

Classical origin for a negative magnetoresistance and for its anomalous behavior at low magnetic fields in two dimensions

Rémi Jullien^a, Alexander Dmitriev^b, and Michel Dyakonov^c

^a*Laboratoire des Verres[†], Université Montpellier 2, place E. Bataillon, 34095 Montpellier, France*

^b*A. F. Ioffe Physico-Technical Institute, 194021 St. Petersburg, Russia*

^c*Laboratoire de Physique Mathématique[†], Université Montpellier 2, place E. Bataillon, 34095 Montpellier, France*

[†] *Laboratoire associé au Centre National de la Recherche Scientifique (CNRS, France).*

Recibido el 24 de noviembre de 2003; aceptado el 12 de octubre de 2004

The classical two-dimensional problem of non-interacting electrons scattered by a static impurity potential in the presence of a magnetic field is investigated both analytically and numerically. A strong negative magnetoresistance is found, due to freely circling electrons, which are not taken into account by the Boltzmann-Drude approach. Moreover, at very low magnetic fields, the resistivity turns out to be proportional to $|B|$, due to a memory effect specific for backscattering events.

Keywords: Magnetotransport; magnetoresistance; semiconductors.

El problema bidimensional de electrones no interactuantes dispersados por un potencial estático en presencia de un campo magnético, se investigó tanto analítica como numéricamente. Se encuentra una fuerte magneto-resistencia negativa debida a los electrones libres circulantes, los cuales no se contemplan en la aproximación de Boltzman-Drude. Mas aún, a un campo magnético muy pequeño, la resistividad se sale de la proporcionalidad de $|B|$, debido al efecto de memoria específico para los eventos de retrodispersión.

Descriptores: Magneto-transporte; magneto-resistencia; semiconductores.

PACS: 05.60.+w; 73.40.-c; 73.50.Jt

The negative magnetoresistance, *i.e.* decrease of resistance in magnetic field, frequently observed in semiconductors and as in metals, remained a mystery for a long time. The first interpretation of Altshuler *et al.* [1] based on quantum interference effects (weak localization) might explain the drop of resistivity often observed at very low values of the classical parameter $\beta = \omega_c \tau$ ($\omega_c = eB/mc$ is the electron cyclotron frequency, τ is the momentum relaxation time, B is the magnetic field, e and m are the electron charge and effective mass, respectively). However, in some experiments, a relatively large (up to 50%) decrease of the resistivity is observed up to $\beta \gtrsim 1$ or even at $\beta \gg 1$. This high-field effect is not so well understood, and is either attributed to the effect of electron-electron interaction [2], which was considered theoretically in Refs. 3, or left without any explanation. Moreover, in some experiments [4], the resistivity is found to decrease quasi-linearly with the applied field for very small values of β , in contrast with the generally expected quadratic behavior. In this paper, we show that all these phenomena can be recovered in the framework of a simple classical approach that we have already proposed [5, 6] and which takes into account memory effects not present in the conventional Boltzmann-Drude (BD) approach.

We first recall that the BD approach predicts zero magnetoresistance. The Drude conductivity tensor is given by:

$$\sigma_{xx} = \frac{\sigma_0}{1 + \beta^2}, \quad \sigma_{xy} = \frac{\sigma_0 \beta}{1 + \beta^2}, \quad (1)$$

where $\sigma_0 = ne^2\tau/m$ is the zero-field conductivity, and n is the electron concentration. For the resistivity tensor, it follows that $\rho_{xx} = \rho_0 = 1/\sigma_0$, $\rho_{xy} = \beta/\sigma_0 = B/nec$,

and therefore the longitudinal resistivity is independent of the magnetic field. This result applies to degenerate electrons for which the time τ , entering Eq. (1) should be taken at the Fermi energy (for non-degenerate electrons one should take into account the dependence of the scattering time τ on the electron energy which, after averaging Eqs. (1) over the Boltzmann energy distribution, results in a *positive* magnetoresistance). Therefore, to explain the experimental facts in a classical framework, one should go beyond the BD approximations.

