



Necessary and sufficient condition for longitudinal magnetoresistance

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Since the Lorentz force is perpendicular to the magnetic field, it should not affect the motion of a charge along the field. This argument seems to imply absence of longitudinal magnetoresistance (LMR) which is, however, observed in many materials and reproduced by standard semiclassical transport theory applied to particular metals. We derive a necessary and sufficient condition on the shape of the Fermi surface for nonzero LMR. Although an anisotropic spectrum is a prerequisite for LMR, not all types of anisotropy can give rise to the effect: a spectrum should not be separable in any sense. More precisely, the combination $k_\rho v_\phi / v_\rho$, where k_ρ is the radial component of the momentum in a cylindrical system with the z axis along the magnetic field and $v_\rho (v_\phi)$ is the radial (tangential) component of the velocity, should depend on the momentum along the field. For some lattice types, this condition is satisfied already at the level of nearest-neighbor hopping; for others, the required non-separability occurs only if next-to-nearest-neighbor hopping is taken into account.

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I. INTRODUCTION

Magnetoresistance, i.e., a change in the resistance due to a magnetic field, can be distinguished into two types depending on the mutual orientation of the current and the magnetic field: transverse (TMR) and longitudinal (LMR). Although a change in the transverse resistance due to a magnetic field is natural because electrons experience Lorentz force in that direction, the very existence of LMR is somewhat surprising, at least at first glance. Indeed, since Lorentz force is perpendicular to the field, one does not expect the motion of electrons along the field to be affected. A weak point of this argument is that it applies, strictly speaking, only to free electrons but not to electrons in metals. Moreover, LMR is absent in a more realistic (yet still incomplete) “damped Bloch electrons model” (DBEM), in which a phenomenological damping term is introduced into the semiclassical equations of motion for an arbitrary electron spectrum.¹⁻³ However, we will argue in this paper that the “damped Bloch electrons model” is not equivalent to the Boltzmann equation, which provides the only complete description of semiclassical dynamics of electrons in solids in the presence of scattering. Therefore, absence of LMR in DBEM does not imply its absence in reality.

Experimentally, LMR has been observed in many materials.^{4,5} Theoretically, a general solution of the Boltzmann equation in the magnetic field does not exclude LMR (Ref. 6); calculations performed for particular metals, e.g., copper, do yield finite LMR.^{4,5} However, it is not clear from this general solution which symmetries must be broken, i.e., how anisotropic the electron spectrum should be for LMR to occur. It is probably why LMR is sometimes viewed as a kind of surprise.^{7,8} In addition to anisotropic spectrum, several more special models have been invoked to explain LMR. It was shown, for example, that LMR can arise due to anisotropic scattering,⁹ macroscopic inhomogeneities,¹⁰ including barrier inhomogeneities in superlattices,⁸ as well as due to a modification of the density of states by the magnetic field in the ultraquantum regime, when all but the lowest Landau levels are depopulated.¹¹ Whereas observed LMR in

many cases is likely to be caused by these more evolved mechanisms, it is still necessary to explore whether LMR can arise simply due to anisotropy of the Fermi surface (FS) and to formulate a minimal condition for LMR to occur.

Magnetotransport in nonquantizing fields is described by the Boltzmann equation which gives the conductivity tensor. To find magnetoresistance, one inverts this tensor. It is well known that for any isotropic spectrum and also for isotropic scattering, the magnetic field dependences of the diagonal and off-diagonal conductivities cancel out, so that both TMR and LMR are absent. While TMR can be made finite by either invoking any kind of anisotropy of the Fermi surface or introducing a multiband picture while keeping the spectrum isotropic, the story with LMR is not so simple. As is shown in this paper, not all types of anisotropy give rise to LMR, e.g., deforming a spherical Fermi surface into an ellipsoidal one is not enough. We derive the necessary and sufficient condition the spectrum must satisfy for LMR to occur and discuss the implications of this condition for several types of band structure. The condition serves as a minimal condition, demonstrating how LMR can arise purely due to Fermi surface geometry even if scattering is simply isotropic. For example, metals with face-centered cubic (FCC) and body-centered cubic (BCC) lattices satisfy the necessary and sufficient condition even if only nearest-neighbor hopping is taken into account, whereas a simple cubic (SC) lattice has LMR only due to hopping between next-to-nearest neighbors. The same is true for layered structures, such as hexagonal planes stacked on top of each other, where one has to include out-of-plane next-nearest-neighbor interactions to see the effect.

