Fermi surfaces which produce large transverse magnetoresistance

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Abstract

The Boltzmann equation is used with elastic s-wave scattering to consider the relationship between the Fermi surface and the magnetoresistance. Specifically discussed are properties of two-dimensional Fermi surfaces which cause the low-field magnetoresistance, to be large. Models such as the tight-binding model and the nearly free electron model are used, as well as fabricated potentials to demonstrate other features of the Fermi surface which cause large magnetoresistance.

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I. BACKGROUND

For the past 45 years, many studies have used magnetoresistance to determine the shape of the Fermi surface of materials, and there are many techniques to do this [1]. The converse, however, is not very well understood. We do not yet know what shape of Fermi surface will produce large magnetoresistance in a material. Producing a material with large magnetoresistance will allow great improvements in the magnetic field sensors used in magnetic data storage [2]. We attempt to understand the characteristics of a Fermi surface which cause the material to have a large magnetoresistance at low field. Some work has been done studying the magnetoresistance of various materials, many of which have Fermi surfaces similar to those we consider here [3, 4].

Much of the remainder of this section is from Ashcroft and Mermin [5].

The first assumption we make is that metals are crystals. We model them as a periodic potential that acts on the electrons. We can then study the motion of the electrons as they carry charge and thus conduct electricity. The consequences of this assumption are as follows. We have a large number, \( N \), of identical primitive cells which make up the crystal. We define the direct lattice, which is the set of all vectors \( \mathbf{R} \) from any primitive cell to the equivalent point in any other primitive cell. The direct lattice along with a suitable boundary condition gives rise to the reciprocal lattice in \( k \)-space. This lattice is the set of wave vectors \( \mathbf{K} \) for which

\[
\mathbf{R} \cdot \mathbf{K} = 2n\pi
\]

where \( n \) is an integer for every \( \mathbf{R} \) in the direct lattice. The reciprocal lattice partitions \( k \)-space into cells in a way analogous to how the direct lattice partitions real space into cells.

We now have two lattices – the direct lattice of vectors \( \mathbf{R} \) in position space which relate any \( \mathbf{r} \) to its equivalent points \( \mathbf{r} - \mathbf{R} \) in the other direct lattice cells, and the reciprocal lattice of vectors \( \mathbf{K} \) in \( k \)-space which relate any \( \mathbf{k} \) to its equivalent vector \( \mathbf{k} - \mathbf{K} \) in the other reciprocal lattice cells. We will define a periodic potential \( U(\mathbf{r}) \) with the condition

\[
U(\mathbf{r}) = U(\mathbf{r} - \mathbf{R})
\]

for all \( \mathbf{R} \) in the direct lattice. The Hamiltonian is then

\[
H = \frac{\mathbf{p}^2}{2m} + U(\mathbf{r}),
\]
and is periodic. Because of this periodicity, we find that $H$ has simultaneous eigenstates with the wave vector $k$ so that we can label the eigenstates $\psi_k$. Further, we find that

$$
\psi_k = \psi_{k-K},
$$

(4)

for any $K$ in the reciprocal lattice. This means that we can relocate any $k$ to a particular cell of our choice.

When we label the eigenstates with $k$ (and thus the energies $E_k$), the Schrödinger equation becomes

$$
\left( \frac{\hbar^2}{2m} (k - K)^2 - E_k \right) c_{k-K} + \sum_{K'} U_{K'-K} c_{k-K'} = 0
$$

(5)

where $U_K$ are the Fourier components of the potential and $\psi_k = e^{-iK\cdot r} \sum_K c_{k-K} e^{iK\cdot r}$. This equation has an infinite number of solutions for any given $k$, so we must introduce another quantum number called the band index $n$. Thus, we can describe the eigenstates uniquely (up to spin) by $k$ and $n$, as $\psi_{nk}$.