In our classical picture, we consider non-interacting 2D electrons with a given energy scattered by short-range impurity centers in the presence of a magnetic field perpendicular to the 2D plane, and we show that for any type of scattering, a strong negative magnetoresistance exists up to $\beta \gg 1$. We perform computer simulations of the electron dynamics in such a system with hard disk impurities (the so-called Lorentz model [7, 8] and variants), and find an excellent agreement between the numerical results and a very simple theory which is based on previously known results [7, 8]. Moreover a thorough analysis of our numerical results, at very small β , reveals that the resistivity varies linearly with the field, an anomaly that we explain by invoking memory effects associated with backscattering.

The main idea put forward in Refs. 7 and 8 is that, except for the case of small β , the BD approach does not work, even as a first approximation, because of the existence of “circling” electrons, that never collide with the short-range scattering centers, the fraction of such electrons being [8]

$$P = \exp(-2\pi R/\ell) = \exp(-2\pi/\beta), \quad (2)$$

where $R = v/\omega_c$ is the cyclotron radius, v is the electron (Fermi) velocity, and $\ell = v\tau$ is the electron mean free path. Contrary to the intrinsic assumption in the BD approach, an electron that happens to make one collision-less cycle will stay on its cyclotron orbit forever. The behavior of the rest of the electrons, the “wandering” electrons, in terms of Ref. 8, whose fraction is $1 - P$, is controlled by the parameter NR^2 , the number of scatterers within the cyclotron orbit, N being the impurity concentration. For $NR^2 \gg 1$ they behave basically as predicted by the BD theory, with an important modification: after a collision with a given scatterer there is a probability P that the electron will re-collide with the same scatterer without experiencing any other collisions. As a result, for $\beta \gg 1$, the electron will re-collide with the same impurity center many times, and its trajectory will have the form of a rosette, sweeping a circular area of radius $2R$ around the impurity center [7]. Since the number of impurities inside this area, $4\pi NR^2$, is large, the electron will eventually collide with one of them, and thus continue its diffusion in the 2D plane. As it follows from the results of Ref. 8, frequent re-collisions with the same center, will lead to the isotropization of scattering, so that the effective τ in Eq. (1) becomes field-dependent. This effect is absent if the scattering is isotropic. At strong fields, when the parameter NR^2 becomes small enough, the rosettes around different scatterers do not overlap anymore, the colliding electrons become localized and give zero contribution to both σ_{xx} and σ_{xy} . This means that a percolation transition should occur [7]. The calculated threshold is $(NR^2)_c = 0.36$ [8]. Thus, there are two characteristic values of the magnetic field, B_1 defined by $\omega_c = 1/\tau$ ($\beta = 1$), and B_2 defined by $\omega_c = v\sqrt{N}$ ($NR^2 = 1$). The ratio $B_1/B_2 = (Nd^2)^{1/2} \ll 1$, where d is the scattering cross-section, is the small parameter of the theory.

It follows, that from the results of Ref. 8 for the simple cases of isotropic scattering and $B \ll B_2$ ($NR^2 \gg 1$), that the conductivity tensor for wandering electrons is simply given by the BD expressions, Eq. (1), with an additional factor $(1 - P)$ in both σ_{xx} and σ_{xy} . The circling electrons behave like free electrons with an effective concentration nP , giving a zero contribution to σ_{xx} , but contributing a term $P\sigma_0/\beta = Pnec/B$ to σ_{xy} ; and this is the reason why the magnetoresistance is negative. This role of circling electrons was overlooked in Ref. 8, but was recognized later [9] (see also Refs. 10 and 11).

