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Magnetic Breakdown and Hall Effect in Iron

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We develop a theory which seems to reproduce qualitatively the experimental features observed in the Hall resistivity of iron at very high magnetic fields (B ~ 200 kG). Magnetic breakdown in invoked to explain transitions between two linear behaviors of the Hall resistance, which in iron may be due to transitions from closed compensated orbits (low-field regime), to open and closed orbits (high-field regime). Several model calculations are done, considering spherical Fermi surfaces and different effective masses for electron and hole-like carriers, thus yielding a linear Hall resistance in the low-field region, when compensation dominates.

Desenvolvemos uma teoria que reproduz qualitativamente o comportamento experimental observado na resistividade de Hall do Ferro a campos magnéticos muito altos (B ~ 200 kG). Transições entre dois comportamentos lineares da resistividade de Hall, as quais no Ferro podem ser devido a transições de órbitas compensadas (regime de baixo campo) para órbitas abertas e fechadas (regime de alto campo), são explicadas pela ruptura magnética. Estudam-se vários modelos, conside-

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rando superfícies de Fermi esféricas e diferentes massas efetivas para portadores do tipo elétron e buraco, obtendo-se uma resistividade de Hall linear na região de campo baixo onde domina a compensação.

1. INTRODUCTION

The galvanomagnetic properties of ferromagnetic metals at very high magnetic fields are currently being the subject of intensive experimental studies, yielding some not completely understood results for the transverse magnetoresistance and Hall effect in iron[1-4]. Experiments done at low temperature and up to 200 kOe [3,4] show field dependent as well as oscillatory behaviors of magnetoresistance which strongly suggest that magnetic breakdown is playing an important role.

One of these effects, such as that shown in Fig.10 of reference 3, concerns the value of the exponent η in the relation $[\Delta\rho/\rho_0] \approx B^{\eta}$, where ρ is the transverse magnetoresistance and B the magnetic field. At low fields the magnetoresistance exhibits the typical behavior of a compensated metal ($\eta \approx 2$ for all directions). However for fields above 100 kG the exponent η decreases to values close to 1 for any general field direction. It has been suggested that this phenomenon is associated to magnetic breakdown between two orbital regimes which yield quadratic behaviors ($\eta = 2$) of magnetoresistance, being the high-field coefficient smaller than the low-field one[5]. In the case of iron this can be accomplished through transitions from compensated to open orbits or from a compensated regime to another compensated regime. Evidence of high-field open orbits has been found recently by a number of authors for some field directions[4,5].

The Fermi surface of ferromagnetic iron[6,7] is enough intricate to allow many instances of the above transitions. The spin-orbit interaction removes the accidental degeneracy at some symmetry points yielding many gaps capable of undergoing magnetic breakdown[8].

The experimental results for the Hall resistance (see for example Fig. 7 and 14(d) of reference 3) also show evidence of interband tunneling and close relationship with the behavior observed in the transverse magnetoresistance.

In this work we want to suggest that the same effect, which seems to explain the anomalous field dependence of the transverse magnetoresistivity, can account for the facts observed in studying the Hall effect.

In order to get that goal, we have made a series of model calculations using spherical Fermi surfaces for electron and hole bands. To remove, in first approximation, the spherical symmetry (very convenient for calculation) we have considered different effective masses for electron-like and hole-like carriers. All the orbits in the low -field limit are compensated (which seems to be the case of iron) and break down to at least one open orbit in the high field regime. The method to calculate the resistivity tensor is exactly the same as that of Falicov and Sievert[9]. Basically, it consists of a semiclassical solution of the Boltzmann equation for a set of electronic orbits in $\vec{k}$--space coupled by means of magnetic breakdown at some points, called breakdown junctions. This is discussed briefly in section 2.

In section 3 we present our results and make the final conclusions. It will be seen that close agreement with experiments (for example with Fig. 7 of reference 3) is achieved for some values of our parameters.

