(ap_z/\hbar)$. The corresponding DOS $g(\varepsilon)$ and the velocity $v_z(\varepsilon)$ in this model are

$$g(\varepsilon)=\frac{1}{\pi}(t^2-\varepsilon^2)^{-1/2},\qquad(8)$$

$$v_z(\varepsilon)=\frac{a}{\hbar}(t^2-\varepsilon^2)^{1/2}.\qquad(9)$$

The Kubo Eq. (1) now takes the form

$$\sigma_{zz}=\frac{2\hbar e^2}{\pi V}\sum_n\int dEd\varepsilon g(\varepsilon)v_z^2(\varepsilon)[\mathrm{Im}\,G_{n,\varepsilon}(E)]^2\left(-\frac{\partial f}{\partial E}\right).\qquad(10)$$

Equation (10) is written in terms of the energy and formally does not require a conservation of the momentum p_z. This provokes a natural question concerning the applicability of Eq. (10) to a more general (incoherent) case when both the DOS and $v_z^2(\varepsilon)$ deviate from the simple form of Eqs. (8) and (9). More precisely, the question is, does Eq. (10) work at least for the weakly incoherent interlayer electron hopping? The analysis of this point done in Appendix A gives a positive answer.

It is shown in Appendix A that in the limit $\Omega\tau\gg 1$, necessary for the quantum oscillations, and under the condition of the weak incoherence, only states with $\varepsilon=\varepsilon'$ contribute into Eq. (6) for the conductivity which takes very much the same form as that in Eq. (10)

$$\sigma_{zz}=\frac{e^2a}{\hbar A}\sum_n\int g(\varepsilon)|t_{\varepsilon,\varepsilon}|^2\left(-\frac{\partial f}{\partial E}\right)[\mathrm{Im}\,G_{n,\varepsilon}(E)]^2dEd\varepsilon.\qquad(11)$$

The weak incoherence means that neither the intralayer scattering nor the interlayer hopping cannot mix Landau levels with different indices n in the quantum limit $\Omega\tau\gg 1$. The latter also implies that the width of the DOS $g(\varepsilon)$ (i.e., the typical value of the hopping integrals t) is much less than the Landau levels separation $\hbar\Omega$. Under these conditions it is reasonable to approximate the tunneling matrix elements by

$$t_{\eta,\eta'}\approx t_{\varepsilon,\varepsilon'}\delta_{n,n'}.\qquad(12)$$

Comparing Eqs. (10) and (11) we see that they become identical if one takes into account that the velocity $v_z(\varepsilon)$ in the incoherent case is determined by the diagonal tunneling matrix elements only

$$v_z(\varepsilon)=\frac{|t_{\varepsilon,\varepsilon}|a}{\hbar\sqrt{2}}.\qquad(13)$$

We arrive therefore at the important conclusion that Eq. (10) is valid both for coherent and weakly incoherent cases. In the first case the momentum p_z is preserved and there is a 3D FS in the system. The DOS and the velocity $v_z^2(\varepsilon)$ are functions of p_z in that case. In the incoherent case the DOS $g(\varepsilon)$ is a nontrivial function of the hopping integrals $t_{\varepsilon,\varepsilon}$ and $v_z(\varepsilon)$ is also related to them by Eq. (13).

III. SDH OSCILLATIONS

Using the results, obtained in Eqs. (A11) and (A12) in Appendix A, we can rewrite Eq. (10) in the following form:

$$\sigma_{zz} = \sigma_0 \operatorname{Re} \sum_{p=-\infty}^{\infty} (-1)^p N_{zz}(p) \int \frac{dE}{2\pi} A_p(E)\left(-\frac{\partial f}{\partial E}\right), \quad (14)$$

where $\sigma_0 = e^2\Phi/V\Phi_0\Omega$ (Φ is the flux through the sample and $\Phi_0 = 2\pi\hbar c/e$ is the flux quantum). The other quantities in Eq. (14) are

$$N_{zz}(p) = \int d\varepsilon g(\varepsilon) v_z^2(\varepsilon) \exp\left(\frac{2\pi i p\varepsilon}{\hbar\Omega}\right), \quad (15)$$

$$A_p(E) = \exp\left(\frac{2\pi i p E}{\hbar\Omega}\right)\left(\frac{1}{|\operatorname{Im}\Sigma(E)|} + \frac{2\pi|p|}{\hbar\Omega}\right) R_D(p,E). \quad (16)$$