The rest of the paper is organized as follows. In Sec. II we show that LMR is absent in DBEM and analyze the differences between this and Boltzmann-equation approach. In Sec. III, we derive the necessary and sufficient condition for LMR in the Boltzmann-equation formalism and discuss the implications of this condition. As a particular example, we consider the case of Bernal-stacked graphite in Sec. IV. In graphite, the necessary and sufficient condition is satisfied due to trigonal warping of the Fermi surface. We find, how-

ever, that strong non-parabolic LMR observed in highly oriented pyrolytic graphite (HOPG) samples¹² cannot be accounted for LMR arising simply from anisotropy of the Fermi surface. Our conclusions are given in Sec. V.

II. SEMICLASSICAL EQUATIONS OF MOTION

The effect of weak electric and magnetic fields on electrons in solids can be described by the semiclassical equations of motion¹³

$$\mathbf{v} = \frac{\partial \varepsilon_{\mathbf{k}}}{\partial \mathbf{k}}, \quad (1a)$$

$$\frac{d\mathbf{k}}{dt} = e(\mathbf{E} + \mathbf{v} \times \mathbf{B}), \quad (1b)$$

where e is the electron charge and we set $\hbar=1$. We neglect here the anomalous terms in the velocity which, even if present, are small in weak magnetic fields.^{14,15} In the absence of scattering, Eqs. (1a) and (1b) are valid for an arbitrary spectrum $\varepsilon(\mathbf{k})$ and provide an invaluable tool for analyzing collisionless dynamics of electrons in solids. To account for scattering of electrons by impurities, phonons, etc., it is customary to replace Eqs. (1a) and (1b) by a phenomenological “damped Bloch electrons model” (DBEM) with a damping term $-\mathbf{k}/\tau$ inserted into the right-hand side of Eq. (1b).¹⁻³ In steady-state, DBEM reduces to

$$\frac{\mathbf{k}}{\tau} = e(\mathbf{E} + \mathbf{v} \times \mathbf{B}). \quad (2)$$

We are now going to show that this approach eliminates LMR not only for an isotropic but also for an arbitrary spectrum. To find LMR, we assume that the current $\mathbf{j}=en_c\mathbf{v}$, where n_c is the number density of conduction electrons, is along \mathbf{B} chosen as the z -axis. Then,

$$v_z(k_x, k_y, k_z) = \frac{j_z}{n_c e}, \quad (3a)$$

$$v_x(k_x, k_y, k_z) = 0, \quad (3b)$$

$$v_y(k_x, k_y, k_z) = 0. \quad (3c)$$

Furthermore, the equation of motion (2) for the k_z component gives

$$k_z = e\tau E_z. \quad (4)$$

The set of four Eqs. (3a)–(3c) and (4) defines an inhomogeneous system for four unknowns: k_x , k_y , k_z , and E_z . In general, such a system has a unique solution. Therefore, E_z can be found as a function of j_z using only Eqs. (3a)–(3c) and (4). Since none of these equations involve the magnetic field, the longitudinal resistivity $\rho_{zz}=j_z/E_z$ does not depend on B either, which implies that LMR is absent for an arbitrary spectrum. On the other hand, components E_x and E_y have to be found from the equations of motion for k_x and k_y which do involve B , and hence TMR is not zero for an arbitrary spectrum.

If the above conclusion were correct, it would be in variance with experimental observations. As we will show shortly, nonzero LMR can be understood only by using the Boltzmann equation

$$\frac{df_{\mathbf{k}}}{dt} = \frac{\partial f_{\mathbf{k}}}{\partial t} + \mathbf{v} \cdot \frac{\partial f_{\mathbf{k}}}{\partial \mathbf{r}} + \dot{\mathbf{k}} \cdot \frac{\partial f_{\mathbf{k}}}{\partial \mathbf{k}} = I_c[f_{\mathbf{k}}], \quad (5)$$

