# Sensitivity of the interlayer magnetoresistance of layered metals to intralayer anisotropies

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Many of the most interesting and technologically important electronic materials discovered in the past two decades have both a layered crystal structure and strong interactions between electrons. Two fundamental questions about such layered metals concern the origin of intralayer anisotropies and the coherence of interlayer charge transport. We show that angle dependent magnetoresistance oscillations (AMROs) are sensitive to anisotropies around an intralayer Fermi surface and can hence be a complementary probe of such anisotropies to angle-resolved photoemission spectroscopy and scanning tunneling microscopy. However, AMROs are not very sensitive to the coherence of the interlayer transport which has implications for recent AMRO experiments on an overdoped cuprate.

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# I. INTRODUCTION

For elemental metals, such as tin and sodium, it is well established that a Fermi liquid description is valid. Thus, the Bloch wave vector is a good quantum number for electronic excitations and there is a well-defined three-dimensional Fermi surface (FS).<sup>1</sup> Any variation of properties over the FS is of secondary interest. In contrast, many layered metals (e.g., cuprates and layered manganites) are distinctly different. Their properties cannot be described in terms of a Fermi liquid picture.<sup>2</sup> Even when one sees signatures of an intralayer FS, suggesting quantum coherence of excitations within individual layers, there is controversy over what length and time scales the electronic excitations are coherent between layers.<sup>3</sup> Furthermore, in the cuprates, properties such as the pseudogap, the quasiparticle spectral weight, and scattering rate vary significantly over the intralayer FS.<sup>2</sup> These variations, also seen in angle-resolved photoemission spectroscopy (ARPES)<sup>4</sup> and scanning tunneling microscopy,<sup>5</sup> may be key to understanding the origin of the superconductivity and the unusual properties of the metallic and pseudogap phases.<sup>2</sup> Significant anisotropies in quasiparticle weight were also seen recently in layered manganites.<sup>6</sup> We show here how the dependence of the interlayer magnetoresistance on the magnetic field orientation is quite sensitive to intralayer anisotropies.

Angle dependent magnetoresistance oscillations. The dependence of the interlayer magnetoresistance on the magnetic field direction has been used to map out a threedimensional (3D) FS in a chemically diverse range of layered metals, including organic charge transfer salts,<sup>7,8</sup> ruthenates,<sup>9,10</sup> semiconductor heterostructures,<sup>11</sup> tungsten bronzes,<sup>12</sup> intercalated graphite,<sup>13</sup> and an overdoped thallium cuprate.<sup>14,15</sup> However, most of the observed angle dependent magnetoresistance oscillations (AMROs) are also consistent with a two-dimensional FS, i.e., a FS existing only within the individual layers and weakly incoherent interlayer transport.<sup>16</sup> Hence, it is difficult to experimentally distinguish the two physically distinct pictures summarized in Fig. 1.<sup>16</sup> AMROs are essentially a geometric resonance involving the cyclotron orbits projected onto the plane parallel to the layers.<sup>17</sup> In this sense, they are similar to geometric commensurability oscillations in magnetoresistance seen for two-dimensional electron gases in semiconductor heterostructures.<sup>18–20</sup>

In this paper, we present the following results for interlayer magnetotransport in a layered Fermi liquid metal. (i) We give a general expression for the interlayer conductivity in a tilted magnetic field including the effects of anisotropy around the FS of the Fermi wave vector, Fermi velocity, scattering rate, quasiparticle weight, and interlayer hopping integral. (ii) We derive (i) for both coherent interlayer transport (a three-dimensional FS) and for weakly incoherent interlayer transport (where the FS is only well defined within the layers) (see Fig. 1). Furthermore, we elucidate the physics behind why the same result is obtained for both types of interlayer transport.<sup>21</sup> (iii) Our results show that a threedimensional FS is not necessary to give a quantitative description of AMRO experiments on an overdoped cuprate.<sup>14</sup> The data can be reproduced by the weakly incoherent model. Others have considered the effect on AMRO of various specific anisotropies and specific field directions,<sup>7,10,22,23</sup> but not the general case considered here.

The paper is structured as follows. In Sec. II, we introduce the anisotropies in FS properties that we consider and state our main result [Eq. (9)] for interlayer conductivity in the presence of these anisotropies. In Sec. III, we discuss the derivation of our main result for the interlayer conductivity for both coherent and weakly incoherent interlayer transport. In Sec. IV, we explore the implications of these results for AMRO experiments on thallium cuprate.<sup>14</sup> Finally, in Sec. V, we conclude and give a discussion of our results.