2. MODEL CALCULATIONS

In the absence of magnetic breakdown, and in the relaxation time approximation the solution of the Boltzmann equation for the electronic distribution along a circular orbit is given by

$$g_\nu(\phi_{\vec{k}}) = g_\nu(\phi_0) \exp\left[-(\phi_{\vec{k}} - \phi_0)/\omega_c\tau\right] +$$

$$+ \int_{\phi_0}^{\phi_{\vec{k}}} d\phi_{\vec{k}'} \exp\left[(\phi_{\vec{k}'} - \phi_{\vec{k}})/\omega_c\tau\right] \cdot \left[-\frac{|e|v_F}{\omega_c} \cdot \frac{\vec{E}\cdot\vec{k}'}{k_F}\right] \quad (2.1)$$

where $g_\nu(\phi)$ is the deviation of the distribution function from equilibrium at the Fermi surface, ν is a band index, τ is the relaxation time, ω_c is the cyclotron frequency corresponding to that orbit, and v_F and k_F are the Fermi velocity and wave vector respectively.

In relation (2.1) we are mapping the $\vec{k}$-space using the well known set of variables (ε, k_H, ϕ) [10], where the energy ε is a constant and equal to the Fermi energy, k_H is the constant projection of the $\vec{k}$--vector along the magnetic field direction and ϕ is an angle which describes our orbit in the plane perpendicular to the magnetic field. The solution (2.1) is then a path integral which goes backwards in time, relating the value of g_ν at a given point $\vec{k}$ with the values at previous points along the orbit. Perturbations from equilibrium are driven by the electric ($\vec{E}$) and magnetic ($\vec{H}$) fields, while decaying with a life-time τ.

When magnetic breakdown is taken into account interband transitions are possible at some points in $\vec{k}$-space (junctions), with a tunneling probability given by

$$T = \exp(-H_0/H) \quad , \tag{2.2}$$

where H_0 is the breakdown field

$$H_0 = \alpha \; \frac{|V_G|^2 mc}{\varepsilon_F |e| \hbar} \quad , \tag{2.3}$$

$2|V_G|$ being the energy gap between bands and α a numerical factor of the order of unity.

The breakdown junctions divide the coupled orbits into n different segments and the problem reduces to a set of n linear equations for the g_ν at the junctions[9]. With the knowledge of this initial values we can easily calculate the conductivity tensor through the relation

$$\vec{j} = - \frac{|e|}{8\pi^3} \sum_\nu \int \vec{v}_\nu(\vec{k}) \; g_\nu(\vec{k}) \; \delta(\varepsilon_\nu(\vec{k}) - \varepsilon_F) d^3k = \vec{\sigma}\cdot\vec{E} \tag{2.4}$$

and then the resistivity tensor by means of matrix inversion

$$\rho_{ij} = \left[\sigma_{ij}\right]^{-1} \quad . \tag{2.5}$$

The case of no breakdown can be obtained by putting $T=0$ in relation (2.2). Within the two bands-model (one Fermi sphere for electrons and one Fermi sphere for holes) we get the usual result

$$\sigma = \sigma_e + \sigma_h, \tag{2.6}$$

where

$$\sigma_e = \frac{e^2 \tau n_e}{m_e(1+\omega_{ce}^2 \tau^2)} \cdot \begin{pmatrix} 1 & \omega_{ce}\tau \\ -\omega_{ce}\tau & 1 \end{pmatrix}, \tag{2.7}$$

$$\sigma_h = \frac{e^2 \tau n_h}{m_h(1+\omega_{ch}^2 \tau^2)} \cdot \begin{pmatrix} 1 & -\omega_{ch}\tau \\ \omega_{ch}\tau & 1 \end{pmatrix} \tag{2.8}$$

The indexes (e,h) are used to denote electrons and holes respectively.

For a compensated metal the concentrations of carriers n_e and n_h are equal. If we also take equal effective masses we get the well known result

$$\sigma = \frac{2e^2 \tau n}{m(1+\omega_c^2 \tau^2)} \cdot \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \tag{2.9}$$

yielding a vanishing Hall resistivity.