where I_c denotes the collision integral. Although the Boltzmann equation is a semi-classical description just like the previous method, there is some conceptual difference between the two approaches. The problem is that while the equations of motions in the absence of scattering can be derived from the Schrödinger equation, the DBEM does not follow from any microscopic approach. Indeed, the momentum \mathbf{k} in the absence of scattering still has the meaning of the quantum number parameterizing the Bloch state $\psi_{\mathbf{k}}(\mathbf{r})$. Hence a (slow) evolution of \mathbf{k} with time in the presence of electric and magnetic fields describes the evolution of $\psi_{\mathbf{k}}(\mathbf{r})$. In the presence of scattering, e.g., by disorder, $\psi_{\mathbf{k}}(\mathbf{r})$ becomes a random quantity whose average over disorder realizations does not have a particular meaning. Therefore, it is not surprising that an *ad hoc* insertion of the damping term into the equation of motion does not capture essential physics. Even in the absence of the magnetic field the shortcomings of this procedure become obvious—e.g., it is easy to show that the conductivity calculated by DBEM method does not coincide with that calculated from the Boltzmann equation for a general band structure, the exception being only in the case of a simple isotropic spectrum.

III. MINIMAL CONDITIONS FOR LONGITUDINAL MAGNETORESISTANCE

A. Necessary condition

Having dealt with the inconsistencies of the “damped Bloch electrons model,” we now return to the original problem of finding the minimum requirement for nonzero LMR for an arbitrary spectrum $\varepsilon=\varepsilon(\mathbf{k})$. In the linear-response regime, one can rewrite Eq. (5) for the nonequilibrium part of the distribution function $g(\mathbf{k})=f_{\mathbf{k}}-f_{\mathbf{k}}^0$ as

$$(1 + \hat{\Omega})g(\mathbf{k}) \equiv \left[1 + e\tau(\mathbf{v} \times \mathbf{B}) \cdot \frac{\partial}{\partial \mathbf{k}} \right] g(\mathbf{k}) = -e\mathbf{E} \cdot \mathbf{v} \frac{\partial f_{\mathbf{k}}^0}{\partial \varepsilon_{\mathbf{k}}}, \quad (6)$$

where we have also adopted the relaxation-time approximation (which is exact for isotropic impurity scattering). Since we are interested in the minimal condition, we allow τ to depend only on ε but not on the direction of \mathbf{k} and assume that all components of \mathbf{k} relax at the same rate, i.e., that $1/\tau$ is a scalar rather than a tensor. We will come back to this point later in the paper. For $\mathbf{B} \parallel \hat{z}$,

$$\hat{\Omega} = \tau e(\mathbf{v} \times \mathbf{B}) \cdot \frac{\partial}{\partial \mathbf{k}} = e\tau B \left(v_y \frac{\partial}{\partial k_x} - v_x \frac{\partial}{\partial k_y} \right). \quad (7)$$

Following the Zener-Jones method,¹⁶ we express $g(\mathbf{k})$ via an infinite series in the operator $\hat{\Omega}$:

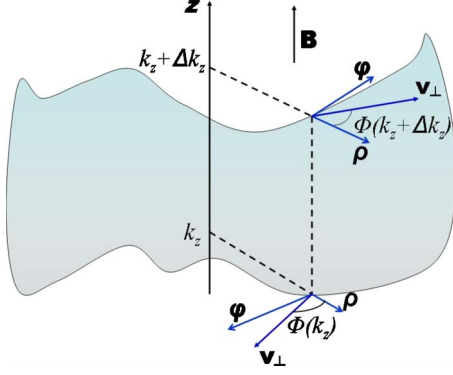


FIG. 1. (Color online) Geometric interpretation of the necessary condition for longitudinal magnetoresistance. Here, \mathbf{v}_\perp is the component of the electron velocity perpendicular to the field.

$$g(\mathbf{k}) = (1 + \hat{\Omega})^{-1} \left(-\tau e \mathbf{E} \cdot \mathbf{v} \frac{\partial f_{\mathbf{k}}^0}{\partial \varepsilon_{\mathbf{k}}} \right) = \sum_{n=0}^{\infty} (-\hat{\Omega})^n \left(-\tau e \mathbf{E} \cdot \mathbf{v} \frac{\partial f_{\mathbf{k}}^0}{\partial \varepsilon_{\mathbf{k}}} \right). \quad (8)$$