## II. ANISOTROPIES IN THE FERMI SURFACE AND TRANSPORT

There are a number of FS properties that can be anisotropic in layered metals. We discuss intralayer anisotropy in the Fermi surface, dispersion and in-plane scattering, and anisotropy in the interlayer hopping. All these anisotropies have been considered in earlier works, but not simultaneously, which is the generic situation.



FIG. 1. (Color online) Two pictures of interlayer transport. (a) The Fermi surface (FS) is three dimensional and warped by the quantum coherence of electron transport between layers and the variation of the interlayer hopping with the intralayer wave vector (Refs. 10 and 14). (b) The FS is only well defined within individual layers. The interlayer transport is weakly incoherent, i.e., momentum parallel to the layers is conserved but coherence is only between neighboring layers. The thickness of the line is proportional to the magnitude of the interlayer hopping.

We will consider the interlayer conductivity in a tilted magnetic field,

$$\mathbf{B} = B(\sin \theta \cos \varphi, \sin \theta \sin \varphi, \cos \theta), \tag{1}$$

which is at an angle  $\theta$  to the *c* axis and makes an azimuthal angle  $\varphi$  to the *a* axis in the *ab* plane (see the inset of Fig. 2).

#### A. Intralayer anisotropies

We use the angle  $\phi$  to parametrize the intralayer FS defined by

$$\mathbf{k}_F(\phi) = k_F(\phi)(\sin\phi, \cos\phi). \tag{2}$$

For an anisotropic in-plane dispersion,  $\epsilon_{2D}(k_x, k_y)$ , the Fermi wave vector  $\mathbf{k}_F$ , which maps out a surface (strictly speaking, a curve) of constant energy surface, is defined by  $\epsilon_{2D}(\mathbf{k}_F(\phi)) = E_F$ , where  $E_F$  is the Fermi energy. The Fermi velocity is defined by



FIG. 2. (Color online) Calculated angular dependence of the interlayer resistance for several different azimuthal angles. The parameters are chosen (see Sec. IV for precise parametrization) so that the calculated curves agree essentially perfectly with the measured curves for the overdoped cuprate Tl2201 (Ref. 14). The inset shows the direction of the magnetic field relative to the layers of the crystal.

$$\mathbf{v}_{F}(\varphi) = \frac{1}{\hbar} \left. \frac{\partial \epsilon}{\partial \mathbf{k}} \right|_{\mathbf{k}=\mathbf{k}_{F}}$$
(3)

and is always normal to the Fermi surface. Hence, if there is intralayer anisotropy in the dispersion relation, there must also be anisotropy in *both* the Fermi surface and the Fermi velocity.

*Cyclotron frequency.* The semiclassical equations of motion<sup>1</sup> for an electron moving on the intralayer FS in a magnetic field with component  $B \cos \theta$  perpendicular to the layers can be solved given the variation of the angular speed due to cyclotron motion around the intralayer FS as

$$\omega_0(\phi) = eB \cos \theta \frac{\mathbf{k}_F(\phi) \cdot \mathbf{v}_F(\phi)}{\hbar k_F(\phi)^2},\tag{4}$$

where  $\mathbf{v}_F(\phi)$  is the Fermi velocity. For a circular FS,  $\omega_0(\phi)$  has a constant value,  $\omega_c \cos \theta$ , with  $\omega_c = eB/m^*$  the cyclotron frequency. However, for an anisotropic FS,  $\mathbf{k}_F$  and  $\mathbf{v}_F$  are not parallel and  $\omega_0(\phi)$  will vary around the FS.

Scattering rate. The variation of the transport lifetime over the FS is given by  $\tau(\phi)$ . The probability of an electron not being scattered in moving between two points on the intralayer FS, defined by angles  $\phi_2$  and  $\phi_1$ , is

$$G(\phi_2, \phi_1) = \exp\left(-\int_{\phi_1}^{\phi_2} \frac{d\psi}{\omega_0(\psi)\tau(\psi)}\right).$$
 (5)

In what follows, an important quantity is  $P \equiv G(2\pi, 0)$ , the probability that an electron makes a complete orbit of the intralayer FS without being scattered.