The function $R_D(p,E) = \exp(-2\pi|p||\operatorname{Im}\Sigma(E)|/\hbar\Omega)$ generalizes the Dingle factor to the case of the energy-dependent self-energy $\Sigma(E)$. The factor $N_{zz}(p)$ is determined by the DOS $g(\varepsilon)$ and valid both for coherent and incoherent interlayer electron hopping. The function $A_p(E)$ was calculated provided that $\Sigma(E)$ depends only on the energy which is always the case for large LL number $n \approx E/\hbar\Omega \gg 1$, so that $\Sigma(E,n) \approx \Sigma(E)$. The inverse scattering time $1/\tau(E) = |\operatorname{Im}\Sigma(E)|/\hbar$ in the self-consistent Born approximation (SCBA) is proportional to the total DOS, i.e., $N(E)/N(0) = \tau_0/\tau(E)$,[17,18] where $N(0)$ is the DOS for the 2D electron gas and τ_0 is the intralayer scattering time. The oscillations of the $N(E)/N(0)$ for the arbitrary layer-stacking [arbitrary $g(\varepsilon)$] and the corresponding oscillations of the $\tau_0/\tau(E)$ can be presented as a series of the following form:[19]

$$\frac{\tau_0}{\tau(E)} = 1 + 2 \operatorname{Re} \sum_{p=1}^{\infty} (-1)^p R_D(p,E) I_p \exp\left(\frac{2\pi i p E}{\hbar\Omega}\right). \quad (17)$$

Here, as in Refs. 15 and 16, we adopt that electrons scatter only within the layers and the interlayer hopping is independent of scattering. This permits us to study different regimes within the one approach: $2\pi t \gg \hbar/\tau_0$ (Ref. 15) and $2\pi t \ll \hbar/\Omega$.[16] In the case $2\pi t \ll \hbar/\tau_0 \ll \hbar\Omega$, which we call the strong 2D regime in what follows, the hopping integrals are very small and the system, in fact, is nearly two-dimensional. The validity conditions of the SCBA in this case are the same as those established in Ref. 20 for the 2D case. Namely, the random impurity potential correlations must decay at the spatial scale much less than the magnetic length $l = (\hbar e/cB)^{1/2}$. The strong 2D regime implies as well the incoherence as it was defined in Ref. 10 since the tunneling time $\hbar/t \gg \tau_0$ and many intralayer scattering events occur before the electron hopping to the neighboring layer.

The layer-stacking influences the $\tau(E)$ through the factor I_p in Eq. (17),

$$I_p = \int d\varepsilon g(\varepsilon) \exp\left(\frac{2\pi i p\varepsilon}{\hbar\Omega}\right). \quad (18)$$

The irregular layer-stacking produces peaks in $g(\varepsilon)$ which alike the intralayer scattering yield a Dingle-like exponents in I_p.[21] Magnetic breakdown[5] and superconductivity[22] modulate the factor I_p too producing effects in the scattering rate which will be discussed elsewhere.

Using the condition $\int d\varepsilon g(\varepsilon) = 1$ and the summation rule

$$S(\lambda,\delta) = \sum_{p=-\infty}^{\infty} (-1)^p e^{-|p|\lambda} \cos p\delta = \frac{\sinh\lambda}{\cosh\lambda + \cos\delta} \quad (19)$$

one can rewrite Eq. (17) in the integral form

$$\frac{1}{\tau(E)} = \frac{1}{\tau_0} \int d\varepsilon g(\varepsilon) S[\lambda, \delta(E,\varepsilon)] \quad (20)$$

$[\lambda(E) = 2\pi/\Omega\tau, \delta(E,\varepsilon) = 2\pi(E+\varepsilon)/\hbar\Omega]$. Combining Eqs. (19), (20), and (14) we can write the SdH conductivity as a sum of the Boltzmann (σ_B) and quantum (σ_Q) terms $\sigma_{zz} = \sigma_B + \sigma_Q$, where

$$\sigma_B = \sigma_0 \int d\varepsilon \frac{dE}{\pi} g(\varepsilon) v_z^2(\varepsilon)\left(-\frac{\partial f}{\partial E}\right) \tau S[\lambda, \delta(E,\varepsilon)], \quad (21)$$

$$\sigma_Q = \sigma_0 \int d\varepsilon \frac{dE}{\pi} g(\varepsilon) v_z^2(\varepsilon)\left(\frac{\partial f}{\partial E}\right)\frac{2\pi}{\Omega}\frac{\partial}{\partial\lambda} S[\lambda, \delta(E,\varepsilon)]. \quad (22)$$