Note that the operator $\hat{\Omega}$ always yields zero when it acts on any function that depends on $\varepsilon_{\mathbf{k}}$ only. Hence, in Eq. (8), $\hat{\Omega}$ acts only on \mathbf{v} . Substituting Eq. (8) into the current $\mathbf{j} = 2e \int d^3k v g(\mathbf{k}) / (2\pi)^3$, we find the conductivity as

$$\sigma_{\alpha\beta} = 2e^2 \tau \int \frac{d^3k}{(2\pi)^3} \left(-\frac{\partial f_{\mathbf{k}}^0}{\partial \varepsilon_{\mathbf{k}}} \right) v_\alpha \sum_{n=0}^{\infty} (-\hat{\Omega})^n v_\beta. \quad (9)$$

In the LMR geometry, $\mathbf{E} \parallel \mathbf{B} \parallel \hat{z}$. If $\hat{\Omega} v_z = 0$, all but the $n=0$ term in Eq. (9) are equal to zero. Therefore, a *necessary* condition for σ_{zz} to depend on the magnetic field is

$$\hat{\Omega} v_z \neq 0. \quad (10)$$

Rewriting $\hat{\Omega}$ in cylindrical coordinates, the condition (10) can be re-expressed as

$$\left(\frac{\partial \varepsilon}{\partial \phi} \frac{\partial}{\partial k_\rho} - \frac{\partial \varepsilon}{\partial k_\rho} \frac{\partial}{\partial \phi} \right) v_z \neq 0, \quad (11)$$

or

$$\frac{\partial}{\partial k_z} \left(\frac{\partial \varepsilon / \partial \phi}{\partial \varepsilon / \partial k_\rho} \right) \neq 0. \quad (12)$$

On the other hand, Eq. (12) is *not* a sufficient condition because even if $\hat{\Omega}^n v_z \neq 0$ for the n^{th} term in the series, the contribution of this term to σ_{zz} may vanish upon integrating over the Fermi surface. For example, since σ_{zz} must be an even function of B , all odd terms in the series must vanish.

Equation (12) implies that the minimum condition on the spectrum is that the ratio of $\partial \varepsilon / \partial \phi$ and $\partial \varepsilon / \partial k_\rho$ (equal to $k_\rho v_\phi / v_\rho$) must depend on k_z . Geometrically, this means that the angle between the component of velocity perpendicular to the field and the radial direction at a given point on the Fermi surface must vary with k_z (Fig. 1). It can be easily seen that if the spectrum does not depend on ϕ , condition (12) is trivially violated and there is no LMR. Therefore, angular

anisotropy of the FS about the magnetic-field direction is a prerequisite. However, anisotropy must be of a special kind. For example, spectra such as $\varepsilon_{\mathbf{k}} = \varepsilon_1(k_\rho, \phi) + \varepsilon_2(k_z)$ and $\varepsilon_{\mathbf{k}} = \varepsilon_1(k_\rho, \phi) \varepsilon_2(k_z)$, which are arbitrarily anisotropic in the ϕ direction but separable in k_z , violate condition (12) and thus do not lead to LMR. As an example, let us consider a SC lattice with lattice parameter a . In the tight-binding model with nearest-neighbor hopping (parameterized by coupling t_1), the energy spectrum is given by $\varepsilon_{\mathbf{k}} = -2t_1 [\cos(k_x a) + \cos(k_y a) + \cos(k_z a)]$ which, being separable in all three coordinates, clearly violates the LMR condition. If next-to-nearest-neighbor hopping (parameterized by coupling t_2) is taken into account, additional terms $-4t_2 [\cos(k_x a) \cos(k_y a) + \cos(k_y a) \cos(k_z a) + \cos(k_z a) \cos(k_x a)]$ occur in the spectrum, which no more violates the LMR condition. Thus, the effect comes only from next-to-nearest-neighbor hopping for an SC lattice. On the other hand, an FCC lattice satisfies the condition already at the nearest-neighbor level because the spectrum in this case $\varepsilon_{\mathbf{k}} = -4t_1 [\cos(k_x a/2) \cos(k_y a/2) + \cos(k_y a/2) \cos(k_z a/2) + \cos(k_z a/2) \cos(k_x a/2)]$ is non-separable; the same is true for a BCC lattice. On the other hand, layered, e.g., hexagonal, structures, will require coupling between an atom located in one plane and another atom in the adjacent plane but situated obliquely from the former, if the magnetic field is perpendicular to the planes (more on this later for the specific case of graphite).