*Interlayer hopping*. The Hamiltonian for hopping between the layers is

$$\mathcal{H}_{\perp} = \sum_{ij} t_{\perp} (\mathbf{r}_i - \mathbf{r}_j) [c_i^{\dagger} c_j e^{i\Phi_{ij}} + c_j^{\dagger} c_i e^{-i\Phi_{ij}}], \qquad (6)$$

where  $\Phi_{ij} = (ec/\hbar)[A_z(\mathbf{r}_i) - A_z(\mathbf{r}_j)]$  is the Aharonov-Bohm (AB) phase acquired by an electron hopping between  $\mathbf{r}_i$  in

one layer and  $\mathbf{r}_j$  in the other layer,<sup>17</sup> with layer separation *c* and  $\mathbf{A}_{\parallel} = A_z(\mathbf{r})\hat{\mathbf{z}} = \frac{1}{2}(\mathbf{B}_{\parallel} \times \mathbf{r})$  the vector potential for the magnetic field parallel to the layers,  $\mathbf{B}_{\parallel}$ . Momentum anisotropy in  $t_{\perp}$  is present in the Fourier transform of the hopping matrix element  $t_{\perp}(\mathbf{r}_i - \mathbf{r}_j)$  via

$$t_{\perp}(\phi) = \int d^2 \mathbf{r} \exp(i\mathbf{k}_F(\phi) \cdot \mathbf{r}) t_{\perp}(\mathbf{r}).$$
(7)

In momentum space, the difference in AB phases acquired in hopping between layers for positions  $\phi_1$  and  $\phi_2$  on the FS is

$$\Phi(\phi_2, \phi_1) = c \tan \theta [k_F(\phi_1) \cos(\phi_1 - \varphi) - k_F(\phi_2) \cos(\phi_2 - \varphi)].$$
(8)

We will also see that for a coherent three-dimensional FS, this quantity can be related to the Bloch wave vector perpendicular to the layers [see Eq. (15) below].

### B. Main result

We now state the result central to this paper. The interlayer conductivity  $\sigma_c$  in a tilted magnetic field [Eq. (1)] at zero temperature is

$$\sigma_{c}(\theta,\varphi) = \frac{s_{0}eB\cos\theta}{(1-P)} \int_{0}^{2\pi} \frac{d\phi_{2}}{\omega_{0}(\phi_{2})} \int_{\phi_{2}-2\pi}^{\phi_{2}} \frac{d\phi_{1}}{\omega_{0}(\phi_{1})} \times t_{\perp}(\phi_{2})t_{\perp}(\phi_{1})\cos(\Phi(\phi_{1},\phi_{2}))G(\phi_{2},\phi_{1}), \quad (9)$$

where  $s_0 = (e^2 c / \pi^2 \hbar^4)$ . The factor 1/(1-P) in the conductivity comes from noting the  $2\pi$  periodicity of the integrand and reducing the integration region for  $\phi_1$ . The factor  $eB \cos \theta / \omega_0(\phi_2)$  can also be interpreted as anisotropy in the density of states.<sup>23</sup> Equation (9) does not explicitly take into account possible anisotropy in the quasiparticle weight  $Z(\phi)$ due to many-body effects. The hopping matrix elements  $t_{\perp}(\phi)$  should be understood as  $t_{\perp}(\phi) = Z(\phi)t_{\perp}^0(\phi)$ , where  $t_{\perp}^0(\phi)$  is the bare hopping. It should be stressed that Eq. (9) depends *only* on *intralayer* FS properties and holds irrespective of the particular form of those anisotropies.

In Sec. III, we give the derivation of this result both for coherent transport perpendicular to the layers and for weakly incoherent interlayer hopping (see Fig. 1), provided  $t_{\perp} \ll E_F$ . Below, in Fig. 2 we show the calculated AMRO for parameters that fit the experimental data for the overdoped thallium cuprate in Ref. 14. The fitting procedure in Ref. 14 allowed for anisotropy in the FS, but not in the Fermi velocity [i.e., in  $\omega_0(\phi)$ ] or in the intralayer scattering. Allowing for both of these factors, we find a very high quality, quantitative fit to the data, which for clarity of presentation is not shown since it lies virtually on top of our calculated magnetoresistance.