Each band has a finite range of allowed energies. Since electrons are Fermions, two electrons cannot occupy the same state, so in the ground state (the lowest possible energy configuration) at zero temperature, they will fill up the eigenstates starting from those of lowest energy. If there is a partially-filled band after all the electrons are accommodated, then the material is a metal and will conduct electricity. Moreover, the energy of each electron is less than or equal to the Fermi energy $E_F$. The equal-energy surface in $k$-space that separates the occupied states from the unoccupied states is called the Fermi surface. Since different bands may have overlapping energies, there may be several partially filled bands, in which case the Fermi surface to have several branches. The Fermi surface is important in determining the properties such as magnetoresistance of a material and is determined by the periodic potential.

To determine the magnetoresistance of a material, we begin with the periodic potential and thus its Fermi surface. We use the Boltzmann equation to model the motion of the electrons. We begin with the Liouville theorem which is a restatement of the continuity equation. Let $f$ be a distribution function, so that the number of electrons in a box from $(r,k)$ to $(r+dr,k+dk)$ in phase space is $N = f(r,k)drdk$. Then

$$
\frac{df}{dt} = \frac{\partial f}{\partial t} + \nabla_r f \cdot \frac{dr}{dt} + \nabla_k f \cdot \frac{dk}{dt} = 0.
$$

(6)
We assume a steady state \( \partial f / \partial t = 0 \) and a uniform space \( \nabla_r f = 0 \) and note that \( \hbar \Delta k / C \tau = F = -e(v \times B + E) \), where the velocity \( v \) satisfies \( v = \frac{1}{\hbar} \nabla_k \mathcal{E}_k \). Finally, we account for scattering. We assume elastic s-wave scattering and use a relaxation time approximation. This means that a scattering electron is equally likely to scatter in any direction and its energy will not change. This approximation is important for these initial results, but may be reconsidered later. Thus, the number of electrons scattering out of a state \( (k, n) \) in a unit time is \( f / \tau \) and the number scattering into a state \( \bar{f} / \tau \), where \( \bar{f} \) is the average of \( f \) over the equal-energy surface. Thus, the Boltzmann equation is

\[
-e(v \times B) \cdot \nabla_k f - eE \cdot \nabla_k f = -\frac{f - \bar{f}}{\tau / \hbar}.
\]

Finally, we define a scalar quantity to represent the magnetoresistance. We will look at quasi-two dimensional Fermi surfaces and transverse magnetoresistance, in which \( B \) is perpendicular to the plane of the Fermi surface. We define this scalar quantity by expanding the resistivity \( \rho(B) \) in powers of \( B \) about zero, as

\[
\rho(B) = \rho^{(0)} + \rho^{(1)}B + \rho^{(2)}B^2 + \ldots.
\]

We then define the magnetoresistance ratio by

\[
\rho_B = \frac{\rho^{(2)}}{\rho^{(0)}}.
\]

This quantity is zero for the spherical free energy Fermi surface in the first Brillouin zone. However, that is not always the case. Nonconstant magnetoresistance may be caused by several factors. There may be more than one band, or more complex scattering may be taking place. A third factor may be the shape of the Fermi surface, which we consider here.

II. FORMALISM

Much of this section is from discussions with Selman Hershfield [6].

A. Boltzmann equation

Here we describe the model we use for our calculations. We begin with the Boltzmann equation, Eq. (7),

\[
-eE \cdot \nabla_k f - ev \times B \cdot \nabla_k f = -\frac{f - \bar{f}}{\tau / \hbar}.
\]
where \( f \) is the distribution function, \( \tau \) is the relaxation time for our scattering approximation, and \( \overline{f} = \frac{\int_S f ds}{\int_S ds} \) is the average of \( f \) over the equal-energy surface. We assume a small electric field and linear response, that is \( f = f^{eq} + \delta f \) where \( f^{eq} \) is independent of \( E \) and \( \delta f \) is linear in \( E \). (We note also that \( f^{eq} \) is independent of \( B \) since there is no equilibrium current caused by a magnetic field and the dependence of \( \delta f \) on \( B \) is still arbitrary.) Thus,

\[
-e(\mathbf{v} \times \mathbf{B}) \cdot \nabla_k \delta f - e \mathbf{E} \cdot \nabla_k f^{eq} = -\frac{\delta f - \overline{f}}{\tau/\hbar}.
\]

