Incoherent Interlayer Transport and Angular-Dependent Magnetoresistance Oscillations in Layered Metals

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The effect of incoherent interlayer transport on the interlayer resistance of a layered metal is considered. We find that for both quasi-one-dimensional and quasi-two-dimensional Fermi liquids the angular dependence of the magnetoresistance is essentially the same for coherent and incoherent transport. Consequently, the existence of a three-dimensional Fermi surface is *not* necessary to explain the oscillations in the magnetoresistance that are seen in many organic conductors as the field direction is varied. [S0031-9007(98)07660-1]

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One of the most fundamental concepts in solid state physics is that in most metallic crystals the electronic conduction occurs through the coherent motion of electrons in band states associated with well-defined wave vectors [1]. There is currently a great deal of interest in whether this concept is valid for interlayer transport in high-T_c superconductors [2,3], organic conductors [4], and layered manganite compounds with colossal magnetoresistance [5]. Incoherent transport means that the motion from layer to layer is diffusive and band states and a Fermi velocity perpendicular to the layers cannot be defined. The Fermi surface is then not three-dimensional and Boltzmann transport theory cannot describe the interlayer transport.

In organic conductors [6] large variations in the magnetoresistance are observed as the direction of the magnetic field is varied and are referred to as angular-dependent magnetoresistance oscillations (AMRO) [7]. These effects in quasi-one-dimensional systems are known as Danner [8], Lebed [9–11], and third angular effects [12], depending on whether the magnetic field is rotated in the **a**-**c**, **b**-**c**, or **a**-**b** plane, respectively. (The **a** and **c** axes are the most- and least-conducting directions, respectively). Oscillations in quasi-two-dimensional systems include the Yamaji [13] oscillations and the anomalous AMRO in the low-temperature phase of α-(BEDT-TTF)$_2M$Hg(SCN)$_4$[$M = \mathrm{K, Rb, Tl}$] [7,14].

We focus on the Danner and Yamaji oscillations here because their explanation in terms of a three-dimensional Fermi surface has generally been accepted. The resistance perpendicular to the layers is a maximum when the field direction is such that the electron velocity (perpendicular to the layers) averaged over its trajectories on the Fermi surface is zero [8,15]. In contrast, it is not clear that coherent transport models can explain the angle-dependent magnetoresistance in the quasi-one-dimensional $(\mathrm{TMTSF})_2\mathrm{PF}_6$ at pressures of about 10 kbar [4,9,10,16,17]. The main result of this Letter is that coherent interlayer transport is not *necessary* to explain the Yamaji and Danner oscillations. In contrast, the observation of beats in the magneto-oscillations of quasi-two-dimensional systems and a peak in the magnetoresistance when the field is parallel to the layers is evidence for a three-dimensional Fermi surface. We now define precisely what we mean by coherent and incoherent transport (see Fig. 1) and how to calculate the associated conductivity.

Coherent interlayer transport.—A three-dimensional dispersion relation $\epsilon_{3D}(\vec{k})$ can be defined where

$$\epsilon_{3D}(\vec{k}) = \epsilon(k_x, k_y) - 2t_c \cos(k_z c), \tag{1}$$

where t_c is the interlayer hopping integral, c is the layer separation, and $\epsilon(k_x, k_y)$ is the intralayer dispersion relation, simple examples of which are given in Table I. The electronic group velocity perpendicular to the layers is

$$v_z = \frac{1}{\hbar}\frac{\partial \epsilon_{3D}(\vec{k})}{\partial k_z} = \frac{2t_c c}{\hbar}\sin(k_z c). \tag{2}$$

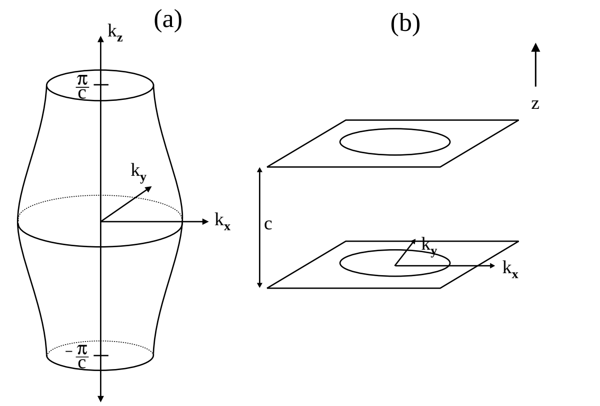

FIG. 1. The pictures relevant to coherent and incoherent interlayer transport in a quasi-two-dimensional system. (a) If the transport between layers is coherent then one can define a three-dimensional Fermi surface which is a warped cylinder. The interlayer conductivity is determined by correlations of the electronic group velocity perpendicular to the layers. [See Eq. (3).] (b) For the incoherent interlayer transport considered here a Fermi surface is only defined within the layers and the interlayer conductivity is determined by the interlayer tunneling rate. [See Eq. (5).]