Thus, the conductivity tensor is given by:

$$\sigma_{xx} = \sigma_0 \frac{1 - P}{1 + \beta^2}, \quad (3)$$

$$\sigma_{xy} = \sigma_0 \left((1 - P) \frac{\beta}{1 + \beta^2} + P \frac{1}{\beta} \right). \quad (4)$$

As a consequence, for the resistivity tensor we obtain

$$\rho_{xx} = \rho_0 \frac{1 - P}{1 + P^2/\beta^2}, \quad \rho_{xy} = \rho_0 \beta \frac{1 + P/\beta^2}{1 + P^2/\beta^2}. \quad (5)$$

Formulas equivalent to Eqs. (3,4) were previously obtained by Baskin and Entin [11] for scattering by randomly posi-

tioned antidots. The expression for ρ_{xx} clearly exhibits negative magnetoresistance. Since the terms P/β^2 and P^2/β^2 are small for any β , Eqs. (4) are very similar to

$$\rho_{xx} = \rho_0(1 - P), \quad \rho_{xy} = \rho_0\beta = \frac{B}{nec}, \quad (6)$$

with better accuracy than than 2% for ρ_{xx} , and 4% for ρ_{xy} . Note that at low fields, Eqs. (4) and (5) predict an exponentially small magnetoresistance.

Let us now present the results of our numerical simulations. In our model, a point particle (electron) with a given absolute value of velocity, v , is scattered by disks of diameter d randomly positioned on a plane inside a square box of edge length L (we take $L/d = 1000$ to be sure that L stays more than an order of magnitude larger than the electronic mean-free path). Periodic boundary conditions are imposed at the edges of the square box. Both the hard-disk (Lorentz) model, which exhibits anisotropic scattering, and a modified model with isotropic scattering are studied. To characterize the coverage, we introduce a dimensionless concentration of scatterers $c = \pi Nd^2/4$, which was changed from $c = 0.025$ to $c = 0.2$. Studies of the percolation phenomena are beyond the scope of the present study.

In the simulation, we first choose an initial electron position at random with an initial velocity along the x -direction. In a magnetic field perpendicular to the plane, the electron trajectory is made of successive circular arcs of radius R . For each collision, we determine the intersections of the trajectory with the disk periphery (the impact point), which gives us the impact parameter b , and the scattering angle ϕ , accordingly. We follow the electron velocities $v_x(t)$, and $v_y(t)$ during a time $t = 20\tau$ to get reliable results for the integral below, and calculate the components of the diffusion tensor by the standard formula:

$$D_{ij} = \frac{1}{2} \int_0^\infty \langle v_i(0)v_j(t) \rangle dt. \quad (7)$$

For each value of the field and the disk concentration, we take the average over 10^2 independent disk configurations, and for each configuration, over 10^6 independent trials for the initial electron position. Of course, at $B = 0$, the trajectories are straight-line segments, and D_{xy} should vanish (this provides a nice test for the numerical precision). The conductivity tensor, being proportional to the diffusion tensor, and the components of the resistivity ρ_{ij} are calculated as $D_{ij}/(D_{xx}^2 + D_{xy}^2)$, with an appropriate normalization. For the Lorentz model, numerical calculations of this type were previously performed [10] with an emphasis on the percolation phenomenon.

The numerical results for ρ_{xx} , as a function of β for the model with isotropic scattering, are presented in Fig. 1 (top). The resistivity is normalized to the BD zero-field value, ρ_0 . The thick line is the theoretical curve predicted by Eq. (4). One can see that the theoretical and numerical curves are