(11)

Next we assume low temperature, so that \( f^{eq} = \Theta(\mathcal{E}_F - \mathcal{E}) \) and we can write \( \delta f = (\frac{\partial f^{eq}}{\partial \mathcal{E}})g = \delta(\mathcal{E}_F - \mathcal{E})g \). Finally, defining \( h = g - \overline{g} \) yields

\[
-e(\mathbf{v} \times \mathbf{B}) \cdot \nabla_k h + e \mathbf{E} \cdot \mathbf{v} = -\frac{h}{\tau/\hbar}.
\]

(12)

In two dimensions, we can further reduce the Boltzmann equation to

\[
\frac{e \tau B v}{\hbar} \frac{dh}{ds} + e \tau \mathbf{E} \cdot \mathbf{v} + h = 0,
\]

(13)

where \( s \) is the arclength along the surface. For convenience, we define \( \tilde{B} = \frac{e \tau}{\hbar} B \) and \( h = -e \tau E \tilde{h} \), so that

\[
\tilde{B} v \frac{d \tilde{h}}{ds} + \tilde{h} = \hat{\mathbf{E}} \cdot \mathbf{v}.
\]

(14)

**B. Conductivity**

Next we look at the current. Starting with

\[
\dot{\mathbf{j}} = -e \int \frac{d^2 k}{(2\pi)^2} \mathbf{v} f,
\]

(15)

we expand \( f \) in terms of \( \tilde{h} \), yielding

\[
\dot{\mathbf{j}} = \frac{e^2 \tau}{\hbar(2\pi)^2} \int_{\mathcal{E}_F} \tilde{h} \mathbf{v} ds,
\]

(16)

where \( \int_{\mathcal{E}_F} ds \) is an integral over the entire Fermi surface. We note that \( \mathbf{v} \) is the outward (or inward?) normal to the Fermi surface. From Ohm’s law,

\[
\begin{pmatrix} j_x \\ j_y \end{pmatrix} = \begin{pmatrix} \sigma_{xx} & \sigma_{xy} \\ \sigma_{yx} & \sigma_{yy} \end{pmatrix} \begin{pmatrix} E_x \\ E_y \end{pmatrix},
\]

(17)
we see that
\[
\sigma_{\alpha\beta} = \frac{e^2 \tau}{\hbar E(2\pi)^2} \oint_{\mathcal{E}_F} \hat{v}_\alpha \tilde{h}_\beta \, ds,
\]  
(18)
where \( \tilde{h}_\beta \) is \( \tilde{h} \) when \( \hat{E} = \hat{\beta} \). We can ignore the constant prefactors to \( \sigma \) because they will be divided out in the magnetoresistance ratio. When the current is at an angle \( \gamma \) with the \( x \)-axis, the resistivity is
\[
\rho = \frac{\sigma_{xx} \sin^2 \gamma + \sigma_{yy} \cos^2 \gamma}{\sigma_{xx} \sigma_{yy} - \sigma_{xy} \sigma_{yx}}.
\]  
(19)