In order to get a contribution to the off-diagonal elements of the resistivity tensor for the compensated case, we have introduced different isotropic effective masses for electrons and holes all along our calculations.

All the cases correspond to orbits with Fermi wave vector of constant magnitude, and no k_H dependence is included, so that the models are supposed to arise from small cylindrical slabs of the Fermi surface.

3. RESULTS AND DISCUSSIONS

Our results are shown in Fig. 1 to 3. In the low-field limit all the models calculated correspond to closed compensated orbits. Transitions to the high field limit are shown in each figure.

The parameters used in our calculation are defined as

$$\omega_0\tau \equiv \frac{|e|H_0}{m_e c}\tau \quad ,$$

and

$$r \equiv m_e/m_h$$

where H_0 is the breakdown field given by relation (2.3), τ is the relaxation time, and m_e and m_h are the effective masses of electrons and holes respectively.

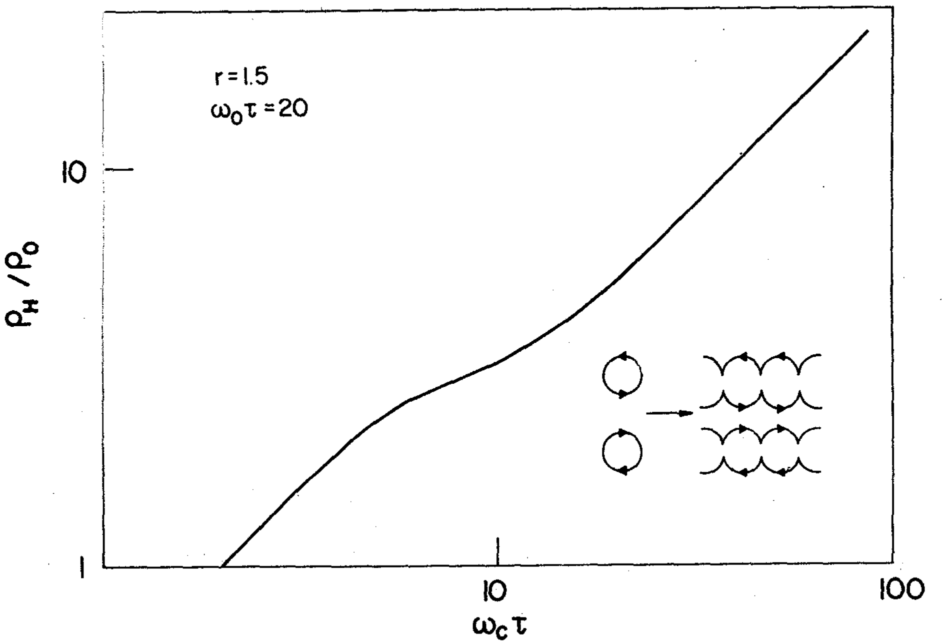

Fig.1 - Hall resisitivity as a function of $\omega_c\tau$ in double logarithmic scale for the case $r = 1.5$ and $\omega_0\tau = 20$ when we have a transition from closed compesated orbits to open orbits along the same direction. The Hall resistivity is normalized to the value of resistivity at zero field.