A quantity measured in a typical experiment is not the conductivity but the resistivity. Generally speaking, the dependence of the conductivity on the magnetic field does not automatically imply a dependence of the resistivity on the field—a well known case is the isotropic spectrum, when the (transverse) diagonal components of the conductivity depend on B but the diagonal components of the resistivity do not. It is necessary, therefore, to make sure that Eq. (12) is not only a necessary condition for longitudinal magnetoconductance but also for magnetoresistance. It is difficult to prove that nonzero magnetoconductance implies nonzero LMR for an arbitrary spectrum. To proceed further, we relax a condition on the energy spectrum, assuming that B is perpendicular to the plane of symmetry, i.e., that $\varepsilon(k_x, k_y, k_z) = \varepsilon(k_x, k_y, -k_z)$. This constraint is stronger than that imposed by time reversal symmetry (in the absence of the spin-orbit interaction and magnetic structure), i.e., in this case, v_z is odd while v_x and v_y are even in k_z , and the off-diagonal components $\sigma_{\alpha z}$ ($\alpha \neq z$) vanish both in zero and finite magnetic fields. For example, all terms in the expression for σ_{xz} vanish upon integration over k_z :

$$\sigma_{xz} = 2e^2 \tau \sum_{n=0}^{\infty} (-e\tau B)^n \int \frac{d^3k}{(2\pi)^3} v_x \left(v_y \frac{\partial}{\partial k_x} - v_x \frac{\partial}{\partial k_y} \right)^n v_z \frac{\partial f_{\mathbf{k}}^0}{\partial \varepsilon_{\mathbf{k}}} = 0. \quad (13)$$

By the Onsager principle, $\sigma_{z\alpha} = \sigma_{\alpha z}$ as well. Therefore, the matrix of $\sigma_{\alpha\beta}$ is block-diagonal and $\rho_{zz} = 1/\sigma_{zz}$. Thus Eq. (12) is a *necessary* condition for nonzero LMR as well, provided that the spectrum is symmetric on inversion of k_z .

B. Sufficient condition

The condition presented in Eq. (12) is only a necessary condition for LMR, as the integral in Eq. (9) may still vanish due to some symmetry even if the integrand satisfies Eq. (12). To formulate a sufficient condition, we approach the problem from the strong-magnetic-field limit. In this limit, it is convenient to use the method of Lifshitz, Azbel' and Kaganov,^{6,17,18} in which the k -space is mapped onto a space defined by the set of variables $\varepsilon \equiv \varepsilon_{\mathbf{k}}$, k_z and t_1 , where t_1 , defined by the equation

$$\frac{d\mathbf{k}}{dt_1} = e\mathbf{v} \times \mathbf{B}, \quad (14)$$

is the time spent by an electron on the orbit in the k -space in the presence of the magnetic field only. Accordingly, the integration measure is transformed as

$$\int \int \int dk_x dk_y dk_z = eB \int \int \int dt_1 d\varepsilon dk_z. \quad (15)$$

The nonequilibrium correction to the distribution function can be written as

$$g = e \frac{\partial f^0}{\partial \varepsilon} \mathbf{E} \cdot \mathbf{s}, \quad (16)$$

where \mathbf{s} satisfies

$$\frac{\partial \mathbf{s}}{\partial t_1} = I_c[\mathbf{s}] + \mathbf{v}. \quad (17)$$

Adopting the relaxation-time approximation for I_c and keeping only the leading term in $1/B$, it is easy to see that⁶

$$s_z = \tau \langle v_z \rangle, \quad (18)$$

where $\langle v_z \rangle = \frac{1}{T} \int v_z dt_1$ with T being either the period of an orbit (for closed orbits) or the time over which an orbit reaches the boundary of the Brillouin zone (for open orbits). The σ_{zz} component of the conductivity tensor in this limit is then equal to

$$\begin{aligned} \sigma_{zz}(\infty) &= \frac{2e^2\tau}{(2\pi)^3} eB \int \int \int d\varepsilon dk_z dt_1 v_z \langle v_z \rangle \left(-\frac{\partial f^0}{\partial \varepsilon} \right) \\ &= \frac{2e^2\tau}{(2\pi)^3} \oint d\ell \int dk_z \int \frac{d\varepsilon}{v_{\perp}} v_z \langle v_z \rangle \left(-\frac{\partial f^0}{\partial \varepsilon} \right), \end{aligned} \quad (19)$$

where $d\ell$ is a line element along the orbit and $v_{\perp} = \sqrt{v_x^2 + v_y^2}$. Obviously, $\sigma_{zz}(\infty)$ does not depend on B . On the other hand, the zero-field value of σ_{zz} is

$$\sigma_{zz}(0) = \frac{2e^2\tau}{(2\pi)^3} \int d^3k v_z^2 \left(-\frac{\partial f^0}{\partial \varepsilon} \right). \quad (20)$$