In the β'' salt the strong 2D regime $2\pi t \ll \hbar/\tau_0 \ll \hbar\Omega$ holds.[13,14] This implies that one can put $\delta \approx \Delta(E) = 2\pi E/\hbar\Omega$ in Eq. (20) which becomes

$$\tau(E) S(\lambda,\Delta) = \tau_0. \quad (23)$$

Equation (23) has an important consequence. It means a cancellation of the oscillations in the Boltzmann term σ_B, and for σ_{zz}, we have

$$\sigma_{zz} = \sigma_\tau \int \frac{dE}{\pi}\left(-\frac{\partial f}{\partial E}\right)\left[1 - \lambda_0 \frac{\partial}{\partial\lambda} S(\lambda,\Delta)\right], \quad (24)$$

where $\sigma_\tau = \sigma_0 \langle v_z^2\rangle \tau_0$ and $\lambda_0 = 2\pi/\Omega\tau_0$. The average of the velocity squared is given by $\langle v_z^2\rangle = \int d\varepsilon g(\varepsilon) v_z^2(\varepsilon)$. The function $\lambda_0 \partial/\partial\lambda S(\lambda,\Delta)$ has sharp peaks at the LL $E_n = \hbar\Omega(n+1/2)$ in the case $\lambda_0 \ll 1$. Under these conditions, $\cos\Delta(E_n) \approx -1$ and Eq. (23) can be written as $\lambda \approx \lambda_0 \coth(\lambda/2)$, which has only the one root $\lambda \approx (2\lambda_0)^{1/2}$. Finally, we obtain (see Appendix B for details)

$$\sigma_{zz} \approx \sigma_\tau \int \frac{dE}{\pi}\left(-\frac{\partial f}{\partial E}\right)[1 + \sqrt{\lambda_0/2} N(\nu,E)], \quad (25)$$

where

$$N(\nu,E) = \frac{1}{\pi}\sum_{n=-\infty}^{\infty} \frac{\nu}{(n+1/2 - E/\hbar\Omega)^2 + \nu^2} \quad (26)$$

and $\nu = \sqrt{2\lambda_0}/2\pi = 1/\sqrt{\pi\Omega\tau_0}$. We conclude, therefore, that the oscillations in σ_{zz} in the strong 2D regime arise from the quantum term only, which cannot be obtained using the BE approach. In the opposite limit, $2\pi t > \hbar\Omega, \lambda_0 \simeq 1$, the quantum term σ_Q gives small corrections to the BE oscillating σ_B term in σ_{zz}.[15] In the dirty case, $\lambda \gg 1$ and $\sigma_Q \propto \exp(-\lambda) \ll 1$.

For the temperature $T \gg \hbar/\tau_0$, the oscillating part of the conductivity Eq. (25) becomes

$$\widetilde{\sigma}_{zz} \approx \sigma_t \frac{\hbar\Omega}{4T} \sum_n \cosh^{-2}\left(\frac{E_n - \mu}{T}\right), \qquad (27)$$

where $\sigma_t = \sigma_\tau / \sqrt{\pi\Omega\tau_0}$. The sharply peaked function in the right-hand-side (rhs) of Eq. (27) is well known. It describes the quantum magnetic oscillations of the ultrasound absorption in metals.[14] Under the condition $\hbar\Omega/T \gg 1$, the conductivity $\widetilde{\sigma}_{zz}$ at the maxima (i.e., when $E_n = \mu$) is given by $\widetilde{\sigma}_{zz} = \sigma_t \hbar\Omega/4T$. At the minima (i.e., when the chemical potential μ falls between the LL) the conductivity $\widetilde{\sigma}_{zz}$ is exponentially small: $\widetilde{\sigma}_{zz} = \sigma_t \hbar\Omega/4T \exp[-(\hbar\Omega - E_0)/T]$ (E_0 is a position of the μ between the LL). Such behavior of the $\widetilde{\sigma}_{zz}$ was found in the β'' salt at fields 20-60T and temperatures 1–4 K.[13] At $T \ll \hbar/\tau_0$ one can approximate $(-\partial f/\partial E)$ by $\delta(E-\mu)$, to obtain