## C. Mapping out Fermi surface anisotropies at high magnetic fields

We now consider AMRO in high magnetic fields ( $\omega_{00}\tau_0 \gg 1$ ), since such experiments have previously been used to map out the FS for very clean organic materials.<sup>7,8,24</sup> When  $ck_F \tan \theta \gg 1$  and  $cv_F \tau_0 eB/\hbar^2 \gg 1$ , the method of steepest descents may be used to evaluate the integrals in Eq. (9).<sup>25</sup> The

integrals are dominated by the angles near  $\phi_0$  which is where the Fermi wave vector  $k_F(\phi)$  has the maximum projection along the direction of the intralayer magnetic field,  $\mathbf{b}_{\parallel} \equiv (\cos \varphi, \sin \varphi)$ .  $\phi_0$  is a  $\varphi$  dependent quantity and is found from the solution of

$$\frac{\partial}{\partial \phi} [\mathbf{b}_{\parallel}(\varphi) \cdot \mathbf{k}_{F}(\phi)] = 0.$$

This leads to

$$\sigma_{c}(\theta,\varphi) \simeq \frac{2\pi s_{0}}{(1-P)} \frac{t_{\perp}(\phi_{0})^{2}}{[\omega_{0}(\phi_{0})]^{2}} \frac{eB\cos\theta}{|\mu(\phi_{0})|c\,\tan\theta} \times [1+2P^{1/2}\sin(2c\,\tan\theta\mathbf{b}_{\parallel}(\varphi)\cdot\mathbf{k}_{F}(\phi_{0}))],$$
(10)

where  $\mu(\phi) = \frac{\partial^2}{\partial \phi^2} [\mathbf{b}_{\parallel}(\varphi) \cdot \mathbf{k}_F(\phi)]$ . This expression shows that the interlayer magnetoresistance oscillates as a function of the field tilt angle, and for a fixed value of  $\varphi$  the magnetoresistance will be a maximum when the field is at angles  $\theta_n$  given by<sup>7,24,25</sup>

$$\mathbf{b}_{\parallel}(\boldsymbol{\varphi}) \cdot \mathbf{k}_{F}(\boldsymbol{\phi}_{0})c \tan \theta_{n} = \pi(n - 1/4), \quad (11)$$

where n=1,2,... This expression has been used to map out the intralayer FS for a wide range of metallic organic charge transfer salts.<sup>7,24</sup> We point out that our expression (10) will also be sensitive to angular variations in the interlayer hopping and cyclotron frequency. Interestingly, when  $\omega_{00}\tau_0 \ge 1$ , there is no  $\phi_0$  dependence from the angular variation in the scattering rate since the only dependence on the scattering rate is through the quantity *P*, which involves an average over the FS. Hence, the FS shape may be determined independent of scattering, which can then be used to determine the anisotropy in scattering at smaller fields.<sup>26</sup>

### III. DERIVATIONS FOR COHERENT AND INCOHERENT INTERLAYER TRANSPORT

We now sketch the derivation of Eq. (9) for the cases of coherent and weakly incoherent interlayer transport.

#### A. Coherent interlayer transport

If  $t_{\perp} \gg \hbar/\tau$ , then there is a well-defined Bloch wave vector perpendicular to the layers,  $k_z$ , and the three-dimensional dispersion is

$$\mathcal{E}_{3D} = \mathcal{E}_{2D}(k_x, k_y) - 2t_{\perp}^0(k_x, k_y)\cos(ck_z).$$
(12)

To obtain Eq. (9) within a picture of coherent interlayer transport, one starts from the dispersion, which can be used to determine the Fermi velocity, and semiclassical equations of motion for motion on the FS. Solution of the appropriate Boltzmann equation, to leading order in  $(t_{\perp}/E_F)^2$ , leads to Eq. (9) as a generalization of the Shockley-Chamber (SC) formula.<sup>1,27</sup>

A useful relation between the projection of the motion in real space onto the plane of the layers and *c*-axis momentum (where  $\mathbf{R}_{\parallel}$  is the position in the plane) comes from considering the equation of motion (we neglect higher order terms in  $t_{\perp}/E_F$ ). Integrating to get in-plane and *c*-axis momentum gives

$$\mathbf{k}_{\parallel}(t) = \mathbf{k}_{\parallel}(0) + \frac{eB_{\perp}}{\hbar} [\mathbf{R}_{\parallel}(t) - \mathbf{R}_{\parallel}(0)] \times \hat{\mathbf{z}}, \qquad (13)$$

$$k_{z}(t) = k_{z}(0) + \frac{\mathbf{B}_{\parallel} \cdot [\mathbf{k}_{\parallel}(t) - \mathbf{k}_{\parallel}(0)]}{B_{\perp}}.$$
 (14)