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TABLE I. Different physical quantities relevant to angular-dependent magnetoresistance oscillations for the cases where intralayer Fermi surface is quasi-one-dimensional (open) and quasi-two-dimensional (closed). In a magnetic field the electrons oscillate on the Fermi surface with frequency ω_0 when the field B is perpendicular to the layers. The geometric factor γ determines the field directions at which the interlayer resistivity is a maximum [see Eq. (9)]. The magnitude of the Fermi wave vector is denoted k_F. For the quasi-one-dimensional case, v_F is the Fermi velocity, t_b the interchain hopping integral, and b the interchain distance. For the quasi-two-dimensional case, m^* is the effective mass.

Quantity	Symbol	Quasi-1D	Quasi-2D
Intralayer dispersion	$\epsilon(k_x, k_y)$	$\hbar v_F(\lvert k_x \rvert - k_F) - 2t_b \cos(k_y b)$	$\frac{\hbar^2}{2m^*}(k_x^2 + k_y^2)$
Oscillation frequency	ω_0	$\frac{e v_F b B}{\hbar}$	$\frac{eB}{m^*}$
Geometric factor	γ	$\frac{2t_b c}{\hbar v_F}$	$k_F c$
Zero-field interlayer conductivity	σ_{zz}^0	$\frac{4e^2 c t_c^2 \tau}{\pi \hbar^3 b v_F}$	$\frac{2e^2 m^* c t_c^2 \tau}{\pi \hbar^4}$

The interlayer conductivity involves correlations of this velocity and is given by Chambers formula [1]

$$\sigma_{zz} = \frac{e^2\tau}{4\pi^3} \int d^3k\, v_z(\vec{k})\overline{v}_z(\vec{k})\delta(E_F - \epsilon_{3\mathrm{D}}(\vec{k}))\,, \quad (3)$$

where E_F is the Fermi energy, τ the scattering time, and $\overline{v}_z(\vec{k})$ is the velocity averaged over a trajectory on the Fermi surface ending at $\vec{k}$:

$$v_z(\vec{k}) = \frac{1}{\tau} \int_{-\infty}^{0} dt \exp(t/\tau) v_z(\vec{k}(t))\,. \quad (4)$$

If the magnetic field is tilted sufficiently far away from the layers that $t_c c \tan\theta \ll \hbar v_F$, where θ is the angle between the field and the normal to the layers, then to lowest order in t_c the expression (3) can be evaluated analytically. This means neglecting the effects of closed orbits that become important when the field direction is close to the layers [18]. After long calculations the results for both the quasi-one-dimensional and quasi-two-dimensional cases can be written in the form (8) given below.

Incoherent interlayer transport.—If the intralayer scattering rate $1/\tau$ is much larger than the interlayer hopping integral t_c [19] then the interlayer transport will be incoherent [20] in the sense that successive interlayer tunneling events are uncorrelated [21]. The interlayer conductivity is then proportional to the tunneling rate between just two adjacent layers (see Fig. 1). This rate can be calculated using standard formalisms for tunneling in metal-insulator-metal junctions [22,23] which assume that the intralayer momentum is conserved. The result (for temperatures much less than the Fermi energy and $\hbar = 1$) is

$$\sigma_{zz} = \frac{e^2 t_c^2 c}{\pi L^2} \int d^2r_a d^2r_b A_1(\vec{r}_a, \vec{r}_b, E_F) A_2(\vec{r}_b, \vec{r}_a, E_F)\,, \quad (5)$$

where L^2 is the area of the layer and $A_j(\vec{r}_a, \vec{r}_b, E)$ $(j = 1, 2)$ are the spectral functions for layers 1 and 2. It will be seen below that in the presence of a tilted magnetic field A_1 and A_2 are not identical. The zero-field limit of this expression has been used in treatments of incoherent interlayer transport in the cuprate superconductors [24].