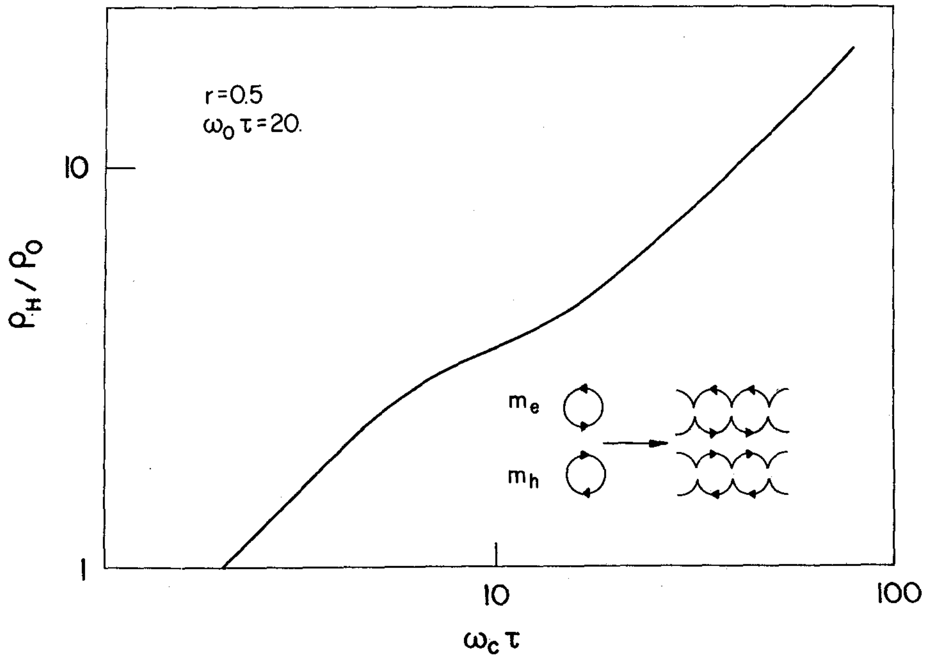

Fig.2 - The normalized Hall resistivity (ρ_{xy}/ρ_0) as a function of $\omega_c\tau$ in double logarithmic scale for the same topologies of orbits shown in Fig.1, but for different values of the parameters. We get here, as in Fig.1, a smooth transition between two linear behaviors which strongly resembles the experimental results.

Fig.1 and 2 correspond to the case when both, an electron orbit and a hole orbit break down to open orbits along the same direction. The related Hall resistivities exhibit a transition from a linear behavior to another linear behavior, going through an intermediate region which shows a more complicated dependence on magnetic field.Fig. 1, 2 resemble quite closely the experiments done in iron, with a smooth transition between linear Hall resistivities. For comparisons look at Fig. 7 and 14 (d) of reference 3. Note that Fig. 1 and 2 in our work are plotted in double logarithmic scale and then the positive value of the Hall resistivity is taken.

Finally in Fig. 3 we display a combination of compensated orbits which breaks down into an open orbit and a hole-like closed orbit. The results for various values of r are plotted. For $r<1$, the low -field behavior is hole-like, while for $r>1$ the electron character domi-

