Comment on "Anisotropic scattering in angular-dependent magnetoresistance oscillations of quasi-two-dimensional and quasi-one-dimensional metals: Beyond the relaxation-time approximation"

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Recently, Smith and McKenzie [Phys. Rev. B **77**, 235123 (2008)] used Boltzmann theory to calculate expressions for the interlayer resistivity in quasi-one-dimensional and quasi-two-dimensional metals for an arbitrary elastic collision integral. In this Comment I point out that their treatment of the equations of motion leads to an error in their expressions, and I derive corrected expressions for the interlayer conductivity in quasi-one-dimensional and quasi-two-dimensional metals in the presence of anisotropic scattering.

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In recent work, Smith and McKenzie[1] have calculated expressions for the interlayer conductivity in quasi-one-dimensional and quasi-two-dimensional metals when scattering is anisotropic in momentum space. Smith and McKenzie give expressions for the finite frequency and dc resistivity that generalize existing expressions.[2,3] These expressions are obtained from solving the Boltzmann equation for the electron distribution function and solving the equations of motion for the electron velocity in the z direction, and combining these to calculate the interlayer conductivity. In this Comment, I point out that the approach taken to the equations of motion by Smith and McKenzie leads them to derive incorrect expressions for the conductivity. I provide a derivation of correct expressions for the interlayer conductivity for both quasi-one-dimensional and quasi-two-dimensional metals.

In the presence of spatially uniform, but potentially time-varying fields, the Boltzmann equation can be written as

$$\frac{\partial f}{\partial t} + \mathbf{F} \cdot \frac{\partial f}{\partial \mathbf{p}} = I[f], \tag{1}$$

where $I[f]$ is the collision integral and $f(p_x,p_y,p_z,t)$ is the distribution function. I now discuss the solution of the Boltzmann equation to determine the c-axis conductivity in quasi-one-dimensional and quasi-two-dimensional metals.

In order to solve the Boltzmann equation for a quasi-two-dimensional metal, we need to specify the dispersion, which we take to have the same form as in Ref. 1

$$\epsilon = \frac{1}{2m^*}(k_x^2 + k_y^2) - 2t_c \cos(k_z c), \tag{2}$$

where m^* is the electron effective mass, t_c is the interlayer hopping along the c axis, and c is the layer spacing. For a quasi-two-dimensional metal $t_c \ll \epsilon_F$, where ϵ_F is the Fermi energy. For an electron subject to a magnetic field oriented in the x-z plane, at an angle θ_B to the z axis, then to lowest order in t_c, the equations of motion are

$$\mathbf{F} = \frac{d\mathbf{p}}{dt} = \hbar \frac{d\mathbf{k}}{dt} = \omega_c(-k_y, k_x, \tan\theta_B k_y),$$

where $\omega_c = \frac{eB}{m^*}\cos\theta_B$. It is convenient to make the change in variables $k_x = k\cos\phi$, $k_y = k\sin\phi$, and then k is a constant of the motion, and

$$\frac{d\phi}{dt} = \omega_c.$$

The equation of motion for k_z can be written as

$$\frac{dk_z}{d\phi} = \frac{dk_z}{dt}\frac{dt}{d\phi} = k\tan\theta_B \sin\phi,$$

which has the solution $k_z(\phi) = k_z^0 - k\tan\theta_B\cos\phi$, where k_z^0 is a constant of integration. As k_z is a function of k_z^0 and ϕ, it is possible to change variables in the distribution function from

$$(k_x,k_y,k_z) \to (k,\phi,k_z^0).$$

For $t_c \ll \epsilon_F$, we can relate k directly to the energy ϵ, and we can consider $f(k_x,k_y,k_z,t)$ as $f(\epsilon,\phi,k_z^0,t)$. Define

$$g(\phi,k_z^0,t) = \int d\epsilon\, f(\epsilon,\phi,k_z^0,t),$$

and integrate the Boltzmann equation over energy. In the presence of an electric field along the z direction it takes the form

$$\frac{\partial g}{\partial t} + \omega_c \frac{\partial g}{\partial \phi} - I[g] = -eE_z(t)v_z(\phi,k_z^0), \tag{3}$$

where

$$v_z(\phi,k_z^0) = \frac{1}{\hbar}\frac{\partial \epsilon}{\partial k_z} = \frac{2ct_c}{\hbar}\sin(ck_z)$$
$$= \frac{2ct_c}{\hbar}\sin(ck_z^0 - ck_F\tan\theta_B\cos\phi).$$

Equation (3) highlights a distinction between the calculation above and that performed in Ref. 1, where the analogous equation, Eq. (14), contains only one partial derivative term, rather than two. [The equations would be equivalent if the electric field considered in Ref. 1 were time independent as

the time derivative in Eq. (3) would vanish in the equation for the steady-state distribution function. In this case, where the Boltzmann equation is the same, the results still differ.]