The magnetic field $\vec{B} = (B_x, 0, B_z) = (B\sin\theta, 0, B\cos\theta)$ is described by a vector potential $\vec{A}$, which in the Landau gauge has only one nonzero component, $A_y = B_z x - B_x z$. The Hamiltonian for layer 1 $(z = 0)$ is then the same as that for a single layer in a perpendicular field $B\cos\theta$. The Hamiltonian for layer 2 $(z = c)$ is the same as for layer 1 except x is replaced with $(x - c\tan\theta)$. This displacement actually corresponds to a gauge transformation [25], $\vec{A} \rightarrow \vec{A} - \nabla\Lambda$ where $\Lambda(\vec{r}) = B\sin\theta c y$. Wave functions transform according to $\psi(\vec{r}) \rightarrow \psi(\vec{r})\exp[ie\Lambda(\vec{r})]$. The Green's functions in layers 1 and 2 are then related by

$$G_2(\vec{r}_a, \vec{r}_b) = \exp[ie\Lambda(\vec{r}_a)] G_1(\vec{r}_a, \vec{r}_b) \exp[-ie\Lambda(\vec{r}_b)]\,. \quad (6)$$

Substituting this in (5) gives

$$\sigma_{zz} = \frac{2e^2 t_c^2 c}{\pi} \int d^2r \lvert G_1(\vec{r}, 0, E_F)\rvert^2 \cos(eB\sin\theta c y)\,. \quad (7)$$

We have evaluated (7) for the simplest possible situation, a Fermi liquid within each layer, with the dispersion relations given in Table I. The complete details of the calculations will be given elsewhere [26]. For the quasi-two-dimensional case we followed a procedure similar to that used by Hackenbroich and von Oppen [27] in their study of magneto-oscillations in antidot lattices. In the semiclassical approximation the Green's function is written as a sum over classical trajectories from $\vec{r}_a$ to $\vec{r}_b$. For the quasi-one-dimensional case the quasiclassical Green's function [28] was used.

In a tilted magnetic field the interlayer conductivity for *both* coherent and incoherent interlayer transport is

$$\sigma_{zz}(\theta) = \sigma_{zz}^0 \left[J_0(\gamma \tan\theta)^2 + 2\sum_{\nu=1}^{\infty} \frac{J_\nu(\gamma \tan\theta)^2}{1 + (\nu\omega_0\tau\cos\theta)^2} \right], \quad (8)$$

where σ_{zz}^0 is the zero-field conductivity, $J_\nu(x)$ is the νth order Bessel function, ω_0 is the oscillation frequency associated with the magnetic field, and γ is a constant that depends on the geometry of the Fermi surface (see Table I). This expression was previously derived by Yagi et al. [29] for coherent interlayer transport for a quasi-two-dimensional Fermi surface [30]. If $\omega_0\tau\cos\theta \gg 1$ then the first term in (8) is dominant. However, if $\gamma\tan\theta$ equals a zero of the zeroth order Bessel function then at that angle σ_{zz} will be a minimum and the interlayer resistivity will be a maximum. If $\gamma\tan\theta \gg 1$, then the zeros occur at angles θ_n given by

$$\gamma \tan\theta_n = \pi\left(n - \frac{1}{4}\right) \qquad (n = 1, 2, 3, \ldots). \quad (9)$$

Determination of these angles experimentally provides a value for γ and thus information about the intralayer Fermi surface. The values of the Fermi surface area of quasi-two-dimensional systems determined from AMRO are in good agreement with the Fermi surface areas determined from the frequency of magneto-oscillations [7].

Figure 2 shows the angular dependence of the interlayer resistivity $\rho_{zz} \equiv 1/\sigma_{zz}$ for parameter values relevant to $(TMTSF)_2ClO_4$. The results are similar to the experimental results in Ref. [8] and the results of numerical integration of Chambers formula for coherent transport (3) except near 90°. For coherent transport there is a small peak in $\rho_{zz}(\theta)$ at $\theta = 90°$. This is due to the existence of closed orbits on the Fermi surface when the field lies close to the plane of the layers [18]. For incoherent transport these orbits do not exist and so the associated magnetoresistance is not present. Hence, except close to 90°, the Danner oscillations can be explained equally well in terms of incoherent transport. Hence, contrary to the claims of Ref. [9], the observation of Danner oscillations is not necessarily evidence for the existence of a three-dimensional Fermi surface. Similarly, the suppression of the Danner oscillations by the introduction of a small component of the magnetic field in the **b** direction, as is observed in $(TMTSF)_2PF_6$ at pressures of about 10 kbar [9], does not necessarily imply that the field is destroying the three-dimensional Fermi surface.