Hence, the interlayer velocity is

$$v_{z}(\phi) = \frac{2ct_{\perp}^{0}(\phi)}{\hbar} \sin(ck_{z}(0) + ck_{F}(\phi)\tan\theta\cos(\phi - \phi)).$$
(15)

The SC formula<sup>1</sup> involves correlations in this velocity at different times (equivalently different  $\phi$ ),

$$\sigma = \frac{e^2}{4\pi^3} \int d^3 \mathbf{k}_1 v_z(\mathbf{k}_1) \left(-\frac{\partial f_T}{\partial \epsilon}\right) \int_{-\infty}^{\phi_1} d\phi_2 \frac{v_z(\phi_2)}{\omega_2(\phi_2)} G(\phi_2, \phi_1),$$
(16)

where  $G(\phi_2, \phi_1)$  was defined in Eq. (5),  $f_T$  is the Fermi-Dirac distribution, and the limits of integration for  $k_z$  are between  $\pm \frac{\pi}{c}$ . The expressions in Eqs. (13)–(15) [when the integral over  $k_z$  is performed in Eq. (16)] allow one to see how the term associated with an Aharonov-Bohm phase for weakly incoherent transport [see Eq. (8)] arises for coherent interlayer transport.<sup>17</sup>

#### B. Weakly incoherent interlayer transport

The interlayer current at  $\mathbf{r}_1$  from layer 2 is<sup>28</sup>

$$j_{\perp}(\mathbf{r}_{1}) = ie \int d^{2}\mathbf{r}_{2}t_{\perp}(\mathbf{r}_{1} - \mathbf{r}_{2})[c_{2}^{\dagger}(\mathbf{r}_{2})c_{1}(\mathbf{r}_{1})e^{i\Phi_{12}} - \text{H.c.}],$$

where  $\Phi_{12}$  is the gauge phase for hopping between the layers. Note that  $t_{\perp}(\mathbf{r}_1, \mathbf{r}_2)$  contains the variation of the interlayer hopping over the FS [Eq. (7)].

In linear response, the Kubo formula for the interlayer conductivity at zero temperature  $is^{16,28}$ 

$$\sigma_{c} = \frac{2ce^{2}}{\hbar L_{x}L_{y}} \operatorname{Re}\left[\int d^{2}\mathbf{r}_{1} \int d^{2}\mathbf{r}_{2} \int d^{2}\mathbf{r}_{3} \int d^{2}\mathbf{r}_{4}t_{\perp}(\mathbf{r}_{1},\mathbf{r}_{4}) \times t_{\perp}(\mathbf{r}_{3},\mathbf{r}_{2})e^{i(\Phi_{12}-\Phi_{34})}K_{E_{F}}(\mathbf{r}_{1},\mathbf{r}_{2},\mathbf{r}_{3},\mathbf{r}_{4})\right], \qquad (17)$$

where<sup>29</sup>  $K_{\epsilon}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3, \mathbf{r}_4) = G_{2,\epsilon}^R(\mathbf{r}_1, \mathbf{r}_2)G_{1,\epsilon}^A(\mathbf{r}_3, \mathbf{r}_4)$  and  $G_{1,\epsilon}^R$  is the retarded one-electron Green's function within layer 1. Now,  $K_{\epsilon}$  oscillates rapidly as a function of the spatial coordinates, with a period comparable to the Fermi wavelength. We can separate the nonoscillatory part by introducing coordinates  $\mathbf{R}_1 = \frac{1}{2}(\mathbf{r}_1 + \mathbf{r}_4)$  and  $\mathbf{R}_2 = \frac{1}{2}(\mathbf{r}_2 + \mathbf{r}_3)$  and write

$$K_{\epsilon}(\mathbf{r}_{1},\mathbf{r}_{2},\mathbf{r}_{3},\mathbf{r}_{4}) = \int \frac{d^{2}\mathbf{k}_{1}}{(2\pi)^{2}} \int \frac{d^{2}\mathbf{k}_{2}}{(2\pi)^{2}} K_{\epsilon}(\mathbf{k}_{1},\mathbf{R}_{1};\mathbf{k}_{2},\mathbf{R}_{2})$$
$$\times e^{i\mathbf{k}_{1}\cdot(\mathbf{r}_{1}-\mathbf{r}_{4})+i\mathbf{k}_{2}\cdot(\mathbf{r}_{3}-\mathbf{r}_{2})}.$$
(18)