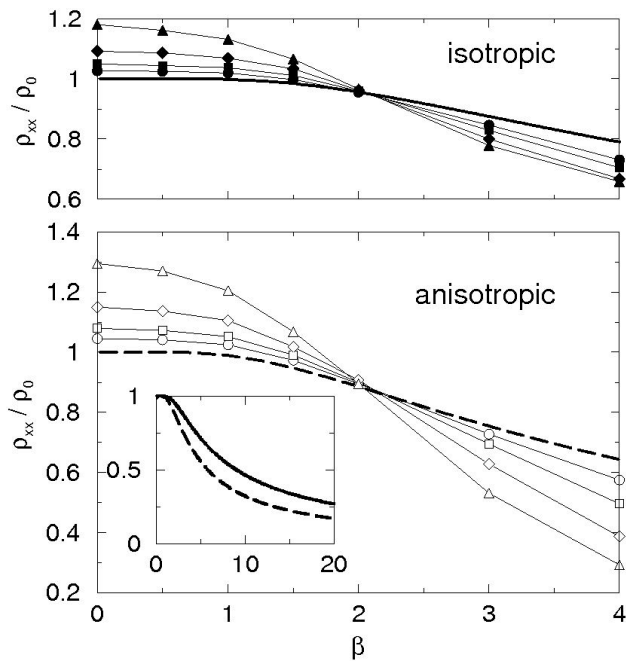


FIGURE 1. Numerical results for the resistivity as a function of $\beta = \omega_c \tau$ for different impurity concentrations, compared to the theoretical curve given by Eq. (4) for the isotropic scattering model (top) and for the Lorentz model with anisotropic scattering (bottom). Circles, squares, diamonds, and triangles correspond to $c = 0.025, 0.05, 0.1, 0.2$, respectively. The continuous and dashed thick lines are the theoretical curves in the isotropic and anisotropic cases, respectively; and they are depicted in the inset on a larger scale. Note the surprising crossings at $\beta = 2$.

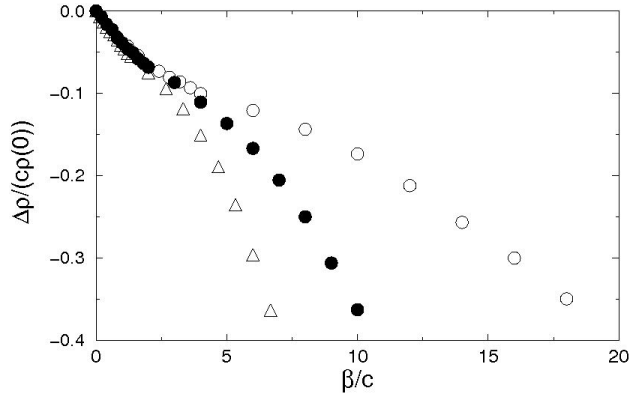


FIGURE 2. Numerical results for the magnetoresistance $\Delta\rho/\rho(0)$ as a function of $\beta = \omega_c \tau$ for different impurity concentrations. Open circles, filled circles, and open triangles correspond to $c = 0.05, 0.1, 0.15$, respectively. Both quantities have been divided by c to better show the universal behavior at low field predicted by Eq. (7).

qualitatively similar and that the quantitative agreement improves as c decreases. In the limit $c \rightarrow 0$, the numerical results converge to the theoretical curve, as they should.

Note that for a finite c , the value of the zero-field resistivity is higher than the BD value ρ_0 . The relative correction for small c is proportional to $c \ln(1/c)$, and is due to re-collisions with the same impurity, which are not accounted for by the

Boltzmann equation [12]. Note also that the numerical results for a finite c approach the limiting theoretical curve from above for $\beta < 2$, and from below for $\beta > 2$. This may be qualitatively explained as follows. On the one hand, at small β the resistivity for a finite c is higher than the $c \rightarrow 0$ BD value due to the $c \ln(1/c)$ correction. On the other hand, at large β we are on the way to the percolation threshold, where ρ_{xx} (but not ρ_{xy} !) becomes zero. So, obviously, for large β and finite c , the resistivity should be lower than the limiting value given by Eq. (4).

Figure 1 (bottom) displays quite similar results obtained for the hard disk Lorentz model (anisotropic scattering). The theoretical curve (thick dashed line) was calculated using the results of Ref. 8 for the wandering electrons, adding the contribution of circling electrons, as explained above. In both cases, all the numerical curves for different c cross the limiting theoretical curve at the same point $\beta = 2$ (within our numerical precision). We have no explanation for this surprising finding so far.

When analyzing our numerical results for very small β values, we have lots of difficulties in recovering a clear quadratic behavior, in contrast with what we previously claimed [5]. Therefore, we have re-done our simulations in the Lorentz case (anisotropic scattering) by running many more β values in the range $0 < \beta < 1$ with a higher precision (the average is now performed over ten times more trajectories). The results for the three concentration values are reported in Fig. 2 as a plot of $\Delta\rho/(c\rho(0))$ versus β/c , where $\Delta\rho = \rho_{xx}(\beta) - \rho_{xx}(0)$, and $\rho(0) = \rho_{xx}(0)$ is the zero field value of the resistivity. In this figure, one clearly observes a characteristic anomalous linear behavior for $\beta \lesssim 2c$ followed by a more conventional parabolic dependence on β .