C. Expanding the Boltzmann equation

Beginning with Eq. (14), we expand \( \tilde{h} \) in powers of \( B \), yielding
\[
\tilde{h}_\beta^{(0)} = v_\beta, \quad \tilde{h}_\beta^{(n+1)} = -v \frac{d\tilde{h}_\beta^{(n)}}{ds}.
\]  
(20)
(21)
This gives results for \( \sigma_{\alpha\beta}^{(n)} \) as follows. We begin by substituting Eq. (20) into Eq. (18) which yields
\[
\sigma_{\alpha\beta}^{(0)} \propto \oint_{\mathcal{E}_F} \frac{v_\alpha v_\beta}{v} \, ds.
\]  
(22)
Next we substitute Eq. (20) into Eq. (21) to get \( \tilde{h}_\beta^{(1)} = v \frac{dv_\beta}{ds} \), so that
\[
\sigma_{\alpha\beta}^{(1)} \propto -\oint_{\mathcal{E}_F} v_\alpha \frac{dv_\beta}{ds} \, ds = \oint_{\mathcal{E}_F} v_\beta \frac{dv_\alpha}{ds}.
\]  
(23)
Finally, repeating the process again, we find \( \tilde{h}_\beta^{(2)} = v^2 \frac{d^2 v_\beta}{ds^2} + v \frac{dv_\beta}{ds} \frac{dv_\alpha}{ds} \), so that
\[
\sigma_{\alpha\beta}^{(2)} \propto \oint_{\mathcal{E}_F} v_\alpha \left( v \frac{d^2 v_\beta}{ds^2} + \frac{dv_\beta}{ds} \frac{dv_\alpha}{ds} \right) \, ds = -\oint_{\mathcal{E}_F} v \frac{dv_\beta}{ds} \frac{dv_\alpha}{ds} \, ds.
\]  
(24)
Finally, expanding \( \sigma_{\alpha\beta} \) in the magnetoresistance ratio gives
\[
\rho_B = \frac{\sigma_{xx}^{(2)} \sin^2 \gamma + \sigma_{yy}^{(2)} \cos^2 \gamma}{\sigma_{xx}^{(0)} \sin^2 \gamma + \sigma_{yy}^{(0)} \cos^2 \gamma} - \frac{\sigma_{xx}^{(0)} \sigma_{yy}^{(2)} + \sigma_{xx}^{(2)} \sigma_{yy}^{(0)} - \sigma_{xy}^{(1)} \sigma_{yx}^{(1)}}{\sigma_{xx}^{(0)} \sigma_{yy}^{(0)}}.
\]  
(25)

D. Angular dependence

Consider the angle-dependent part of Eq. (25). The extrema satisfy
\[
0 = \frac{\partial}{\partial \gamma} \left( \frac{\sigma_{xx}^{(2)} \sin^2 \gamma + \sigma_{yy}^{(2)} \cos^2 \gamma}{\sigma_{xx}^{(0)} \sin^2 \gamma + \sigma_{yy}^{(0)} \cos^2 \gamma} \right) = \frac{\sin(2\gamma)(\sigma_{yy}^{(2)} \sigma_{xx}^{(0)} - \sigma_{yy}^{(0)} \sigma_{xx}^{(2)})}{(\sigma_{xx}^{(0)} \sin^2 \gamma + \sigma_{yy}^{(0)} \cos^2 \gamma)^2}.
\]  
(26)
We restrict $0 \leq \gamma \leq \frac{\pi}{2}$ and see that the extrema are always at $\gamma = 0$ or $\gamma = \frac{\pi}{2}$. Specifically, the magnetoresistance is greatest at

\[
\begin{cases} 
\gamma = 0 & \text{if } \sigma_{xx}^{(2)} \sigma_{yy}^{(0)} > \sigma_{xx}^{(0)} \sigma_{yy}^{(2)} \\
\gamma = \frac{\pi}{2} & \text{if } \sigma_{xx}^{(2)} \sigma_{yy}^{(0)} < \sigma_{xx}^{(0)} \sigma_{yy}^{(2)} \\
\text{any } \gamma & \text{if } \sigma_{xx}^{(2)} \sigma_{yy}^{(0)} = \sigma_{xx}^{(0)} \sigma_{yy}^{(2)}
\end{cases}
\quad \text{(27)}
\]

### III. RESULTS

In optimizing the magnetoresistance, we look at several different cases.