The issue that leads to incorrect results in Ref. 1 is the treatment of the solutions of the equations of motion. The authors obtain solutions for k_z and ϕ in terms of the variable t and introduce two constants of integration in doing so. However, the variable t in the equations of motion (as far as the Boltzmann equation is concerned) should be understood as a parameter with the units of time, that parametrizes the motion, rather than the physical time, which enters elsewhere in the Boltzmann equation. This is not immediately obvious when starting from a semiclassical point of view but is required if the Boltzmann equation is to correspond to the semiclassical limit of the quantum kinetic equation.[4]

The consequence of this can be easily seen in the case of a dc electric field, although the same problems persist for time-dependent electric fields. For time-independent fields, the steady-state distribution function (which is used to determine the steady-state current, and hence conductivity) depends only on the independent variables (k_x,k_y,k_z), which, after changes in variable and integration over energy, lead to a distribution function g which depends on just two independent variables: ϕ and k_z^0.[5] However, the approach of the authors of Ref. 1 leads to a distribution function g which for a dc electric field depends on three variables: $k_z(0)$, $\phi(0)$, and t, all of which are treated as independent. This mathematical issue, in which a function of two independent variables is represented by a function of three independent variables, leads to the incorrect results for the conductivity obtained in Ref. 1. The variables t, $\phi(0)$, and $k_z(0)$ used in Ref. 1 are related to ϕ and k_z^0 in the presentation I have given above by

$$t = \frac{\phi - \phi(0)}{\omega_c}, \quad k_z^0 = k_z(0) + k_F \tan\theta \cos[\phi(0)].$$

Note that t, as used in Ref. 1, plays a similar role to ϕ in the presentation I have given. This is not uncommon usage in the literature on magnetic oscillations and interlayer resistance in layered metals,[6,7] and the distinction between t and physical time is noted by Abrikosov.[6] Once the extra independent variable is introduced into the calculation in Ref. 1, there is an extra integration in the calculation of the interlayer conductivity over $\phi(0)$, which leads to an expression that involves a sum over a product of four Bessel functions rather than an expression involving a sum over a product of two Bessel functions, which I derive below.

I now provide a derivation of the conductivity that does not suffer from the deficiencies identified above. The mechanics of the calculation are relatively similar to those in Ref. 1. For an ac electric field along the z direction I expand the distribution function g, the collision integral $I[g]$, and v_z in a similar way to Ref. 1, but using the variables k_z^0, ϕ, and t (note that ϕ and t are independent in my treatment). The expansions are as follows:

$$g(k_z^0,\phi,t) = \sum_{m,n} g_{mn}(t) e^{imck_z^0} e^{in\phi}, \tag{4}$$

$$v_z(k_z,\phi) = \sum_{m,n} u_{mn} e^{imck_z^0} e^{in\phi}, \tag{5}$$

$$I[g] = -\sum_{m,n} \lambda_{mn} g_{mn}(t) e^{imck_z^0} e^{in\phi}. \tag{6}$$

The coefficients λ_{mn} parametrize the anisotropic scattering and have the same meaning as in Ref. 1. For an electric field with magnitude E_z at frequency ω, one can substitute these into the Boltzmann equation and find

$$g_{mn}(\omega) = -\frac{eE_z u_{mn}}{in\omega_c - i\omega + \lambda_{mn}},$$

where (dropping the superscript on k_z^0)

$$u_{mn} = \int_0^{2\pi} \frac{d\phi}{2\pi} e^{-in\phi} \int_{-\pi/c}^{\pi/c} \frac{dk_z}{2\pi} e^{-imck_z} v_z(\phi,k_z)$$

$$= \frac{t_c c}{i\hbar} \sum_{s=-\infty}^{\infty} J_s(ck_F \tan\theta)\{\delta_{m,1}\delta_{n,s} e^{-is(\pi/2)} - \delta_{m,-1}\delta_{n,-s} e^{is(\pi/2)}\}. \tag{7}$$