Pippard⁵ suggested that the ratio $\sigma_{zz}(\infty)/\sigma_{zz}(0)$ may be used to get information about the scattering mechanisms on the FS. We, however, use this ratio to construct a sufficient condition for LMR. Keeping the same constraint on the energy spectrum $\varepsilon(k_x, k_y, k_z) = \varepsilon(k_x, k_y, -k_z)$ so that $\rho_{zz} = 1/\sigma_{zz}$, the sufficient condition for LMR can now be formulated as follows: if $\sigma_{zz}(\infty) \neq \sigma_{zz}(0)$, we have nonzero LMR. It is only a

sufficient condition because, even if it is violated, LMR can still exist. Indeed, even if asymptotic limits of the function $\sigma_{zz}(B)$ coincide, it is not necessarily a constant. To formulate the sufficient condition in more transparent terms, we use the following trick. The integration measure in the expression (20) for the zero-field conductivity can formally be rewritten in terms of variables ε , k_z and t_1 , as specified by transformation [Eq. (15)]. Since the result does not depend on the magnetic field, this transformation can be applied for any value of the field but, to compare the zero- and strong-field values, we choose the same B as in the first line of Eq. (19). Then,

$$\sigma_{zz}(0) = \frac{2e^2\tau}{(2\pi)^3} eB \int \int \int d\varepsilon dk_z dt_1 v_z^2 \left(-\frac{\partial f^0}{\partial \varepsilon} \right). \quad (21)$$

Comparing this equation with the first line of Eq. (19), we see that the sufficient condition is equivalent to

$$\int \int \int d\varepsilon dk_z dt_1 \left(-\frac{\partial f^0}{\partial \varepsilon} \right) (v_z \langle v_z \rangle - v_z^2) \neq 0. \quad (22)$$

Integrating over t_1 , we rewrite the last equation as

$$\begin{aligned} &\int \int d\varepsilon dk_z \left(-\frac{\partial f^0}{\partial \varepsilon} \right) (\langle v_z^2 \rangle - \langle v_z \rangle^2) \\ &= \int \int d\varepsilon dk_z \left(-\frac{\partial f^0}{\partial \varepsilon} \right) (\langle v_z - \langle v_z \rangle \rangle^2) \neq 0. \end{aligned}$$

Since the integrand is non-negative, the integral can only vanish if $v_z = \langle v_z \rangle$, which is the case if v_z does not depend on t_1 . Hence, the sufficient condition is equivalent to the requirement that

$$\frac{\partial v_z}{\partial t_1} = \frac{\partial v_z}{\partial k_x} \frac{\partial k_x}{\partial t_1} + \frac{\partial v_z}{\partial k_y} \frac{\partial k_y}{\partial t_1} + \frac{\partial v_z}{\partial k_z} \frac{\partial k_z}{\partial t_1} \neq 0. \quad (23)$$

Recalling that \mathbf{k} satisfies Eq. (14), we re-write the last equation as

$$\left(v_y \frac{\partial}{\partial k_x} - v_x \frac{\partial}{\partial k_y} \right) v_z \neq 0 \quad (24)$$

or, recalling the definition of the operator $\hat{\Omega}$ in Eq. (7), as

$$\hat{\Omega} v_z \neq 0. \quad (25)$$

Since the sufficient condition (25) coincides with the necessary condition in Eq. (10), we conclude that Eq. (12) is both a *necessary* and *sufficient* condition for LMR. As a corollary, it also follows that the strong-field value $\sigma_{zz}(\infty)$ is always smaller than or equal to $\sigma_{zz}(0)$, implying that if LMR is finite, it is positive.