#### A. Tight-binding model

The first model we look at is the tight-binding model. The periodic potential for this model is

\[ E = -W_x \cos(ak_x) - W_y \cos(ak_y). \quad \text{(28)} \]

First we consider the isotropic case, $W_x = W_y = W$. Figs. 1(a-d) show the Fermi surface and magnetoresistance curves for several Fermi energies. Fig. 1(e) shows the magnetoresistance ratio as a function of Fermi energy. We can see that $E_F = 0$, shown in Fig. 1(c), has the largest magnetoresistance ratio of the isotropic Fermi surfaces.

Next we consider the anisotropic case. We fix $W^2 = W_x^2 + W_y^2$ so that the magnetoresistance does not become unbounded. For energies near zero, we find when $W_x \neq W_y$ that the Fermi surface becomes disconnected. Fig. 2 shows several anisotropic tight-binding Fermi surfaces. We see from Fig. 3 that the magnetoresistance increases with increasing anisotropy and decreasing $|E_F|$. We also see that the current angle is an important factor. Indeed, the form of the curve is very different for $\gamma = 0$ than for $\gamma = \frac{\pi}{2}$.

Upon studying the $\gamma = \frac{\pi}{2}$ curve, we see that it has two maxima and a relative minimum at $E_F = 0$. The maxima occur at $\frac{E_F}{W} \approx \pm 0.43$, just outside the energy at which the surface becomes disconnected ($\frac{E_F}{W} = \pm \frac{1}{2}(\sqrt{3} - 1) \approx \pm 0.37$). We note that at this energy (and at $E_F = 0$ for the isotropic case), the surface has cusps. This is not an issue for tight binding because the velocity vanishes at these points, but next we look at the free electron model, in which the velocity is the same everywhere.
FIG. 1: Fermi surfaces and magnetoresistance plots for two isotropic tight-binding Fermi surfaces with different Fermi energies. $\rho_0 = \frac{(2\pi)^2 e^2}{\epsilon^2 W}$, $B_0 = \frac{\hbar^2}{\epsilon^2 e W}$. (a) Fermi surface for $E_F = -0.3W$. (b) Magnetoresistance for $E_F = -0.3W$. (c) Fermi surface for $E_F = 0$. (d) Magnetoresistance for $E_F = 0$. (e) Magnetoresistance ratio vs. Fermi energy.
FIG. 2: Fermi surfaces and magnetoresistance plots for two anisotropic tight-binding Fermi surfaces with different Fermi energies and $W_y/W_x = \sqrt{3}$, $\gamma = \pi/2$. $\rho_0 = (2\pi^2/\hbar e^2 W) \gamma$, $B_0 = \hbar e^2 / a^2 \gamma W$. (a) Fermi surface for $E_F = -0.5W$. (b) Magnetoresistance for $E_F = -0.5W$. (c) Fermi surface for $E_F = 0$. (d) Magnetoresistance for $E_F = 0$.

B. Nearly-free electrons

In this section we will consider free electrons and nearly-free electrons on square lattice. If we look at free electrons inside the first Brillouin zone, the Fermi surface is a sphere, and our model predicts constant magnetoresistance. On the other hand, with larger energies and wave vectors in other Brillouin zones, the Fermi surface has cusps, as shown in Fig. 4.