$$\widetilde{\sigma}_{zz} \approx \sigma_t \frac{\sinh(2\pi\nu)}{\cosh(2\pi\nu) + \cos(2\pi\mu/\hbar\Omega)}. \qquad (28)$$

This regime is more appropriate to the experiments of Ref. 12. The magnetization oscillations in a layered 2D electron gas can be described by the sum

$$\widetilde{M} = M_0 \sum_{p=1}^{\infty} \frac{(-1)^p}{p} \exp(-2\pi\nu p) \sin\left(\frac{2\pi\mu p}{\hbar\Omega}\right). \qquad (29)$$

Neglecting small corrections of the order of $\hbar/\tau_0\mu \ll 1$, we can establish a relation between the SdH conductivity of Eq. (28) and the magnetization

$$\frac{\widetilde{\sigma}_{zz}}{\sigma_t} \approx AB^2 \frac{\partial}{\partial B} \frac{\widetilde{M}}{M_0}, \qquad (30)$$

where $A = e\hbar/\pi mc\mu$. Since $AB \simeq \hbar\Omega/\pi\mu \ll 1$ one may conclude that the relative amplitude of the SdH oscillations $\widetilde{\sigma}_{zz}/\sigma_t$ is much less than the relative magnetization amplitude $\widetilde{M}/M_0$. Equation (30), known for 3D metals, was established experimentally in the β'' salt[12] and proved above for the quasi 2D case.

In ET salts it is believed that 1D sheets of the FS play the role of the electron reservoir, which stabilizes the chemical-potential oscillations.[23–25] In Ref. 16, a semiphenomenological equation for $\mathrm{Im}\Sigma(E)$ was used that has a nearly E-independent solution for some strengths of the model reservoir. The authors gave a thorough numerical analysis of the SdH conductivity in the 2D regime for coherent electron hopping across the layers in the τ-approximation ($\tau(E) = \Gamma$). The τ-approximation means that Eq. (23) is invalid and $\tau = \Gamma$ in Eqs. (21) and (22). In the strong 2D regime, this simply leads to the redefinition of the σ_t and ν in the above equations: $\sigma_t = \sigma_\Gamma / \pi(1 + \sqrt{\pi/\Omega\Gamma})$ where $\sigma_\Gamma = \sigma_\tau$ with $\tau_0 = \Gamma$, $\nu = 1/\Omega\Gamma$.

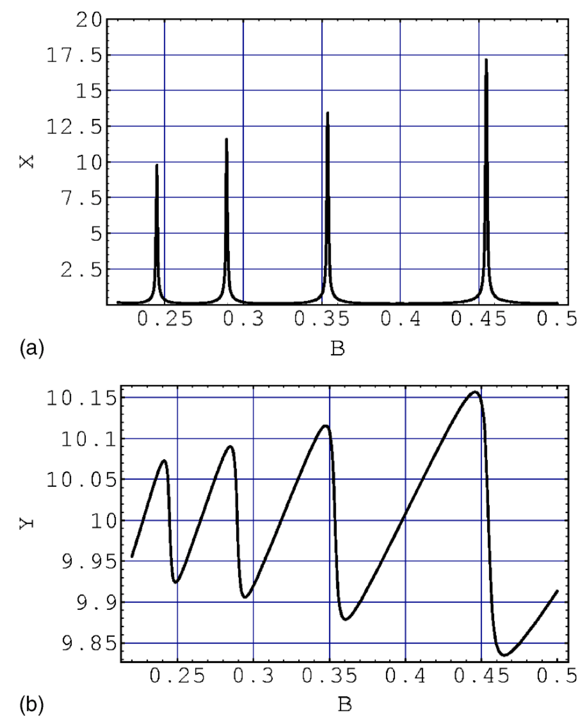

FIG. 1. The SdH conductivity [Eq. (28)] $X = \widetilde{\sigma}_{zz}(B)/\sigma_t$ and the chemical potential $Y = \mu(B)$ as a function of the magnetic field (in arbitrary units). The $\mu(B)$ has a shape of the direct sawtooth [Eq. (31) with $\mu \approx E_f$ in the rhs].