We use a semiclassical approximation since  $K_{\epsilon}$  will be

sharply peaked at energies around the Fermi energy, which enforces the condition that the magnitude of the momentum in the Fourier transform is  $\phi$  dependent and lies on the FS and then  $K_{\epsilon}(\mathbf{k}_F(\phi_1), \mathbf{R}_1; \mathbf{k}_F(\phi_2), \mathbf{R}_2)$  satisfies the Boltzmanntype equation for a diffuson:<sup>29</sup>

$$\begin{bmatrix} \mathbf{v}_F(\phi_2) \cdot \frac{\partial}{\partial \mathbf{R}_2} + \omega_0(\phi_2) \frac{\partial}{\partial \phi_2} - \frac{1}{\tau(\phi_2)} \end{bmatrix} K_{E_F}(\phi_1, \mathbf{R}_1; \phi_2, \mathbf{R}_2)$$
$$= 2\pi \frac{\omega_0(\phi_1)}{eB \cos \theta} \delta(\phi_1 - \phi_2) \delta(\mathbf{R}_1 - \mathbf{R}_2),$$

where the factor of  $\omega_0$  on the right hand side of the equation comes from noting that the Boltzmann equation is initially stated with  $\delta^2(\mathbf{k}_1 - \mathbf{k}_2)$  on the right hand side. We can solve this equation for *K* by Fourier transforming to get a solution in terms of

$$K(\phi_1, \mathbf{R}_1; \phi_2, \mathbf{q}) = \int \frac{d^2 \mathbf{q}}{(2\pi)^2} e^{i\mathbf{q}\cdot\mathbf{R}_2} K(\phi_1, \mathbf{R}_1; \phi_2, \mathbf{R}_2), \quad (19)$$

and then

$$K(\phi_{1}, \mathbf{R}_{1}; \phi_{2}, \mathbf{q}) = 2\pi e^{-i\mathbf{q}\cdot\mathbf{R}_{1}} \int_{-\infty}^{\phi_{2}} d\widetilde{\phi} \frac{\delta(\phi_{1} - \widetilde{\phi})}{\omega_{0}(\widetilde{\phi})} \frac{\omega_{0}(\phi_{1})}{eB\cos\theta}$$
$$\times \exp\left[-\int_{\phi_{2}}^{\widetilde{\phi}} \frac{d\psi}{\omega_{0}(\psi)\tau(\psi)}\right]$$
$$\times \exp\left[i\mathbf{q}\cdot\int_{\phi_{2}}^{\widetilde{\phi}} \frac{\mathbf{v}_{F}(\psi)}{\omega_{0}(\psi)}d\psi\right], \qquad (20)$$

where we can note that

$$\int_{\phi_2}^{\overline{\phi}} \frac{\mathbf{v}_F(\psi)}{\omega_0(\psi)} d\psi = \mathbf{R}_{\parallel}(\widetilde{\phi}) - \mathbf{R}_{\parallel}(\phi_2).$$

Inserting this solution into Eq. (17), using Eq. (13), and integrating over  $\mathbf{R}_1$  and  $\mathbf{R}_2$  forces

$$\Phi = \Phi_{12} - \Phi_{34} = c \tan \theta (k_F(\phi_2)\cos(\phi_2 - \varphi) - k_F(\phi_1) \times \cos(\phi_1 - \varphi)).$$

So, we get as our final result

$$\sigma_{c} = \frac{2ce^{2}}{\hbar L_{x}L_{y}} \operatorname{Re} \int_{0}^{2\pi} d\phi_{2} \int_{-\infty}^{\phi_{2}} d\phi_{1} \int d\mathbf{R}_{1} \int d\mathbf{R}_{2} \frac{eB\cos\theta}{\omega_{0}(\phi_{1})}$$
$$\times \frac{eB\cos\theta}{\omega_{0}(\phi_{2})} t_{\perp}(\phi_{1})t_{\perp}(\phi_{2})\cos[\Phi]K_{\epsilon}(\phi_{1},\mathbf{R}_{1};\phi_{2},\mathbf{R}_{2}),$$
(21)

which is identical to the equation found with the Boltzmann equation for coherent transport in Eq. (9) after using periodicity of the integrand to reduce the interval of integration over  $\phi_1$  to have length  $2\pi$ .

