Reply to "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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In reply to the Comment by Kennett regarding our article [Phys. Rev. B **77**, 235123 (2008)], we clarify the key points at which we disagree with Kennett's derivation of the interlayer magnetoconductivity in layered metals and argue that our original derivation of this quantity is valid.

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In his Comment, Kennett claims that our derivation[1] of the interlayer magnetoconductivity in quasi-two-dimensional (2D) and quasi-one-dimensional (1D) metals with a momentum-dependent scattering potential is incorrect. He presents an alternative derivation, obtaining a different final expression for the conductivity $\sigma(\omega)$. The discrepancy arises in the simplest case of dc conductivity ($\omega=0$), and occurs in exactly the same way for 2D and 1D metals.[2] To most clearly illustrate the disagreement, we focus on the derivation of the dc conductivity in a 2D metal, commenting briefly on finite frequencies near the end.

In two unnumbered equations below Eq. (2K), then in Eq. (3K) of the Comment, Kennett writes the relevant electronic equation of motion and the Boltzmann equation, respectively. (We indicate an equation in Kennett's Comment by using the letter "K" after the equation number. An equation number without a K will always refer to an equation in this reply. Equation numbers in our original article will not be referenced.). As he notes, for dc fields these equations are the same as those appearing in our article.[1] So, our derivations proceed from an identical starting point.

The equations of motion are

$$\frac{d\phi}{dt'} = \omega_C \quad \frac{dk_z}{dt'} = k_f \omega_C \tan\theta_B \sin\phi, \tag{1}$$

where ω_C is the cyclotron frequency, k_f the radius of (the quasicylindrical) Fermi surface, and θ_B the orientation of magnetic field.

The general solution of this 2D equation of motion contains two arbitrary constants (here taken to be the initial values of the coordinates ϕ and k_z) and can be written

$$\phi(t') = \phi(0) + \omega_C t',$$

$$k_z(t') = k_z(0) - k_f \tan\theta_B \{\cos[\phi(t')] - \cos[\phi(0)]\}. \tag{2}$$

The rest of our derivation proceeds as follows (we refer to the same numbered steps when we discuss Kennett's derivation below): (I) substitute $k_z(t')$ into the interlayer velocity appearing in the Boltzmann equation, which is

$$\frac{\partial g}{\partial t'} + \omega_C^{-1} I[g] = -eE_z \omega_C^{-1} v_z[k_z]. \tag{3}$$

So the velocity $v_z(k_z)$ becomes $v_z(k_z[t'])$. Thus, the distribution g formally depends on three variables: t', $\phi[0]$ and $k_z(0)$ (i.e., all three appear in the Boltzmann equation that determines g). (II) Solve Eq. (3) for $g(\phi[0],k_z[0],t')$ via Fourier transform of all three variables. (III) Insert $g(\phi[0],k_z[0],t')$ into the expression for the current j_z. The current is an integral over all momenta so $k_z[0]$ and $\phi[0]$ are integrated to obtain a t'-dependent $j_z(t')$. The dc conductivity is obtained by taking a time-frequency Fourier transform and the $\omega \to 0$ limit.

At intermediate steps of this derivation, we employ a Fermi surface distribution function of three independent variables: $g(\phi[0],k_z[0],t')$. *Kennett states that this is not valid and, in his derivation, takes the distribution to depend on only two Fermi-surface momentum variables, which he calls* ϕ *and* k_z^0. However, since he started from the same 2D equation of motion that we did, he reaches his two-variable description by dropping an initial constant from the general solution of this equation. We believe that this is carried out in an arbitrary manner and leads him to an incorrect result for the conductivity. Thus, while we acknowledge that there are subtleties in our calculation (discussed below) we contend that our approach is on a more solid mathematical footing than Kennett's and that our final expression for the conductivity is more plausible. We justify our approach below. First we criticize Kennett's derivation.

As a solution to the equation of motion for k_z, Eq. (1), Kennett finds

$$k_z(\phi) = k_z^0 - k_f \tan\theta_B \cos\phi. \tag{4}$$

He makes the connection with the general solution above by assigning the variable k_z^0 the value

$$k_z^0 = k_z(0) + k_f \tan\theta_B \cos[\phi(0)] \quad \text{with} \quad \phi = \phi[0] + \omega_C t' \tag{5}$$

so the quantities k_z^0 and ϕ depend on the three parameters of the general solution.