IV. CHEMICAL POTENTIAL OSCILLATIONS AND THE PEAK-SPLITTING EFFECT

The chemical potential in all the above results enters as a parameter. In real systems $\mu(B)$ is an oscillating function of B, depending on the dimensionality, the shape of the FS and other parameters. The inverse sawtooth dHvA oscillations observed in the β'' salt[12] implies a fixed value of $\mu(B)$ in this salt. Theoretical considerations of the chemical-potential oscillations in 2D conductors[23–29] show that the shape of $\mu(B)$ varies from the direct to the inverse sawtooth depending on the different types of reservoirs for the electron states due to impurities, 1D sheets of the FS, etc. The equation for $\mu(B)$ in the 2D case is well known. Its oscillating part $\widetilde{\mu}/\hbar\Omega$ is proportional to the $\widetilde{M}/M_0$, and is given by the sum in Eq. (29), which can be completed to yield

$$\mu = E_f \pm \frac{\hbar\Omega}{\pi} \arctan\left(\frac{\sin(2\pi\mu/\hbar\Omega)}{e^{\nu} + \cos(2\pi\mu/\hbar\Omega)}\right). \qquad (31)$$

The sign $(-)$ here stands for the direct sawtooth and $(+)$ for the inverse sawtooth. The amplitude of these oscillations is of the order of the $\hbar\Omega$ which is small compared with the Fermi energy E_f. Combining Eqs. (28) and (31),we studied numerically how the shape of the chemical-potential oscillations influences the peaks of the SdH conductivity. The results are shown in Figs. 1 and 2. We consider three cases: (i) the fixed value of the chemical potential; (ii) the direct sawtooth shape of $\mu(B)$ (Fig. 1); and (iii) the inverse sawtooth shape of $\mu(B)$ (Fig. 2). Although the relative amplitudes of

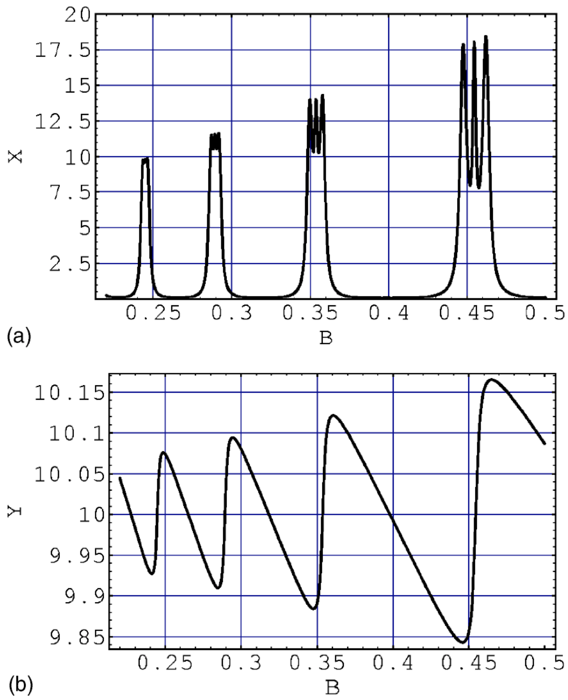

FIG. 2. The same as in Fig. 1 but $\mu(B)$ has a shape of the inverse sawtooth.