### **IV. AMRO IN THALLIUM CUPRATES**

In Secs. II and III, we established Eq. (9) for general forms of anisotropy and interlayer transport mechanisms. To



FIG. 3. (Color online) Calculated angular dependence of the interlayer magnetoresistance for several different azimuthal angles, based on Eq. (9). The parameter values used were  $\eta_1 = 0.675$ ,  $t_{\perp}^0 \approx 13$  meV,  $ck_F^0 = 8.64$ , and  $\omega_{00}\tau_0 = 0.45$ . In (a),  $\alpha = 0.0$ ,  $\kappa = 0.0$ , and u = 0.0, as defined in Eqs. (22)–(25). In (b), we allow anisotropy in  $k_F$ , with  $\kappa = -0.033$ . In (c), we allow anisotropy in  $k_F$  and  $\omega_0$  with  $\kappa = -0.033$  and u = -0.08.

illustrate the use of Eq. (9) and its significance, we fit recent AMRO measurements of a thallium cuprate.<sup>14,15</sup> An important point to note about these experiments is that the data are of very high quality and it is thus possible to fit AMRO to very high precision, which leads to extraction of FS parameters to high accuracy.

Numerical evaluation of Eq. (9) shows that changing the functional forms of the anisotropy in interlayer hopping and intralayer scattering leads to quantitative variations in the AMRO. This can be seen in Figs. 3(a)-3(c) as we add in anisotropies to our fitting of AMRO. To extract deviations of

the FS from circularity in a self-consistent manner from AMRO experiments, one must also take into account the related anisotropy in the Fermi velocity and the resulting anisotropy in the angular speed [see Eq. (4)]. In previous work,<sup>10,14</sup> such effects were not included in the expressions used for fitting experimental data. This omission quantitatively changes the magnitude of anisotropies in  $k_F$  extracted from the fits. Similarly, a self-consistent determination of anisotropy in  $\tau(\phi)$  also requires including anisotropy in  $\omega_0(\phi)$ .

### Model forms for anisotropy in thallium cuprates

We use a form of  $t_{\perp}(\phi)$  which is consistent with the bodycentered-tetragonal crystal structure of thallium cuprate and band structure calculations:<sup>14,30</sup>

$$t_{\perp}(\phi) = t_{\perp}[\sin(2\phi) + \eta_1 \sin(6\phi) + \eta_2 \sin(10\phi)], \quad (22)$$

parametrized by  $\eta_1$  and  $\eta_2$ . The crystal symmetry requires that  $t_{\perp}(\phi) = -t_{\perp}(\phi + \pi/2)$ , implying  $\eta_1 = 1 + \eta_2$ , and that  $t_{\perp}(\phi)$  has eightfold symmetry and vanishes at  $\phi = \frac{n\pi}{4}$ ,  $n = 0, 1, \dots, 7$ .

A number of experiments on the cuprates suggest that the scattering rate has a fourfold variation around the Fermi surface. Such variations are also seen in calculations for a doped Hubbard model, using cellular dynamical mean-field theory.<sup>31</sup> A simple hot or cold spot model of scattering<sup>32,33</sup> yields

$$\frac{1}{\tau(\phi)} = \frac{1}{\tau_0} [1 + \alpha \cos(4\phi)],$$
 (23)

where  $\alpha > 0$  for cold spots located at  $\phi = \pm \frac{\pi}{2}, \pm \frac{3\pi}{2}$ . We parametrize the anisotropy in the FS and the cyclotron frequency as

$$k_F(\phi) = k_F^0 [1 + \kappa \cos(4\phi)], \qquad (24)$$

$$\frac{1}{\omega_0(\phi)} = \frac{1}{\omega_{00}} [1 + u\cos(4\phi)].$$
(25)

