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Magnetoresistance of very pure simple metals

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High-magnetic-field anomalies in pure and simple metals such as Al, K, and In are explained in terms of carrier transport along two-dimensional skipping orbit states. Our approach explains in a very simple way the linear magnetoresistance due to grooves and projections at the sample surface. Our approach also provides an explanation for the negative voltages measured in certain geometries.

Understanding the magnetoresistance data of simple metals such as Al, K, and In has eluded physicists for many decades. Fickett,[1] in his 1971 paper, writes "It has become almost axiomatic that the more simple metals, in the free-electron sense, exhibit magnetoresistance data which are at odds with theory." The general theory[2] predicts that the high-field magnetoresistance should saturate. In contrast, in many experiments the magnetoresistance at high fields increases linearly with magnetic field.[1] A considerable insight into the origin of the linear magnetoresistance was obtained by Bruls *et al.*,[3] who showed that the effect at helium temperature, in millimeter-sized, high-purity samples with a mean free path of 0.3–0.4 mm, is due to sample-thickness variations. Samples with wedges and grooves and protrusions extending across the entire width of the sample were studied (see Fig. 1). Bruls *et al.*[3] also presented a model based on *local* resistivities which is able to explain some of the observations. Subsequently, Soethout *et al.*[4] observed that if a sample of complex geometry is rotated in a magnetic field, the longitudinal resistance is negative over a large range of angular orientations. These observations prompted Overhauser[5] to propose that the negative resistance is a consequence of a magnetoserpentine effect due to charge-density-wave domains.

We present a different point of view: We propose that the high-field magnetoresistance anomalies in these simple metals are due to carriers which for certain geometries and field directions follow skipping orbits along surfaces of the metallic conductor. Our approach bears a close resemblance to a recent discussion[6] of the quantized Hall effect which uses carrier motion along edge states[7] to evaluate transmission probabilities.[8,9] This approach has been successfully applied to a variety of geometries.[10] The close relationship between the phenomena discussed here and electron motion in two-dimensional electron gases is supported by recent work of Hirai *et al.*,[11] who

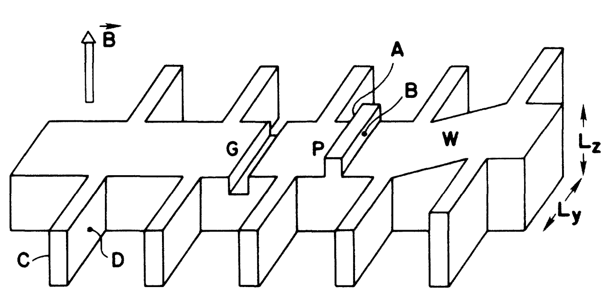

FIG. 1. Conductor consisting of flat portions, grooves (*G*), protrusions (*P*), and wedges (*W*). *A–D* are small contacts. After Bruls *et al.* (Ref. 3).

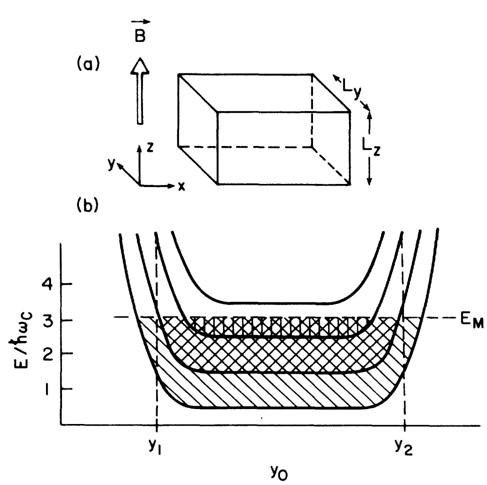

FIG. 2. (a) A rectangular piece of metal of height L_z and width L_y. (b) Energy spectrum of the conductor with side walls at y_1 and y_2 in a large magnetic field.

find that an inhomogeneous two-dimensional conductor also gives rise to a linear magnetoresistance in a certain range of fields. Motion along metallic edge states explains in a natural way the linear magnetoresistance and the conditions under which it occurs.