These cusps provide a very large or infinite magnetoresistance ratio. In actuality, the magnetoresistance is not analytical and has a cusp at $B = 0$. However, the free electron model is not accurate. Near a Bragg plane, as the cusps are, there is a nontrivial perturbation
FIG. 3: $B_0 = \frac{h^2}{e^2 W}$. (a) Magnetoresistance ratio vs. degree of anisotropy ($\tan(W_y/W_x)$) for the anisotropic tight binding. $\mathcal{E}_F = 0$ and $\gamma = 0$. (b) Magnetoresistance ratio vs. Fermi energy for anisotropic tight-binding Fermi surfaces, with $W_y/W_x = \sqrt{3}$. Inset: detail of $\gamma = \pi/2$ on same axes as main plot.

on the order of the strength of the periodic potential $U$. The perturbed potential is then [5]

$$\mathcal{E} = \frac{1}{2} \left( \frac{k^2}{2m} + \frac{(k - K)^2}{2m} \right) + \sqrt{\frac{1}{4} \left( \frac{k^2}{2m} - \frac{(k - K)^2}{2m} \right)^2 + |U|^2}. \quad (29)$$

The result is a Fermi surface such as in Fig. 5.
FIG. 4: Free energy model with $k_F a/2\pi = 0.66$ in the second Brillouin zone. $\rho_0 = \frac{2m\alpha^2}{\varepsilon^* \tau}, B_0 = \frac{2m}{\varepsilon^* \tau}$.

(a) Fermi surface. (b) Magnetoresistance with $\gamma = \pi/2$.

C. Rippled Fermi surface

Finally, we look at a contrived example to achieve arbitrarily large magnetoresistance. We can see from Eq. (25) that the magnetoresistance ratio is large when $\frac{d\rho}{ds}$ is large. So consider the potential

$$\mathcal{E}(k, \theta) = \frac{\hbar^2 k^2}{2m} (1 + \alpha \cos(2N\theta)),$$

for $0 < \alpha < 1$ and $N$ an arbitrarily large integer. Figs. 6(a-d) demonstrate this for $N = 10$ and $N = 100$. We see in Fig. 6(e) that the magnetoresistance ratio grows arbitrarily large as $N$ increases. This comes from our definition of the ratio. Although the curvature, or quadratic term, does not change much, the constant term $\rho(0)$ goes to zero as $N$ gets large, so that the magnetoresistance ratio goes to infinity.

IV. CONCLUSIONS

We have shown that it is possible to produce curves which should yield arbitrarily large magnetoresistance ratio.

For this study we made a number of approximations. First, we used a relaxation-time approximation and only considered elastic $s$-wave scattering. This approximation is not
FIG. 5: Fermi surfaces and magnetoresistance plots for nearly free energy model, \( \mathcal{E}_F = 0.44\mathcal{E}_0 \) and \( \gamma = \pi/2 \). \( \rho_0 = \frac{2m^2a^2}{e^2\tau} \), \( B_0 = \frac{2m}{e\tau} \), \( \mathcal{E}_0 = \frac{\hbar^2}{2ma^2} \). (a) Fermi surface, \( U = 0.01\mathcal{E}_0 \). Inset: detail of left “cusp.” (b) Magnetoresistance, \( U = 0.01\mathcal{E}_0 \). (c) Fermi surface, \( U = 0.1\mathcal{E}_0 \). (d) Magnetoresistance, \( U = 0.1\mathcal{E}_0 \).

very accurate. We also applied linear response and low-temperature limits. Using these approximations we were able to reach our results which show a number of ways of achieving a large magnetoresistance.

Future studies could look further into these topics, perhaps by defining a more accurate scattering model, such as non-\( s \)-wave scattering. Also, another definition for magnetoresistance would certainly provide different results, which may be applicable in other situations. Further study should be done on the Fermi surfaces we studied, both to determine how accurate the magnetoresistance estimates are, as well as to find a real material whose Fermi surface is similar to those presented here.
FIG. 6: Fermi surface and magnetoresistance plots for rippled Fermi surface. $\alpha = .25$, $B_0 = \frac{2m}{e\tau}$, $
abla_0 = \frac{2mk_0^2}{e^2\tau}$. (a) Fermi surface for $N = 10$. (b) Magnetoresistance for $N = 10$. (c) Fermi surface for $N = 100$. (d) Magnetoresistance for $N = 100$. (e) Magnetoresistance ratio vs. $N$. 
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