To understand this result, we have invoked memory effects associated with back scattering events [6]. For simplicity, let us first consider the case $B = 0$ and a particle which, after going a distance $x \gg d$ without collisions, experiences backscattering at an angle $\phi = \pi$, and then returns to the initial point. The probability of this round trip of length $2x$ is proportional to $\exp(-x/\ell)$, not to $\exp(-2x/\ell)$, as would suggest the BD approach, since the existence of a free corridor of width d allowing the first part of the journey guarantees a collision-less return. This is not the case for scattering angles outside the interval on the order of d/x around the value $\phi = \pi$, when the probabilities for a free path x before and after collision become independent and equal to $\exp(-x/\ell)$. Since typically $x \sim \ell$, the probability of backscattering in the interval $\Delta\phi \sim d/\ell$ around $\phi = \pi$ is enhanced, and this should lead to an additional increase of resistivity on the order of $d/\ell \sim c$, i.e. same order of magnitude as the contribution of return loops involving two or more intermediate scatterings. One can say that the existence of a free corridor effectively enhances backscattering in the interval $\Delta\phi$, roughly by a factor of 2, thus increasing the transport cross-section by an amount $\sim d\Delta\phi$.

We attribute the low field anomaly in Fig. 2 to the influence of field on this effect. In the presence of even a

small magnetic field, the electron trajectories before and after collisions can not follow the same path anymore. At high enough fields this kills the memory effect and, as a consequence, reduces the resistivity. Thus a negative magnetoresistance with a characteristic magnetic field defined by the relation $\beta = d/\ell \sim c \ll 1$ appears. We do not have a regular method for calculating analytically the magnetoresistance at low fields. However, some qualitative conclusions may be drawn as follows.

Consider again backscattering by an angle exactly equal to π , but in the presence of magnetic field. In order to have collision-less paths of length x before and after scattering, the centers of all disks should be outside the corridor of width d surrounding these paths. The probability of this is proportional to $P = \exp(-NS)$, where N is the disk concentration and S is the joint area of the two corridors. The overlapping region should not be counted twice. While at $B = 0$ there is full overlap, $S = xd$ and $P = \exp(-x/\ell)$, in the presence of a magnetic field the overlap diminishes and the relevant area increases. In the low-field limit, this increase can be easily calculated to be $\Delta S = x^3/(3R) \sim B$, so that P decreases linearly with B . This means that the (negative) magnetoresistance is linear in B for $R \gg \ell^2/d$, or $\beta \ll d/\ell$. For higher fields, such that $\beta \gg d/\ell$, the two corridors practically cease to overlap and one has $S = 2xd$, $P = \exp(-2x/\ell)$. Similar considerations apply to backscattering in the interval $\Delta\phi \sim d/\ell$.

A similar contribution comes from the influence of a magnetic field on the probability of the simplest re-collision process $1 \rightarrow 2 \rightarrow 1$, which necessarily involves backscattering in the same angular interval $\Delta\phi$. At $B = 0$, the memory effect increases the relative contribution of this process to the resistivity by an amount on the order of c , and again the curving of the trajectories in the magnetic field will increase the total area S , and thus reduce the probability of this process. In the low-field limit, one finds again that the area increase, ΔS , is linear in B . These qualitative considerations lead us to the following conclusions:

- (i) A characteristic magnetic field exists, at which the classical parameter $\beta = \omega_c\tau$ is small: $\beta_c = d/\ell \sim c \ll 1$.
- (ii) The total drop of resistivity in the region $\beta \lesssim \beta_c$ is on the order of $d/\ell \sim c$.
- (iii) At $\beta \ll \beta_c$ the resistivity ρ_{xx} is linear in the magnetic field exhibiting the $|B|$ cusp observed in our simulation [13].
- (iv) For $\beta_c \ll \beta \ll 1$; only quadratic corrections in B remain, which are on the order of $c\beta^2$. (It can be shown that these corrections come from the influence of the magnetic field on the contribution of return loops).