First, we consider the energy spectrum along a portion of a conductor which is perfect (without any impurities). The conductor shown in Fig. 2(a) is rectangular, and the applied magnetic field is aligned along the z axis. We consider a free-electron Hamiltonian with a confining potential which is zero for points in the interior of the conductor and is infinite for points outside the conductor. The energy of an electron in such a conductor consists of two contributions: For L_z of the order of the Fermi wavelength, the electronic spectrum of a thin perfect film is the same as that discussed in connection with the quantized Hall effect.[7] The energies $E_l(y)$, where l is the Landau-level index, are independent of y, if y is not too close to a sample boundary and given by $E_l(y)=\hbar\omega_c(l+\frac{1}{2})$. Near the sample boundary the energy levels rise as shown in Fig. 2(b). For L_z much larger than a Fermi wavelength, the energy for the two-dimensional strip geometry has to be supplemented by kinetic energy associated with the motion along the z direction. Thus the total energy is

$$E_{ln}(y)=E_l(y)+\hbar^2\pi^2n^2/2mL_z^2\,. \tag{1}$$

For a fixed Landau-level index l the motion in the z direction leads to a ladder of energy levels which as a function of y follow the Landau level of the strip geometry. Near the surfaces of the sample, parallel to the applied field, the energies of Eq. (1) are associated with skipping orbits with velocity along the x direction given by

$$v_x=dE/d\hbar k_x=(dE/dy)(dy/d\hbar k_x)\,,$$

where $y=k_xl_B^2$ and $l_B=(\hbar c/|eB|)^{1/2}$ is the magnetic length. The motion along the z direction is associated with a velocity $v_z=\hbar k_z/m=\hbar n\pi/mL_z$. Away from the surfaces the carriers are on helical orbits around a stationary axis parallel to the magnetic field.

A current can be induced in the conductor of Fig. 2(a) by attaching electron reservoirs with differing chemical potentials. The Fermi energy in the presence of a magnetic field is denoted by E_M. Each channel ln which intercepts the Fermi energy permits a current from one electron reservoir to the other which is just $(e/h)(\mu_1-\mu_2)$ independent of the indices of the energy level and its density of states.[6-9] Therefore, to obtain the total current, $I=(e/h)N(\mu_1-\mu_2)$, we need only count the number of energy levels N with energies $E_{ln}\le E_M$. For the free-electron spectrum assumed here the density of states is $dn/dE_z=(mL_z^2/2\pi^2\hbar^2)^{1/2}E_z^{-1/2}$. Hence the lth Landau level contributes

$$N_l=(2mL_z^2/\hbar^2)^{1/2}[E_M-\hbar\omega_c(l+\tfrac{1}{2})]^{1/2}$$

channels. Thus the current is determined by $N=\sum_{l=0}^{l'}N_l$. Here l' is the maximum Landau-level index such that $\hbar\omega_c(l'+\frac{1}{2})\le E_M$. It is useful to express this result not in terms of the Fermi energy E_M in the presence of a magnetic field but in terms of the Fermi energy E_F in zero magnetic field. Since the number of electrons in a large volume element has to be the same in the presence of a magnetic field as in the absence of a magnetic field there exists a relation between these two Fermi energies. Neglecting boundary corrections due to the finite extension of the sample, this calculation gives

$$N=\tfrac{2}{3}(2mL_z^2/\hbar^2)^{1/2}(E_F)^{1/2}E_F/\hbar\omega_c\,.$$

In terms of the equilibrium density of electrons $n=(1/6\pi^2)(2mE_F/\hbar^2)^{3/2}$ and the magnetic length $l_B=(\hbar c/eB)^{1/2}$, we find that the total number of channels is

$$N=2\pi l_B^2L_zn\,. \tag{2}$$

Note that N is equal to a two-dimensional sheet density nL_z measured in units of the density of electrons $1/2\pi l_B^2$ which can be accommodated in one Landau level. Most importantly, Eq. (2) implies a current which is proportional to $1/B$. In the materials considered here N is very large: at $B=1$ T, a concentration of $n=6\times10^{22}$ cm^{-3}, and a height of $L_z=1$ mm, we obtain $N\approx4.14\times10^{11}$.

Now consider a sample with impurities. An impurity which is within a few magnetic lengths of the sample boundary scatters electrons skipping along the surface. However, this does not affect the current as calculated above. Impurities can change the momentum in the z direction but the direction of motion along x cannot be reversed over large distances compared to a magnetic length.[6] Impurity scattering in the bulk can cause backscattering from one sample side to the other if the probability of finding an impurity in the volume of a bulk helical orbit $V=2\pi l_B^2(l'+\frac{1}{2})L_z\approx2\pi l_B^2E_F/\hbar\omega_c$ is of order 1. Therefore, the relation $n_iV=1$, where n_i is the impurity concentration defines a critical field B_c above which backscattering due to bulk impurities is suppressed. For