In Fig. 3, we show the effects of adding various anisotropies to the calculated AMRO. In Fig. 3(a), we show the calculated AMRO only allowing for anisotropic interlayer hopping. This demonstrates that much of the overall form of the magnetoresistance curves is determined by the presence of the eight nodes in the interlayer hopping [Eq. (22)]. Due to this symmetry, we only display AMRO for  $\varphi \in [0, \frac{\pi}{4}]$ . In Fig. 3(b), we add the effects of an anisotropic  $k_F$  which can be seen to depress  $\rho_c(\theta)$  for small  $\varphi$  at large  $\theta$  and enhance  $\rho_c(\theta)$  for larger  $\varphi$  (up to  $\frac{\pi}{4}$ ) at large  $\theta$ . In Fig. 3(c), we make our fit self-consistent by also allowing for anisotropy in  $\omega_0$ , which tends to reduce  $\rho_c(\theta)$  at larger  $\theta$  for larger  $\varphi$ . When we also include scattering anisotropy, we recover the fit that we displayed in Fig. 2 for the following set of parameters:  $\eta_1$ =0.675,  $t_{\perp}^0 \simeq 13$  meV,  $ck_F^0 = 8.64$ ,  $\omega_{00}\tau_0 = 0.45$ ,  $\kappa = -0.033$ , u=-0.08, and  $\alpha = 0.01$ .

The effect of anisotropic scattering on the shape of the curves is most pronounced at large values of  $\theta$  and on the

height of the peak in  $\rho_c(\theta)$  at  $\theta \sim 40^\circ$ , for  $\varphi \sim 0^\circ$ . We use a small value of  $\alpha$  here to fit the data, but larger values tend to be required at higher temperatures.<sup>15</sup> Increasing  $\alpha$  also increases the value of  $\rho(\theta=0)=\rho_0$ .

For the overdoped cuprate we consider, a tight-binding model for the intralayer bands has been fitted to ARPES data for a sample of similar chemical composition.<sup>34</sup> We use this model as an independent check of the reliability of the values we obtain for  $k_F^0$ ,  $\omega_0$ , u, and  $\kappa$ . The tight-binding fit gives comparable values, which increases confidence that the extraction of anisotropies from AMRO is robust.

Equation (9) is valid for both coherent and weakly incoherent transport between layers, except in a small region near  $\theta$ =90°. For coherent transport, but not for incoherent transport, there is a peak in the resistivity at  $\theta = 90^{\circ}$  due to orbits on the 3D FS that do not exist if one can only define a two-dimensional (2D) FS within the layers.<sup>7,16</sup> A second definitive signature of coherent interlayer transport is beats in quantum magnetic oscillations,<sup>16</sup> but these have not been seen in thallium cuprate. For the samples in Ref. 14,  $t_{\perp}$  and  $\hbar/\tau_0$  are of the same order, which would place them at the boundary between coherent and incoherent interlayer transport. However,  $\omega_{00}\tau_0$  is insufficiently large to be able to see either of these definitive signatures of coherence. This implies that further evidence is required to validate the claim of a 3D FS in Ref. 14, and so a 3D FS is not necessary to explain the AMRO data in Ref. 14.

### **V. DISCUSSION**

In conclusion, we have given a general formula for AMRO in layered metals which have anisotropy in interlayer tunneling and in intralayer scattering and an anisotropic FS. We have performed explicit calculations for parameters relevant to experiments on thallium cuprate<sup>14</sup> and have shown that these do not, on their own, imply the coherence of interlayer transport. These fits are very sensitive to the anisotropies of intralayer properties.

While we have focused our attention on the example of AMRO in thallium cuprate, our results have a much wider applicability, in fact, to any layered metal with an anisotropic Fermi surface and anisotropic scattering. Our results have been stated for quasi-two-dimensional systems, but it should be fairly straightforward to generalize our results to quasione-dimensional systems such as Bechgaard salts, for which there is a substantial amount of AMRO data.<sup>7,8</sup> We also discuss how AMRO can be used in conjunction with other techniques such as ARPES to place strong constraints on FS properties. Combined AMRO and ARPES studies of layered metals could give a strong consistency check for the results of both techniques and this suggests many future opportunities ahead for AMRO as a powerful probe of anisotropies in layered metals. In particular, for superconducting organic charge transfer salts, a characterization of intralayer anisotropies could reveal the presence of a pseudogap with *d*-wave symmetry, as predicted by a resonating valence bond theory of these materials.<sup>35</sup>

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