the chemical potential oscillations are small, their shapes have a strong impact on the shape of the SdH peaks. The peaks are split in case (iii). Therefore the shape of the SdH peaks and the type of the function $\mu(B)$ are correlated. All figures are drawn for the same values of the parameters, but have different peak widths. We conclude, therefore, that the shape of the function $\mu(B)$ also influences the peak width. The narrowest peaks are for the direct sawtooth $\mu(B)$ (Fig. 1), and broadest peaks are for the inverse sawtooth (Fig. 2), compared to the (unshown) case of a fixed $\mu(B)$. The reason for the peak-splitting is as follows. The peaks occur if $\mu = \hbar\Omega(n+1/2)$. This condition in terms of the variable $y = \tan \pi x$, where $x = n + 1/2 - E_f/\hbar\Omega$, yields near each peak the equation $[(e^{\nu}+1)(1+y^2)-2\pm 2]y=0$. For the direct sawtooth $(+)$, this equation has only one real root $y_1=0$ and two imaginary roots $y_{2,3}=\pm i$. For the inverse sawtooth, there are three real roots: $y_1=0$, $y_{2,3}=\pm[(3-e^{\nu})/(e^{\nu}+1)]^{1/2}$. This results in three peaks: one at the LL, and two symmetric satellites, as in Fig. 2. The peak-splitting effect is less pronounced for larger ν. For $e^{\nu}>3$ only one root, $y_1=0$, survives, but this is irrelevant to the present case $\nu \ll 1$. One can see in Fig. 2 a decrease of the peak-splitting with decreasing B.

V. RESULTS AND CONCLUSIONS

In this paper we developed an approach to the problem of the SdH oscillations in layered conductors with an arbitrary stacking and valid both for the coherent and incoherent electron hopping between the layers [see Eqs. (10)–(13)]. Above the well-known layer-stacking factor I_p given by Eq. (18) a factor, $N_{zz}(p)$, defined by Eq. (15) was introduced. This factor, contrary to the I_p, enters only to the SdH conductivity Eq. (14).

In the coherent case the DOS is given by Eq. (8) and both factors can be easily calculated: $I_p = J_0(2\pi tp/\hbar\Omega)$ and $N_{zz}(p) = a^2 t\Omega/2\pi\hbar p J_1(2\pi pt/\hbar\Omega)$. Here $J_p(x)$ is a Bessel function. Substituting these factors into Eqs. (14)–(17), we recover the results in Refs. 15 and 16. In the strong 2D regime the conductivity across the layers is proportional to the $\sigma_\tau = \sigma_0 \langle v_z^2\rangle \tau_0$. In the coherent case the average of the velocity squared $\langle v_z^2\rangle = \int \deg(\varepsilon) v_z^2(\varepsilon)$ is easy to calculate. In the strong 2D regime it equals to $\langle v_z^2\rangle = 1/2(at/\hbar)^2$. The same result holds also for the incoherent case if the matrix elements in Eq. (13) independent of the energy $t_{\varepsilon,\varepsilon}=t$. In general, under the conditions of irregular layer-stacking, some states in the DOS $g(\varepsilon)$ can be localized. If all the states are localized then $\langle v_z^2\rangle = 0$. Correspondingly, $\sigma_\tau = 0$ and there is no conductivity across the layers. On the other hand, if $\langle v_z^2\rangle \neq 0$ the quantity $\sigma_\tau \to \infty$ when $\tau_0 \to \infty$. Physically this is because the intralayer scattering is the only channel of scattering in our model and switching it off makes the system an ideal conductor. All the previous theories[10,15,16] display the same behavior in the limit $\tau_0 \to \infty$.

Localization and incoherence effectively change the hopping between the layers. Quantitatively these effects are determined by the $\langle v_z^2\rangle = \int d\varepsilon g(\varepsilon) v_z^2(\varepsilon)$ which is difficult to calculate in general. Qualitatively, the effect can be estimated as follows. In the strong 2D regime the inequality $2\pi t \ll \hbar/\tau_0$ implies that a large number of in-plane scattering takes place before the interlayer hopping. This, as was shown in Ref. 30, makes the hopping time effectively larger by the factor $\gamma = \hbar/t\tau_0 \gg 1$ and the quantity $\langle v_z^2\rangle = 1/2(at/\hbar)^2$ by the factor γ^{-2} smaller than in the coherent case.

In conclusion, we have shown that in the strong 2D regime the quasiclassical Boltzmann contribution to σ_{zz} does not oscillate and SdH effect is entirely due to the quantum-transport mechanism. The $\sigma_{zz}(B)$ minima display thermally activated behavior and $\sigma_{zz} \propto B^2 dM/dB$ in agreement with experiments on the β''. We predict a strong impact of the small chemical-potential oscillations on the shape of peaks in $\sigma_{zz}(B)$. A detailed description and generalization to the magnetic breakdown will be published elsewhere.