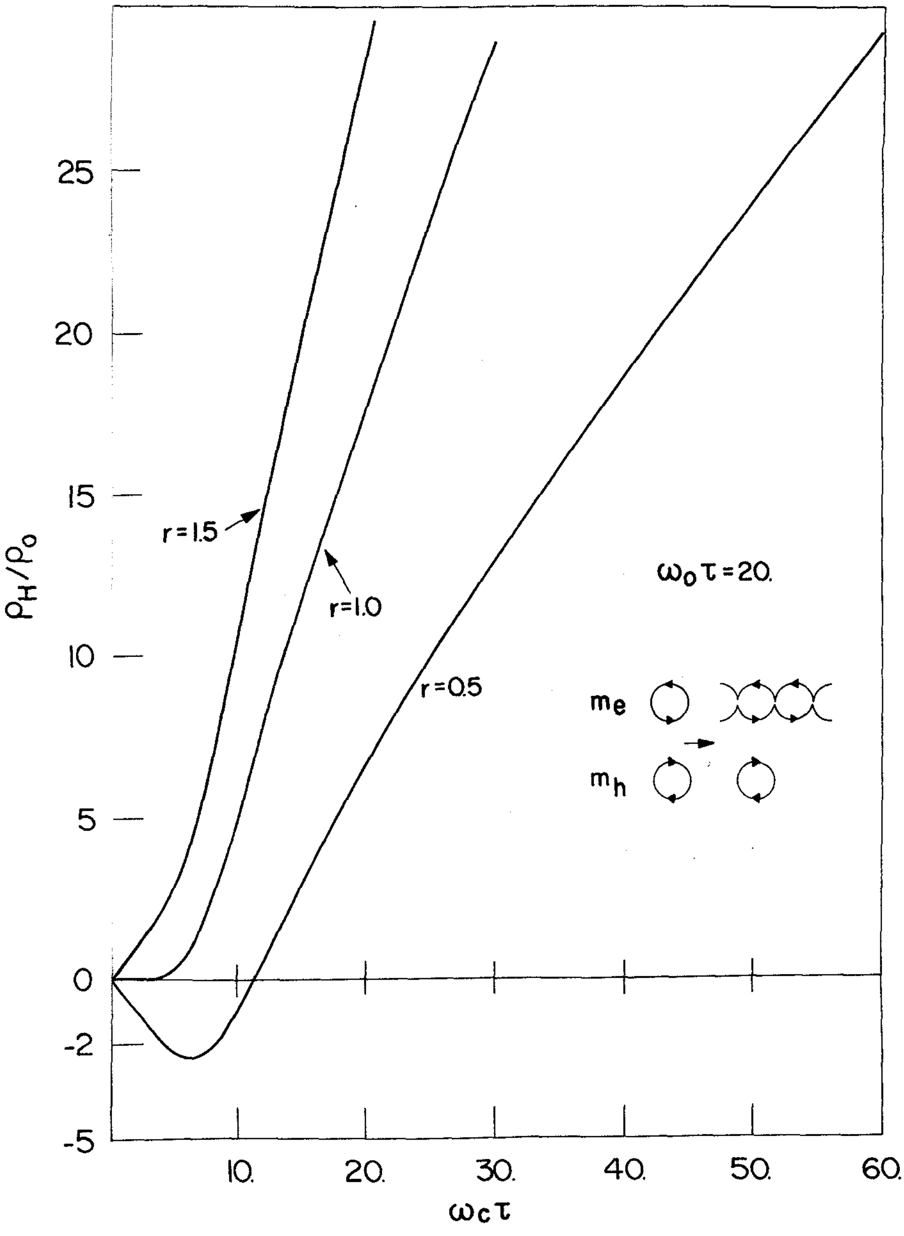

Fig.3 - The normalized Hall resistivity as a function of $\omega_c\tau$ for a transition from closed compensated orbits to an open orbit and a hole-like closed orbit. The parameter r takes the values 0.5, 1.0 and 1.5. For r = 0.5 the low-field behavior is dominated by the hole character and breakdown causes a change in sign of the Hall resistivity.

nates. For high magnetic fields the Hall resistivity is monitored mainly by the open orbit and we get then similar behaviors for the various values of r.

The case r=1 yields a vanishing Hall resistance in the low-field region (due to the total spherical symmetry) and is shown for comparison.

Summarizing we want to make the following comments:

i) In the absence of breakdown, spherical Fermi surfaces with equal effective masses for electrons and holes yield no contribution to the Hall resisitivity for the compensated case. This is a rather pathological case and of little help in our problem.

ii) As soon as closed compensated but non-spherical Fermi surfaces are considered we get non-vanishing contributions to the Hall resistivity which may be non-linear in the magnetic field. Spherical Fermi surfaces with different (but isotropic) effective masses for different kinds of carriers produce a linear behavior for the compensated case. We have taken the latter as our low-field case.

iii) Breakdown with formation of open orbits along a unique direction causes transitions from a linear to another linear regime, passing through an intermediate region where decompensation and coupling between different orbits give rise to a more complex dependence.

iv) Temperatures effects, in first approximation, modify the relaxation time τ, and in second order the position of the Fermi level and the effective masses of carriers. Then, changes in the topology of orbits as well in the mobility of carriers are possible. Under some conditions all these factors together may induce a change in sign of the Hall resistivity at a given temperature.

v) We conclude then that magnetic breakdown may be responsible of the observed behavior of the Hall resistance and a model which explains such behavior has been proposed. Measurements of the Hall resistivity for various directions of the external field, along with the simultaneous study of the transverse magnetoresistivity should be of value in order to test our theory.

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