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LETTER TO THE EDITOR

On the contribution of magnetic scattering to weak localization magnetoresistance

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Abstract. The effect of magnetic scattering on weak localization is investigated. The different contributions of elastic and spin-flip magnetic scattering and their field dependence are used to obtain an expression for three-dimensional, weak localization magnetoresistance.

Weak localization deals with quantum corrections of several electronic properties of disordered systems. These are due to interference between pairs of partial waves of electrons scattered at defects. Magnetoresistance is one of the best probes for these effects; it allows determination of the characteristic electronic scattering rates associated with inelastic spin-orbit and magnetic interaction processes [1].

At present the most complete theoretical expressions for magnetoresistance, which also take into account the Zeeman splitting of the conduction electron sub-bands, are the ones obtained by Maekawa and Fukuyama [2] for 2D films and by Fukuyama and Hoshino [3] with a recent extension by Baxter *et al* [4] for 3D systems. However, none of these methods completely takes into account the specificities of magnetic scattering, either by ignoring the different contributions of elastic and spin-flip magnetic scattering processes or by neglecting the effect of the magnetic field on these mechanisms.

In this letter I present a calculation of the weak localization effect on magnetoresistance in the presence of scattering by magnetic impurities, taking these two aspects into consideration. The final expressions are extracted for the 3D case.

According to the general formalism of weak localization [1, 2] the conducting corrections in d dimensions are given by

$$\sigma = \frac{2}{\hbar^2} N(E_F) \tau^2 e^2 D \int \frac{d^d q}{(2\pi)^d} \sum_{\alpha\beta} \Gamma_{\alpha\beta, \beta\alpha} \quad (1)$$

where D is the diffusion constant, τ is the total electron relaxation time and Γ are the relevant particle-particle propagators depending on the spin index ($\alpha, \beta = \pm$) to be determined by the Dyson equation

$$\Gamma_{\alpha\beta, \gamma\delta} = \Gamma_{\alpha\beta, \gamma\delta}^0 + \sum_{\mu\nu} \Gamma_{\alpha\mu, \gamma\nu}^0 \Pi_{\mu\nu} \Gamma_{\mu\beta, \nu\delta}$$

where, with usual approximations [1, 2], we have

$$\Pi_{\nu\nu} = (2\pi/\hbar) N(E_F) \tau (1 - |\omega_1| \tau - Dq^2 \tau)$$

$$\Pi_{\nu-\nu} = (2\pi/\hbar) N(E_F) \tau (1 - |\omega_1| \tau - Dq^2 \tau + 2i\nu f \tau).$$

ω_1 is an electron frequency and $f = g\mu_B B/2\hbar$ depends on the effective g -factor for electrons and on the magnetic field B .

$\Gamma_{\alpha\beta,\gamma\delta}^0$ is given by three contributions, each one associated with a certain characteristic scattering time. Potential scattering gives $(\hbar/2\pi N(E_F))(1/\tau_0)\delta_{\alpha\beta}\delta_{\gamma\delta}$ and spin-orbit scattering (three components in general) gives

$$-\frac{\hbar}{2\pi N(E_F)} \sum_i \frac{1}{\tau_{so}^i} \sigma_{\alpha\beta}^i \sigma_{\gamma\delta}^i \quad i = x, y, z$$

where σ^i are the Pauli matrices.

Magnetic scattering can be described by the s-d interaction of conduction electrons with a localized spin S [5-7]: $H_{sd} = JS \cdot \sigma$. Its contribution to Γ^0 will in general consist of a sum of terms proportional to

$$\langle S^i S^j \rangle \sigma_{\alpha\beta}^i \sigma_{\gamma\delta}^j \quad i, j = x, y, z$$

where $\langle \rangle$ denotes a thermal average.

When the spins are completely random (isotropy in spin space) all the cross terms with $i \neq j$ vanish and we are left with only the diagonal ones. However, when there is a magnetic field this is not the case in principle, and we must consider all the terms. This is easier if we expand with raising (S^+) and lowering (S^-) operators. Using the properties of the thermal averages of spins, we only get terms of the form

$$\langle (S^z)^2 \rangle \sigma_{\alpha\beta}^z \sigma_{\gamma\delta}^z \quad \langle S^+ S^- \rangle \sigma_{\alpha\beta}^+ \sigma_{\gamma\delta}^- \quad \langle S^- S^+ \rangle \sigma_{\alpha\beta}^- \sigma_{\gamma\delta}^+$$

Associating a scattering time to each one the magnetic contribution to Γ^0 can be written in general as:

$$\frac{\hbar}{2\pi N(E_F)} \left(\frac{1}{\tau_s^z} \sigma_{\alpha\beta}^z \sigma_{\gamma\delta}^z + \frac{1}{2\tau_s^{+-}} \sigma_{\alpha\beta}^+ \sigma_{\gamma\delta}^- + \frac{1}{2\tau_s^{-+}} \sigma_{\alpha\beta}^- \sigma_{\gamma\delta}^+ \right).$$

These same scattering times correspond to the contributions (with and without spin-flip) to the classical magnetic scattering resistivity [6, 7] which has the form

$$\rho_{\text{mag}} = \text{constant} \times (1/\tau_s^z + 1/\tau_s^{+-} + 1/\tau_s^{-+}).$$

Expressing the averages of the raising and lowering operators as a function of the average of S^z we have in the first Born approximation [6, 7]:

$$\frac{1}{\tau_s^z} = \frac{2\pi N(E_F)}{\hbar} c\Omega J^2 \langle (S^z)^2 \rangle \quad \frac{1}{\tau_s^{+-}} = \frac{1}{\tau_s^{-+}} = \frac{1}{\tau_s^z} = \frac{1}{2} \frac{2\pi N(E_F)}{\hbar} c\Omega J^2 \frac{\alpha/2}{\sinh^2(\alpha/2)} \langle S^z \rangle$$

with

$$\alpha = g_S \mu_B B / K_B T \quad (2)$$

where g_S is the g -factor of the magnetic impurities of atomic concentration c and Ω is the average atomic volume.