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APPENDIX A

Substituting Eq. (12) into Eq. (6), we have

$$\sigma_{zz} = \frac{e^2 a}{\hbar A} \int g(\varepsilon) g(\varepsilon') |t_{\varepsilon,\varepsilon'}|^2 \left(-\frac{\partial f}{\partial E} \right) M(E,\varepsilon,\varepsilon') dE d\varepsilon d\varepsilon' , \tag{A1}$$

where

$$M(E,\varepsilon,\varepsilon') = \sum_n \operatorname{Im} G_{n,\varepsilon}(E) \operatorname{Im} G_{n,\varepsilon'}(E). \tag{A2}$$

Using the identity

$$\sum_{n=-\infty}^{\infty} \delta[E - \varepsilon - \hbar\Omega(n+1/2)] = \frac{1}{\hbar\Omega} \operatorname{Re} \sum_{p=-\infty}^{\infty} (-1)^p \exp\left[\frac{i2\pi p(E-\varepsilon)}{\hbar\Omega} \right], \tag{A3}$$

we obtain

$$M(E,\varepsilon,\varepsilon') = \frac{1}{\hbar\Omega} \operatorname{Re} \sum_p (-1)^p \Gamma_p(E,\varepsilon,\varepsilon'). \tag{A4}$$

The function $\Gamma_p(E,\varepsilon,\varepsilon')$ is given by the integral

$$\Gamma_p(E,\varepsilon,\varepsilon') = \int_{-\infty}^{\infty} \frac{\nu^2 \exp(2\pi i p x/\hbar\Omega)}{[(E^* - \varepsilon - x)^2 + \nu^2][(E^* - \varepsilon' - x)^2 + \nu^2]} dx. \tag{A5}$$

Here we denote $\nu = |\operatorname{Im}\Sigma(E)|$ and $E^* = E - \operatorname{Re}\Sigma(E)$. The poles at the complex plane which has the function in the integral (A5) are of the first order if $\varepsilon \neq \varepsilon'$ and of the second order for $\varepsilon = \varepsilon'$. Therefore, the calculation of the function $\Gamma_p(E,\varepsilon,\varepsilon')$ differs for the cases $\varepsilon = \varepsilon'$ and $\varepsilon \neq \varepsilon'$. In the case $\varepsilon \neq \varepsilon'$, we have

$$\Gamma_p(E,\varepsilon,\varepsilon') = \pi\nu \exp\left[2\pi \frac{(ipE^* - |p|\nu)}{\hbar\Omega} \right] F^{\nu}(p,\varepsilon,\varepsilon'), \tag{A6}$$

where we denoted

$$F^{\nu}(p,\varepsilon,\varepsilon') = \frac{1}{\varepsilon - \varepsilon'} \left[\frac{\exp\left(-\frac{2\pi i p\varepsilon}{\hbar\Omega}\right)}{\varepsilon - \varepsilon' - i\nu} + \frac{\exp\left(-\frac{2\pi i p\varepsilon'}{\hbar\Omega}\right)}{\varepsilon - \varepsilon' + i\nu} \right]. \tag{A7}$$

Therefore, $\varepsilon = \varepsilon'$ is a singular point for the function $\Gamma_p(E,\varepsilon,\varepsilon')$. Substituting Eq. (A6) into Eq. (A4) and using the summation rule (19), we have

$$M(E,\varepsilon,\varepsilon') = \frac{\pi f_\gamma(\varepsilon - \varepsilon')}{\hbar^2\Omega^2} [S^*(E,\varepsilon) + S^*(E,\varepsilon')]. \tag{A8}$$

Here the sum $S^*(E,\varepsilon) \equiv S[\lambda, \delta(E,-\varepsilon)]$ is defined by Eq. (19) and

$$f_\gamma(\varepsilon - \varepsilon') = \frac{\gamma}{\left(\frac{\varepsilon - \varepsilon'}{\hbar\Omega}\right)^2 + \gamma^2} \tag{A9}$$

with $\gamma = (2/\Omega\tau)$. In the quantum limit $\Omega\tau \gg 1$ the parameter $\gamma \ll 1$ is small and one can approximate $f_\gamma(\varepsilon - \varepsilon')$ by the δ function

$$f_\gamma(\varepsilon - \varepsilon') \approx \pi\hbar\Omega\, \delta(\varepsilon - \varepsilon'). \tag{A10}$$