Now, Kennett performs step I. But by using the quantity k_z^0 and making the additional substitution $\partial/\partial t' \to \omega_C \partial/\partial\phi$ he obtains a Boltzmann equation that appears to involve only

two momentum variables: k_z^0 and ϕ. (This is his Eq. (3K), with the first term absent for dc fields—note that Kennett's t variable is used only in the case of ac fields, which we are not discussing yet.) He seeks a two-variable distribution function $g(\phi,k_z^0)$ as the solution of the Boltzmann equation. But because ϕ and k_z^0 are functions of the three independent parameters originating from the Eq. (1), there is an implicit ambiguity in this description.

To illustrate the consequences of this ambiguity, consider the Fourier expansion [Eq. (4K)] used in step II

$$g(k_z^0,\phi) = \sum_{mn} g_{mn} \exp(imck_z^0 + in\phi), \tag{6}$$

where c is the lattice constant. If we substitute the expression for k_z^0 in terms of $k_z(0)$ and $\phi(0)$, then it is clear that different choices of the parameter $\phi(0)$ will give different values for the expansion coefficients. Indeed, it is easy to obtain the relation

$$g_{mn}[\phi(0)] = \exp\{-imk_f c \tan\theta_B \cos[\phi(0)]\} g_{mn}[\pi/2]. \tag{7}$$

So the expansion of the distribution function is not specified unless the value of $\phi[0]$ is fixed. By dropping the factor appearing on the right side of Eq. (7), Kennett is tacitly setting $\phi(0)=\pi/2$, though he gives no justification for this choice.

Kennett proceeds through step III where he does the momentum integral in the current j_z by integrating over k_z^0 and ϕ. This procedure amounts to integrating over *one* of the initial coordinates that appeared in the general solution of the equation of motion, while arbitrarily fixing the other. We see no mathematical justification for such an inconsistent treatment of two initial values that arose from the same source. We regard this as a flaw in Kennett's derivation and claim that his subsequent result for $\sigma(\omega)$ is not valid.

We now discuss the reasoning beyond our "three-variable" calculation. The general approach, and particularly the meaning of the time variable t' that appears in Eq. (1), is discussed in Ref. 3. There, it is noted that while the physical time appears in the equation of motion, $d\mathbf{k}/dt=-e\mathbf{v}\times\mathbf{B}-e\mathbf{E}$, the auxiliary time variable t' appears in the corresponding equation *without the electric field*. In the presence of a strong magnetic field and weak electric field there will exist a time scale over which electrons undergo cyclotron motion driven by the magnetic field without feeling any effect of the electric field. On this time scale, the auxiliary time variable t' will correspond exactly to the physical time t.

Equation (1) describes the real cyclotron motion of each thermally excited quasiparticle on this short time scale. The distribution function describes the population of all such orbiting electrons. On the Fermi surface $g[\phi(0),k_z(0),t']$ may be described as a function of three variables: two static momentum variables $\phi(0)$ and $k_z(0)$ and one time variable to describe the phase of the cyclotron motion. (Of course, periodic time dependence driven by the magnetic field does not threaten the stability of a steady state solution. A distribution can be time-independent on the long time scales over which the acceleration in the electric field, and compensating relaxation due to scattering, is relevant. This is enough to ensure a steady state.) Following this approach, as described above, one solves for the time-dependent distribution and current and takes a time-frequency Fourier transform to obtain dc magnetotransport coefficients.

We have confirmed that this approach can be used to obtain the established magnetoconductivity for metals in several geometries. As one example, it yields the known result[4] for the interlayer conductivity in layered metals in the limiting case of isotropic scattering, where the relaxation-time approximation (RTA) can be used. Kennett's conductivity expression also captures this limiting case, though the different manner in which our expression and his reduce to the RTA result is illuminating.

When the RTA is used in our derivation, cancellations of t'-dependent factors result in a current that is independent of t'. So, within the RTA, the ω-t' Fourier transform is trivial and the resulting conductivity has a single factor of a squared Bessel function that originates from the integral over $\phi(0)$. When we go beyond the RTA and use the full collision integral, $j_z(t')$ becomes (periodically) t'-dependent. Upon carrying out the time-frequency Fourier transform and $\omega\to 0$ limit, one obtains an extra squared Bessel function convoluted with the first [the first squared Bessel comes from the $\phi(0)$ integral, the second from the t' integral].

This result has an appealing physical interpretation. When one goes beyond the RTA, the effectiveness of a scattering process becomes dependent on the difference in the distribution at the initial and final scattering momenta. Thus, it is reasonable that one should find such an additional convolution of squared Bessel factors—a reflection of the fact that the conductivity is now sensitive to the value of the distribution at two different positions of the Fermi surface (in the RTA only a single $\mathbf{k}$ value of the distribution is relevant). Going beyond the RTA comes at considerable computational cost in our formulation (the cost of going from a single to a double summation of convoluted Bessel functions).