Before concluding this section, we would like to comment that our aim was to establish a minimal condition for the appearance of LMR in materials. Specifically, we wanted to explore whether, in the simplest model for scattering, anisotropy of the bandstructure alone can give rise to LMR; the answer turns out to be in the affirmative. It should be pointed out that LMR can also occur due to anisotropic scattering. Indeed, as was shown by Jones and Sondheimer¹⁹ who chose a special form of the scattering probability to solve the Boltzmann equation exactly, nonzero LMR can occur even for an

isotropic spectrum, if the scattering probability is appropriately anisotropic. In general, scattering of Bloch electrons is to be described by a tensor of relaxation times, because different components of momentum relax at different rates. In lieu of a fully microscopic description, we adopt here a heuristic model, in which the relaxation time, being still a scalar, depends on the point in the k space, $\tau = \tau(\mathbf{k})$. It is easy to see that the necessary condition for nonzero LMR in this case is modified to:

$$\hat{\Omega}(\tau v_z) \neq 0, \quad (26)$$

That means that even if the spectrum alone violates our previous condition (12), i.e., $\hat{\Omega}v_z = 0$, Eq. (26) may still be satisfied because $\hat{\Omega}\tau$ may be nonzero. If this is the case, LMR is finite as well. On the other hand, an attempt to prove that Eq. (26) is also a sufficient condition in this case fails because of the following reason. With $\tau = \tau(\mathbf{k})$, expressions for the high-field and zero-field longitudinal conductivities are still given by Eqs. (19) and (21), except that now τ is inside the integrals. Following same reasoning as before, a sufficient condition for nonzero LMR would be $\sigma_{zz}(B=\infty) \neq \sigma_{zz}(B=0)$, which now implies that $\int \int (-\partial f^0 / \partial \varepsilon) (\langle v_z^2 \tau \rangle - \langle v_z \rangle \langle v_z \tau \rangle) d\varepsilon dk_z \neq 0$. Unlike the previous case, however, the integrand cannot be proven to be a positive function; therefore, a nonzero integrand does not guarantee that the integral is also nonzero. Therefore, the sufficient condition can only be formulated in the integral form, as given above.

IV. EXAMPLE: LONGITUDINAL MAGNETORESISTANCE IN GRAPHITE

As a particular example of a material with significant LMR, we consider the case of graphite, where a huge—up to three orders of magnitude—LMR effect is observed when both the current and magnetic field are along the c axis.¹² The crystal structure of graphite consists of Carbon atoms arranged in hexagonal layers stacked on top of each other in the Bernal way (ABABAB...). Each unit cell has 4 C atoms with two inequivalent C atoms in each layer. The resulting Brillouin zone is a hexagonal prism with very thin elongated FSs along the edges of the Brillouin zone extended in the direction perpendicular to the plane of the layers. The energy spectrum of graphite is well described by the Slonczewski Weiss McClure (SWMc) model¹² which involves seven parameters $\gamma_0, \dots, \gamma_6$, describing different kinds of interactions between lattice points. Here, γ_0 and γ_1 denote in- and out-of-plane nearest-neighbor interactions, respectively, $\gamma_2, \dots, \gamma_5$ describe various next-nearest neighbor interactions, while γ_6 embodies the difference in the on-site energies of two inequivalent C atoms in each layer. Parameter γ_3 plays a special role as it breaks rotational symmetry of the FS. Without γ_3 , the FS is cylindrically symmetric about the Brillouin zone edge. Therefore, the LMR condition is clearly violated. However, finite γ_3 leads to “trigonal warping,” i.e., a threefold deformation of the FS. An expression for energy spectrum of electrons and holes with γ_3 included in a perturbative way can be written as²⁰

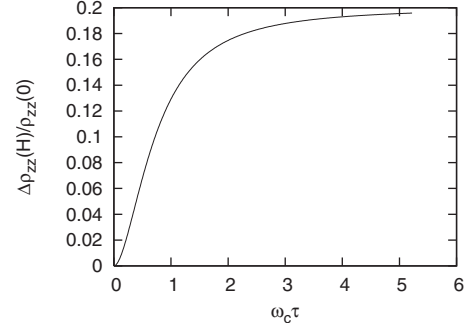


FIG. 2. Calculated dependence of LMR on magnetic field in graphite.