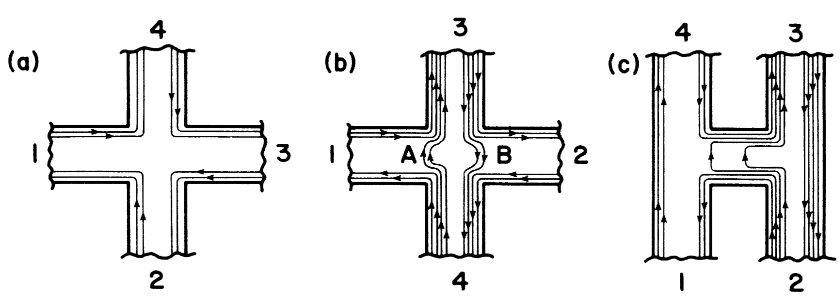

FIG. 3. Schematic quantum channel picture for (a) flat Hall bar cross, (b) protrusion with additional contacts 3 and 4 causing equilibration, and (c) a wedge-shaped sample.

$E_F = 5.6$ eV, a mean free path of 0.3 mm, and a sample size $L_z = 1$ mm, this critical field is extremely low and approximately 860 G. In the high-field regime of interest here ($B \geq 1$ T) elastic backscattering via bulk impurities is completely suppressed.

We now neglect backscattering processes and investigate the results which we obtain by considering the current determined by Eq. (2). Consider first a flat Hall bar cross [see Figs. 1 and 3(a)]. Since the carriers follow the surface, the total transmission probabilities T_{ij} for carriers entering in probe j and transmitted into probe i are given by $T_{41} = T_{34} = T_{23} = T_{21} = N$. All other transmission probabilities are zero in the absence of backscattering. A schematic picture of the connection of the channels with the contacts given in Fig. 3(a). For small temperatures the transmission probabilities evaluated at the equilibrium Fermi energy are the transport coefficients which relate the carrier flux incident at probe i with the chemical potentials μ_i applied at the probes,[9]

$$I_i = (e/h) \left[(M_i - R_{ii})\mu_i - \sum_j T_{ij}\mu_j \right] . \tag{3}$$

Here M_i is the number of channels of the probe i and R_{ii} is the total reflection probability. Assuming no scattering at the contacts, Eq. (3), with the transmission probabilities as specified above,[6] yields a Hall resistance $\mathcal{R}_H = (h/e^2/)N$. It is linear in field B without any features.

Next consider a portion of the conductor with a groove. First consider a two-terminal situation. The height of the conductor away from the groove is L_1 and under the groove it is L_2. Away from the groove the conductor supports $N_1 = N(L_1)$ channels and under the groove $N_2 = N(L_2)$ channels. Hence the maximum transmission probability is $T = N_2$. The portion of the current which is reflected is $R = N_1 - T = N_1 - N_2$. Note that we do not imply that carriers which are reflected skip the entire width of the sample along the vertical wall of the groove. But carriers which leave this wall start a helical orbit until after repeated scattering events the vertical wall is again reached and the carrier proceeds along a differing skipping orbit. If a four-terminal measurement is made with leads on the same side of the conductor on either side of the groove, the resistance is[6,10,12] $\mathcal{R}_L = (h/e^2)R/(N_1 T)$ and hence $\mathcal{R}_L = (h/e^2)(N_1 - N_2)/(N_1 N_2)$. If this is normalized with the Hall resistance we find

$$\mathcal{R}_L/\mathcal{R}_H = (L_1 - L_2)/L_1 . \tag{4}$$

This is a key result of Bruls *et al.*[3] The resistance caused by a groove is proportional to the depth of the groove and proportional to the Hall resistance.

Consider next a portion of the conductor with a protrusion. Here the number of states N_2 of the conductor under the protrusion is larger than the number of states N_1 away from the protrusion. However, Ref. 3 found that a protrusion and a groove of the same height (depth) give rise to the same linear magnetoresistance. Clearly, this is impossible if the conduction electrons would not sense the additional available states in the region of the protrusion. Inelastic scattering is needed to explain this result. To incorporate inelastic scattering inside the protrusion we introduce additional contacts[6] attached in this region of the conductor to either side of the conductor. The channel picture including the fictitious contacts 3 and 4 is depicted in Fig. 3(b). Of the N_2 channels in the region of the protrusion, $N_2 - N_1$ channels are reflected on either side of the protrusion. All N_2 channels enter the fictitious contacts. In the incident carrier stream N_1 channels are occupied up to a common chemical potential μ_1. At contact 3, inelastic scattering occurs and the current is redistributed among all N_2 channels up to a common chemical potential μ_3. At contact 4 we have, therefore, carriers in $N_2 - N_1$ channels which are filled up to a common potential μ_3 and N_1 incident channels filled up to a potential μ_2. Using Eq. (3), we find