It is the averaging of the phase factor over the spatial integral in (7) that gives rise to the Yamaji and Danner effects. The length scale associated with the magnetic field for the quasi-2d system is the cyclotron length R which at the Fermi energy is $R = \hbar k_F/(eB\cos\theta)$. For the quasi-1d case the length scale associated with oscillations perpendicular to the chains is $R = 2t_b/(ev_FB\cos\theta)$ [31]. At this length scale the phase difference between the wave function of adjacent layers is $e\Lambda(R) = eB\sin\theta cR = \gamma\tan\theta$. Naively, we might expect maximum resistivity when this phase difference is an odd multiple of π, leading to a condition different from (9). However, one must take into account averaging of the electron position over the perpendicular direction.

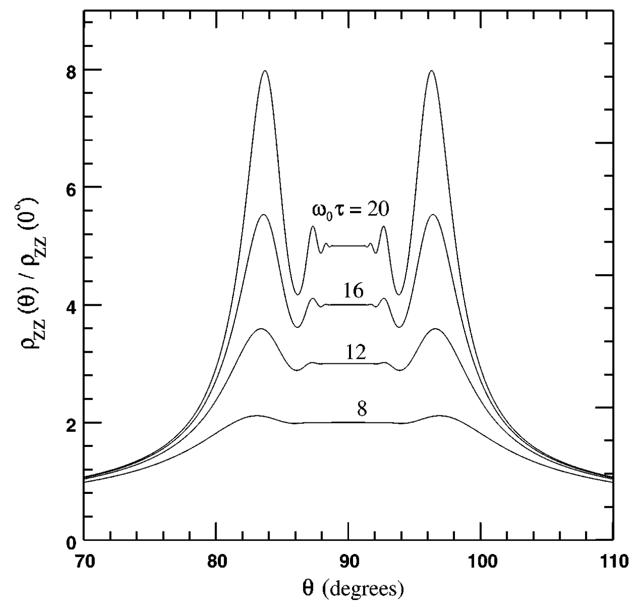

FIG. 2. Dependence of the interlayer resistance of a quasi-one-dimensional system on the direction of the magnetic field for a range of magnetic fields. θ is the angle between the magnetic field and the least conducting direction, with the field in the same plane as the most conducting direction. The parameter which defines the anisotropy of the intralayer hopping $\gamma = 0.25$ (cf. Table I). τ is the intralayer scattering time and ω_0 is the frequency at which the electrons oscillate between the chains when the field is perpendicular to the layers. Except very close to 90°, this figure is similar to the experimental data on $(TMTSF)_2ClO_4$ in Ref. [8].

Given we have shown that the existence of a three-dimensional Fermi surface is not necessary to produce the Yamaji oscillations we consider an alternative test for coherent transport for quasi-two-dimensional systems. Definitive evidence for the existence of a three-dimensional Fermi surface, such as that shown in Fig. 1(a), is the observation of a beat frequency in de Haas-van Alphen and Shubnikov–de Haas oscillations. The frequency of these oscillations is determined by extremal areas of the Fermi surface [7]. For the Fermi surface shown in Fig. 1(a) there are two extremal areas, corresponding to "neck" and "belly" orbits. The small difference between the two areas leads to a beating of the corresponding frequencies with a frequency proportional to t_c/E_F [7]. Such beat frequencies have been observed in β-$(BEDT\text{-}TTF)_2I_3$, β-$(BEDT\text{-}TTF)_2IBr_2$ [7], α-$(BETS)_2KHg(SCN)_4$ at pressures above 4 kbar [32], and Sr_2RuO_4 [33]. In the former it was used to establish that $t_c/E_F \simeq 1/175$ [7]. However, in many other quasi-two-dimensional organics no beat frequency is observed [7]. This could be because the interlayer transport is incoherent or because the interlayer hopping t_c is so small that the beat frequency cannot be resolved experimentally. For κ-(BEDT-TTF)$_2$I$_3$ the absence of beating has been used to establish the upper bound $t_c/E_F < 1/3000$ [7,34]. This implies a conductivity anisotropy $\sigma_{zz}/\sigma_{xx} \sim (t_c/E_F)^2 < 10^{-7}$. However, the observed anisotropy in the κ-(BEDT-TTF)$_2X$ materials is about 10^{-3} [35]. This large discrepancy suggests that the interlayer transport is incoherent in these materials.

We have also examined semiclassical transport models [11] which give Lebed resonances and find that the resonances are still present for incoherent interlayer transport [26]. A much greater challenge than that considered here is to explain the angle-dependent magnetoresistance observed in (TMTSF)$_2$PF$_6$ at pressures of about 10 kbar [9,10]. In particular, the background magnetoresistance is smallest when the field is in the layers, the opposite of what one expects based on the simple Lorentz force arguments relevant to semiclassical magnetoresistance.

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