This means that $M(E,\varepsilon,\varepsilon') \propto \delta(\varepsilon - \varepsilon')$ and only a singular point $\varepsilon = \varepsilon'$ contribute into the conductivity σ_{zz} in the limit of interest $\Omega\tau \gg 1$. From Eq. (6) in this case we have

$$\sigma_{zz} = \frac{e^2 a}{\hbar A} \int g(\varepsilon) |t_{\varepsilon,\varepsilon}|^2 \left(-\frac{\partial f}{\partial E} \right) M(E,\varepsilon,\varepsilon) dE d\varepsilon. \tag{A11}$$

Here the function $M(E,\varepsilon,\varepsilon)$ is given by Eq. (A2) for the coinsiding arguments $\varepsilon = \varepsilon'$. For this case, after the calculation of the integral (A5), it can be also written as a sum (A4) with the

$$\Gamma_p(E,\varepsilon,\varepsilon) = \frac{\pi}{2} \exp\left[2\pi \frac{ip(E^* - \varepsilon) - |p|\nu}{\hbar\Omega} \right] \left(\frac{1}{\nu} + \frac{2\pi|p|}{\hbar\Omega} \right). \tag{A12}$$

Substituting Eq. (A12) into Eq. (A11) we can discard the difference between E and E^* because the steady part of the $\operatorname{Re}\Sigma(E)$ gives just a shift to the Fermi energy E_f. The oscillations in the $\operatorname{Re}\Sigma(E)$ are smooth because of the dispersion relation giving the $\operatorname{Re}\Sigma(E)$ as an integral of the (oscillating) imaginary part $\operatorname{Im}\Sigma(E)$. The amplitude of the oscillations in the $\operatorname{Re}\Sigma(E)$ are much less than $\hbar\Omega$ in the limit $\Omega\tau \gg 1$ and can be neglected (see also Ref. 15 in this connection)

APPENDIX B

Equation (24) for σ_{zz} in an explicit form reads

$$\sigma_{zz} = \sigma_\tau \int \frac{dE}{\pi} \left(-\frac{df}{dE} \right) \left[1 - \lambda_0 \frac{1 + \cosh\lambda \cos\Delta}{(\cosh\lambda + \cos\Delta)^2} \right]. \tag{B1}$$

The quantity $\lambda(E)$ satisfies Eq. (23) which takes the form

$$\lambda = \lambda_0 \frac{\sinh\lambda}{\cosh\lambda + \cos\Delta}. \tag{B2}$$

Using the identity

$$\frac{1}{\pi} \sum_{p=-\infty}^{\infty} \frac{\nu}{(n+a)^2 + \nu^2} = \frac{\sinh 2\pi\nu}{\cosh 2\pi\nu - \cos 2\pi a} \tag{B3}$$

we can rewrite the second term in the brackets in Eq. (B1) as follows:

$$\frac{1 + \cosh\lambda \cos\Delta}{(\cosh\lambda + \cos\Delta)^2} = \frac{1 + \cosh\lambda \cos\Delta}{(\cosh\lambda + \cos\Delta)\sinh\lambda} N(\nu,E), \tag{B4}$$

where

$$N(\nu,E) = \frac{1}{\pi}\sum_{n=-\infty}^{\infty} \frac{\nu}{\left(n+\frac{1}{2}-\frac{E}{\hbar\Omega}\right)^2+\nu^2} \tag{B5}$$

and $\nu=\lambda/2\pi=(\Omega\tau)^{-1}$. Since we are interested in the limit $\lambda \ll 1$ at which $N(\nu,E)$ is a set of sharp delta peaks centered at the Landau levels E_n we can use the relations $\cos\Delta(E_n)=-1$. Equation (B2) can be written in this limit as

$$\lambda \approx \lambda_0 \coth(\lambda/2). \tag{B6}$$

It has only the one root $\lambda \approx (2\lambda_0)^{1/2} \ll 1$. Taking all this into account we can rewrite Eq. (B1) in the following form:

$$\sigma_{zz} = \sigma_\tau \int \frac{dE}{\pi}\left(-\frac{df}{dE}\right)\left[1+\sqrt{\lambda_0/2}N(\nu,E)\right]. \tag{B7}$$

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