$$\mu_3 = \frac{N_1\mu_1 + (N_2 - N_1)\mu_2}{2N_2 - N_1} , \tag{5}$$

$$\mu_4 = \frac{(N_2 - N_1)\mu_1 + N_2\mu_2}{2N_2 - N_1} , \tag{6}$$

and a total two-terminal transmission and reflection probability given by $T = N_1 N_2/(2N_2 - N_1)$, $R = N_1(N_2 - N_1)/(2N_2 - N_1)$. If a longitudinal four-terminal measurement is made, the resistance is given by

$$\mathcal{R}_L = (h/e^2)R/(N_1 T) = (h/e^2)(L_2 - L_1)/(N_1 L_2)$$

or $\mathcal{R}_L/\mathcal{R}_H = (L_2 - L_1)/L_2$. Therefore, a groove and protrusion give rise to the same additional linear magnetoresistance (for small heights, small depths) if the protrusion is wide enough for inelastic scattering to be effective.

There is an important additional test of the picture developed here. Suppose that small contacts can be made on either side of the protrusion. In Figs. 1 and 3(b) these contacts are labeled A and B. Contact A measures carriers which are reflected emanating from reservoir 4 and, therefore, indicates a chemical potential μ_4 given by Eq. (6). Contact B measures carriers emitted by reservoir 3 and indicates a chemical potential μ_3 given by Eq. (5). Hence the voltage measured between contacts A and B is given by

$$\mu_A - \mu_B = \mu_4 - \mu_3 = -[L_1/(2L_2 - L_1)](\mu_1 - \mu_2) . \tag{7}$$

We emphasize that the voltage across contacts A and B has a sign which is opposite to the voltage difference across the protrusion. An effect similar to that predicted by Eq. (7) was indeed observed by Bruls *et al.*[3] If the magnetic field is taken to be parallel to a voltage lead of the conductor in Fig. 1, the voltage lead acts like a very high protrusion. If the voltage is measured on small contacts on either side of such voltage lead (C and D in Fig. 1), a negative voltage is measured.

Finally, we investigate the portion of the conductor with a wedge. An equivalent four-terminal channel picture is shown in Fig. 3(c). On the left-hand side of the wedge the conductor has $N_1 = N(L_1)$ channels. On the right-hand side the conductor supports $N_2 = N(L_2)$ channels. Take contact 4 to be the carrier source and contact 3 to be the carrier sink and measure the voltage between contact 1 and 2. This longitudinal resistance $\mathcal{R}_{43,12}$ is ideally *zero*. Carriers entering contact 4 see an increasing number of available channels and, therefore, can penetrate the wedge without being reflected. Now take contact 2 to be the carrier source and contact 1 to be the sink, and measure the voltage between contact 3 and 4. A portion of the carriers entering from contact 2 is reflected into contact 3 since the number of available channels decreases as the carriers enter the wedge. Determining all transmission probabilities and using Eq. (3) yields $\mathcal{R}_{21,34}=(h/e^2)(N_2-N_1)/(N_1N_2)$, i.e., the same result as for a groove or a protrusion. The asymmetric behavior of the longitudinal resistance measured on either side of a wedge is indeed experimentally observed.[3] The uncorrected data[3] show a linear increase with magnetic field for $\mathcal{R}_{12,43}\equiv\mathcal{R}_{21,34}$. However, $\mathcal{R}_{43,12}$ is not zero but decreases with increasing field. That $\mathcal{R}_{43,12}$ is not zero is to be expected: We have after all completely neglected backscattering. The extent to which this resistance decreases with increasing field gives, therefore, a good indication of the suppression of backscattering.

It is remarkable that by completely neglecting backscattering we have been able to explain the main features of the magnetoresistance size effects in these pure and simple metals. Since skipping along surfaces is required, it is evident from our discussion that protrusions or grooves which do not extend all the way across the width of the sample, ideally, do not give rise to resistance at all. It is also clear that the surface states discussed here provide a very natural explanation for the negative voltages observed in such metallic conductors of complicated geometry.

If it is possible to produce high-purity metallic samples with geometrical dimensions smaller than the mean free path, we expect size effects at much lower magnetic fields. Indeed it should be possible to observe size effects similar to those that have recently found intense interest in ballistic *submicronmeter* conductors.[13,14]

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