$$\varepsilon = \varepsilon_3^0 + A\sigma^2 \pm [B^2\sigma^4 + 2B\gamma_3\Gamma\sigma^3 \cos(3\alpha) + \gamma_3^2\Gamma^2\sigma^2]^{1/2}, \quad (27)$$

where $\sigma = \sqrt{3}a_0k_\rho/2$, $\Gamma = \cos(k_z c_0/2)$, and $\alpha = \pi/2 + \phi$, with a_0 and c_0 being the in-plane and out-of-plane lattice constants, respectively. Also in Eq. (27), ε_3^0 , A and B are all functions of k_z and contain other interaction parameters. Neglecting all the next-to-nearest-neighbor couplings except for γ_3 in the spectrum, we have $\varepsilon_3^0 = A = 0$ and $B = \gamma_0^2 / \gamma_1 \Gamma$. With this approximation, Eq. (27) can be rewritten [up to $\mathcal{O}(\gamma_3^2)$] as:

$$\varepsilon = \pm \left[\frac{k_\rho^2}{2m(k_z)} + \gamma_3\Gamma\sigma \cos(3\alpha) + \frac{\gamma_1\gamma_3^2\Gamma^3}{2\gamma_0^2} \sin^2(3\alpha) \right], \quad (28)$$

where $m(k_z) = 2\gamma_1\Gamma/3a_0^2\gamma_0^2$. As is obvious from Eq. (27), the terms containing α introduce the trigonal warping effect in the spectrum. Due to the presence of these terms, the condition for nonzero LMR is satisfied. Figure 2 shows the calculated dependence of LMR on the magnetic field in units of $\omega_c \tau$, where $\omega_c = 3eB/m_0$ with $m_0 \equiv m(k_z=0)$ in graphite at zero temperature (for $\gamma_0 = 3.16$ eV, $\gamma_1 = 0.39$ eV, and $\gamma_3 = 0.315$ eV).¹² As expected, LMR is quadratic at small fields and eventually saturates at large fields. However, we note that although this explains qualitatively why graphite has nonzero LMR in the first place, the curve does not nearly match the experiment quantitatively. Namely, we find that relative magnetoresistance $\Delta\rho_{zz}(B)/\rho_{zz}(0) \equiv [\rho_{zz}(B) - \rho_{zz}(0)]/\rho_{zz}(0)$ saturates approximately at a value of 0.2. However, observed value of this ratio is higher by orders of magnitude.²² This implies that the mechanism of LMR in real graphite (as opposed to ideal graphite described by the SWMc model) is not simply anisotropy of the FS. The disagreement is not surprising in light of the fact that the mechanism of c -axis transport in graphite (not only in finite but also in zero magnetic field) is still not completely understood and generally believed to be due to processes not described by the standard Boltzmann equations, e.g., phonon-assisted resonant tunneling through macroscopic defects, e.g., stacking faults,^{21,23,24} or disorder-assisted delocalization.²⁵

V. CONCLUDING REMARKS

To conclude, we have derived a necessary and sufficient condition that an electronic spectrum should satisfy in order to show nonzero longitudinal magnetoresistance within the semiclassical regime of electron transport. We find that anisotropy is essential for nonzero LMR although this anisotropy is to be of a special kind, namely, the spectrum must satisfy a particular nonseparability condition given by Eq. (12). We also show that a phenomenological “damped Bloch electrons” model does not capture essential physics of semiclassical transport in anisotropic materials. In particular, this model predicts that LMR is absent not only for isotropic but also for anisotropic transport, which is not consistent either with the predictions of the Boltzmann-equation theory or experiment.

In general, the limiting values of the longitudinal conductivities in the zero- and high-field limits differ only in how the square of the z -component of the electron velocity is averaged over the FS. Excluding some pathological situa-

tions, these two averages can only differ by a numerical coefficient on the order of unity. Therefore, an LMR effect can, in principle, result from FS anisotropy if its magnitude does not exceed or comparable to 100%. If, in addition, the lattice structure is such that LMR is only possible only due nearest-neighbor-hopping, one should expect even smaller values of LMR. In many materials, e.g., copper⁴ and Sr₂RuO₄,⁷ the observed LMR effect is on the order of 10%, which is well within the anisotropic-FS mechanism. However, gigantic LMR effects, such as the one observed in graphite, require explanations which involve macroscopic inhomogeneities of the sample.

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