A standard calculation of the conductivity leads to the following expressions for real and imaginary parts of the conductivity:

$$\mathrm{Re}\left[\frac{\sigma_{zz}(\omega)}{\sigma_0\lambda_0}\right] = \sum_{n=-\infty}^{\infty} \lambda_n \frac{[J_n(ck_F \tan\theta_B)]^2}{\lambda_n^2 + (\omega - n\omega_c)^2}, \tag{8}$$

$$\mathrm{Im}\left[\frac{\sigma_{zz}(\omega)}{\sigma_0\lambda_0}\right] = \sum_{n=-\infty}^{\infty} \frac{(\omega - n\omega_c)[J_n(ck_F \tan\theta_B)]^2}{\lambda_n^2 + (\omega - n\omega_c)^2}, \tag{9}$$

where, as noted in Ref. 1,

$$\sigma_0 = \frac{2e^2 t_c^2 c k_F}{\pi\hbar^3 v_F} \frac{1}{\lambda_0}$$

is the zero-field c-axis conductivity and $\lambda_n = \lambda_{\pm 1 n}$. This expression should be contrasted with the results for the real part of the conductivity presented in Ref. 1, in which the sums are over products of four Bessel functions rather than two Bessel functions. If the frequency ω is taken to zero, then the dc conductivity becomes

$$\frac{\sigma_{\mathrm{dc}}}{\sigma_0\lambda_0} = \sum_{n=-\infty}^{\infty} \frac{\lambda_n [J_n(ck_F \tan\theta_B)]^2}{\lambda_n^2 + (n\omega_c)^2}. \tag{10}$$

In the limit that all of the λ_n are equal, corresponding to isotropic scattering, Eq. (10) reduces to the well-known expression for angle-dependent magnetoresistance oscillations (AMRO).[8] This is also true of the expression obtained in Ref. 1—the issues raised here only affect calculations of the conductivity for anisotropic scattering.

In a quasi-one-dimensional metal, there is hopping along both y and z directions, and the dispersion takes the form

$$\epsilon = v_F|k_x| - 2t_b \cos(bk_y) - 2t_c \cos(ck_z),$$

where t_b is the hopping in the y direction and b is the lattice spacing in this direction. The analysis in Ref. 1 of this case

suffers from the same mathematical problem identified for the quasi-two-dimensional case above and following through a similar calculation for the conductivity to that outlined above, taking into account the fact that the Fermi surface consists of two sheets,[1] one arrives again at an expression for the conductivity that depends on sums of products of two Bessel functions, rather than sums of products of four Bessel functions. The final result for the frequency-dependent conductivity is

$$\mathrm{Re}\left[\frac{\sigma_{zz}(\omega)}{\sigma_0\lambda_0}\right] = \frac{1}{2}\sum_{\nu}\sum_{n=-\infty}^{\infty}\lambda_n^{\nu}\frac{\eta_\nu[J_n(\gamma)]^2}{[\lambda_n^{\nu}]^2+(\omega-n\omega_c)^2}, \quad (11)$$

$$\mathrm{Im}\left[\frac{\sigma_{zz}(\omega)}{\sigma_0\lambda_0}\right] = \frac{1}{2}\sum_{\nu}\sum_{n=-\infty}^{\infty}\frac{\eta_\nu(\omega-n\omega_c)[J_n(\gamma)]^2}{[\lambda_n^{\nu}]^2+(\omega-n\omega_c)^2}, \quad (12)$$

where $\gamma=(2t_bc/v_F)\tan\theta_B$, $\omega_c=(bev_FB/\hbar)\cos\theta_B$, and in the dc limit the conductivity simplifies to

$$\frac{\sigma_{\mathrm{dc}}}{\sigma_0\lambda_0} = \frac{1}{2}\sum_{n=-\infty}^{\infty}\frac{\eta_\nu\lambda_n^{\nu}[J_n(\gamma)]^2}{[\lambda_n^{\nu}]^2+(n\omega_c)^2}, \quad (13)$$

where $\nu=s$ or d labels the sum and difference contributions (relating to the two Fermi sheets) as introduced in Ref. 1, and $\eta_s=1+(-1)^n$, $\eta_d=1-(-1)^n$, with $\lambda_n^{\nu}=\lambda_{\pm 1n}^{\nu}$, similarly to the quasi-two-dimensional case. The constant

$$\sigma_0 = \frac{4e^2t_c^2c}{\pi b\hbar^3v_F}\frac{1}{\lambda_0},$$

which is in agreement with Ref. 8, correcting a missing factor of 2 in the expression in Ref. 1.

The expressions in Eqs. (10) and (13) lead to a very natural way to view the dc resistivity curve, as a sum of peaks indexed by n, whose width is determined by the parameter $\lambda_n/n\omega_c$, and whose height and position are determined by the magnitude and argument of the Bessel function, respectively. This separation of information, so that the nth peak gives information almost exclusively about the nth collision parameter, is actually less complicated than the picture presented in Ref. 1 and gives different quantitative predictions for the interlayer resistivity. These quantitative differences are important if the behavior of anisotropic scattering in quasi-one-dimensional and quasi-two-dimensional metals is to be extracted accurately from AMRO experiments for which momentum-dependent scattering is important.[9,10]

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