In contrast, Kennett's conductivity in the case of the general collision integral is of exactly the same form as that found within the RTA. Both are given by a single sum over squared Bessel functions (to go beyond the RTA and incorporate a full collision integral into his expression, one simply has to replace a constant scattering rate with one that depends on the momentum index). There is no additional convolution of Bessel components. This form results from the usage of a two-variable distribution. It implies that one pays no penalty for going beyond the RTA. This is in stark contrast to virtually all other results in Boltzmann transport theory where one finds that going beyond the RTA entails a significant increase in the complexity of the calculation.[5]

We now briefly address the extension to finite frequency. In Eq. (3K), Kennett writes down a well-known[3] version of the Boltzmann equation that is appropriate for ac fields that differs from the one we used (by the addition of its first term on the left-hand side, mentioned above). Below we justify our use of the simpler equation. However, we must first emphasize that this point is not related to the central disagreement between Kennett's results and our own. As shown above, the discrepancy between our derivations occurs at the level of the dc calculation. Indeed, when one compares the relationship between our expressions for the dc and ac conductivities, one sees that it is analogous to the corresponding

relationship between Kennett's expressions. That is, the discrepancy occurring in the dc calculation propagates to the ac calculation.

We restricted ourselves to the consideration of vanishingly weak ac electric fields and strong, static magnetic fields. In this case, the dominant influence on electron motion is the magnetic field that drives cyclotron motion. The additional electric field is a weak correction that is nonetheless responsible for the interlayer electric current. By dropping the first term included in Kennett's Boltzmann equation, we make the assumption that the quasiparticle distribution, and interlayer current, can be determined to lowest order in electric field by only incorporating the ac electric field into the current source term (which is the only term in which the electric field must be included to obtain finite current). We explicitly described our approach in the article.[1] We concede that there is a valid point of criticism to be made about our calculation—one might be concerned that the omitted term would have a significant effect on our results for the frequency-dependent conductivity. Inclusion of this term would make the calculation far more difficult, however. Kennett is able to incorporate this term into his analysis because of his simpler treatment of the dc current source. But we cannot regard his result for the ac conductivity as an improvement over our expression. It has, we claim oversimplified, properties analogous to those of the dc expression, as we now briefly mention.

The key feature of the ac conductivity expressions obtained in our article and in Kennett's Comment are the resonant peak widths, which contain information about the Fourier components of the scattering potential. According to Kennett's Comment, individual components can simply be read off (as they follow a one-to-one correspondence) from the widths of peaks in the ac conductivity. Our result instead suggests that such peak widths are produced by weighted sums over all possible scattering components (low-frequency peaks being more heavily weighted toward long-wavelength scattering components). We would argue that the latter behavior, in which all allowable scattering processes are entangled in the measurable spectral peaks, more closely follows one's physical intuition for scattering effects. A full discussion of the implications of our ac conductivity expression is given in Ref. 1.

In conclusion, we have replied to Kennett's criticism of our derivation of the interlayer magnetoconductivity in 1D and 2D metals. On the one hand, we have justified our calculation by discussing how it follows a general approach, which successfully accounts for well-known results in magnetotransport, and arguing that our final expression has physically reasonable features. On the other, we have identified what we see as a critical issue in Kennett's alternative derivation: the questionable treatment of initial constants arising from the electronic equation of motion, which is done to reduce from three to two the number of variables in the distribution function. We have also pointed out unusual properties of his final expression. While we appreciate that there are subtle issues at play (especially in the interpretation of the time-dependent distribution and the respective roles of a time-dependent electric field and the cyclotron motion within a static magnetic field) we claim that we have demonstrated that the results of our original article are on a sound theoretical footing, whereas those of Kennett's Comment are more difficult to justify.

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[1] M. F. Smith and R. H. McKenzie, Phys. Rev. B **77**, 235123 (2008).

[2] We are grateful to Kennett for pointing out a factor of 2 missed by us in the 1D metal calculation, but will not discuss the 1D case since it is so similar to 2D.

[3] A. A. Abrikosov, *Fundamentals of the Theory of Normal Metals* (North-Holland, Amsterdam, 1988), Chaps. 3 and 4.

[4] R. H. McKenzie and P. Moses, Phys. Rev. Lett. **81**, 4492 (1998).

[5] J. M. Ziman, *Electrons and Phonons: The Theory of Transport Phenomena in Solids* (Clarendon, Oxford, 1960).