This means that at low fields, $\beta \ll 1$, the magnetoresistance, $\Delta\rho$, is described by the formula:

$$\Delta\rho/\rho(0) = -c(f(\beta/c) + A\beta^2), \quad (8)$$

where A is a numerical constant and $f(\xi)$ is a function which behaves as $|\xi|$ for small values of its argument and saturates at some value on the order of 1 for $|\xi| \gg 1$. This theoretical prediction is in excellent agreement with the simulations results presented in Fig. 2, which allow to estimate $A \simeq 0.3$. Some recent experimental results [4] for magnetoresistance of 2D electrons in a disordered array of antidots, which is almost exactly the experimental realization of the Lorentz model, exhibit such a predicted anomalous behavior. We have also presented a quantitative fit (without any adjusting parameter) in Ref. 5.

In conclusion, we have shown that both a negative magnetoresistance and its low-field anomaly can be explained in a classical framework taking into account corrections to the standard Boltzmann-Drude approach. We are convinced that these results, established here by using the Lorentz model and variants, can apply to any other kind of disordered short range potential. In the future, we will consider the more complicated case of long range disorder in order to check numerically available theoretical predictions [14].

-
- 1. B.L. Altshuler, D. Khmel'nitskii, A.I. Larkin, and P.A. Lee, *Phys. Rev. B* **22** (1980) 5142.
 - 2. M.A. Paalanen, D.C. Tsui, and J.C.M. Hwang, *Phys. Rev. Lett.* **51** (1983) 2226.
 - 3. B.L. Altshuler, A.G. Aronov, and P.A. Lee, *Phys. Rev. Lett.* **44** (1980) 5142; H. Fukuyama, *J. Phys. Soc. Jpn.* **48** (1980) 2169; A. Houghton, J.R. Senna, and S.C. Ying, *Phys. Rev. B* **25** (1982) 2196, 6468; S.M. Girvin, M. Jonson, and P.A. Lee, *Phys. Rev. B* **26** (1982) 1651.
 - 4. G.M. Gusev *et al.*, *Surface Science* **305** (1994) 443; O. Yevtushenko, G. Lütjering, D. Weiss, and K. Richter, *Phys. Rev. Lett.* **84** (2000) 542.
 - 5. A. Dmitriev, M. Dyakonov, and R. Jullien, *Phys. Rev. B* **64** (2001) 233321.
 - 6. A. Dmitriev, M. Dyakonov and R. Jullien, *Phys. Rev. Letters* **89** (2002) 266804.
 - 7. E.M. Baskin, L.N. Magarill, and M.V. Entin, *Sov.Phys. JETP* **48**, 365 (1978).
 - 8. A.V. Bobylev, F.A. Maaø, A. Hansen, and E.H. Hauge, *Phys. Rev. Letters* **75** (1995) 197.
 - 9. A.V. Bobylev, F.A. Maaø, A. Hansen, and E.H. Hauge, *J. Stat. Physics* **87** (1997) 1205.
 - 10. A. Kuzmany and H. Spohn, *Phys. Rev. E* **57** (1998) 5544.
 - 11. E.M. Baskin and M.V. Entin, *Physica B: Condensed Matter* **249-251** (1998) 805.
 - 12. J.M.J. van Leeuwen and A. Weijland, *Physica* **36** (1967) 457; A. Weijland and J.M.J. van Leeuwen, *Physica* **38** (1968) 35; C. Bruin, *Phys. Rev. Letters* **29** (1972) 1670.

13. Strictly speaking, the magnetoresistance is an analytical function of B : a careful analysis shows that, in a very small region around zero field, where $\beta \lesssim c^2$, the dependence on B should be parabolic. This region is not accessible in our simulation. See V. Cheianov, A. Dmitriev, and V. Kachorovskii, to appear in *Phys. Rev. B*.
14. M.M. Fogler, A.Yu. Dobin, V.I. Perel, and B.I. Shklovskii, *Phys. Rev. B* **56** (1997) 6823; A.D. Mirlin *et al.*, *Phys. Rev. Lett.* **83** (1999) 2801.