The total relaxation time due to elastic potential scattering, spin-orbit and magnetic scattering is given by

$$\frac{1}{\tau} = \frac{1}{\tau_0} + \sum_i \frac{1}{\tau_{so}^i} + \frac{1}{\tau_s^z} + \frac{2}{\tau_s^t}.$$

To simplify, we will assume in the following an isotropic spin-orbit scattering, leading to the relation

$$1/\tau_{so}^i = 1/3\tau_{so} \quad i = x, y, z$$

and we will also make the usual assumption that $\tau_0 \ll \tau_{so}, \tau_s^z, \tau_s^t$.

Solving the Dyson equations and introducing the inelastic scattering frequency $(1/\tau_i)$ instead of ω_1 [1], we get

$$\Gamma_{+,+,++} + \Gamma_{-,-,--} = \frac{\hbar}{2\pi N(E_F)\tau^2} \frac{2}{Dq^2 + (1/\tau')}$$

$$\Gamma_{-+,-+} + \Gamma_{+-,+-} = \frac{\hbar}{2\pi N(E_F)\tau^2} \frac{1}{\sqrt{1-\gamma}} \left(\frac{1}{Dq^2 + (1/\tau_+)} - \frac{1}{Dq^2 + (1/\tau_-)} \right)$$

where we defined the frequencies

$$\frac{1}{\tau'} = \frac{1}{\tau_i} + \frac{4}{3\tau_{so}} + \frac{2}{\tau'_s} \quad \frac{1}{\tau_{\pm}} = \frac{1}{\tau_i} + \frac{2}{3\tau_{so}} + \frac{2}{\tau_s^z} + \frac{2}{\tau'_s} \pm 2 \left(\frac{1}{3\tau_{so}} - \frac{1}{\tau'_s} \right) \sqrt{1-\gamma}$$

$$\gamma = \{f/[(1/3\tau_{so}) - (1/\tau'_s)]\}^2.$$

In the following the calculations will be restricted to the 3D case. For each term in Γ associated with a time τ_j , of the type $(\hbar/2\pi N(E_F)\tau^2)(Dq^2 + 1/\tau_j)$, equation (1) gives a contribution [6, 3]

$$\sigma_j(B, T) = (e^2/2\pi^2\hbar) (e/\hbar)^{1/2} [\frac{1}{2}\sqrt{B} f_3(B/B_j) + \sqrt{B_j}]$$

where for each rate $1/\tau_j$ a characteristic field B_j is associated

$$B_j = h/4eD\tau_j \quad j = ', + \text{ and } - \tag{3}$$

and $f_3(x)$ is the Kawabata function

$$f_3(x) = \sum_{n=0}^{\infty} \{2[n+1+(1/x)]^{1/2} - 2[n+(1/x)]^{1/2} - [n+\frac{1}{2}+(1/x)]^{-1/2}\}$$

for which useful compact formulas can be found in [4] and [8].

Finally we can write the expressions for the weak localization correction to conductivity in 3D as a function of temperature and field

$$\sigma_{WL}(B, T) = \frac{e^2}{2\pi^2\hbar} \left(\frac{e}{\hbar} \right)^{1/2} \left[\sqrt{B} \left\{ f_3 \left(\frac{B}{B'} \right) + \frac{1}{2\sqrt{1-\gamma}} \left[f_3 \left(\frac{B}{B_+} \right) - f_3 \left(\frac{B}{B_-} \right) \right] \right\} \right. \\ \left. + 2\sqrt{B'} + (1-\gamma)^{-1/2} (\sqrt{B_+} - \sqrt{B_-}) \right] \tag{4}$$

where the fields B' , B_+ and B_- correspond to the frequencies $1/\tau'$, $1/\tau_+$ and $1/\tau_-$ according to equation (3).

It is important to notice at this point that these fields do not depend only on temperature but also on the magnetic field through the spin-scattering terms. Unlike the other formulations where this implicit field dependence is not taken into account we will have an extra contribution to the magnetoresistance from the $\sqrt{B_j}$ terms.

So we finally obtain

$$(\Delta\rho_{WL}/\rho^2)(B, T) = -[\sigma_{WL}(B, T) - \sigma_{WL}(0, T)] \\ = -\frac{e^2}{2\pi^2\hbar} \left(\frac{e}{\hbar} \right)^{1/2} \left[\sqrt{B} \left\{ f_3 \left(\frac{B}{B'} + \frac{1}{2\sqrt{1-\gamma}} \left[f_3 \left(\frac{B}{B_+} \right) - f_3 \left(\frac{B}{B_-} \right) \right] \right\} \right. \right. \\ \left. \left. + 2(\sqrt{B'} - \sqrt{B'(0)}) + (1-\gamma)^{-1/2} (\sqrt{B_+} - \sqrt{B_-}) \right. \right. \\ \left. \left. - (\sqrt{B_+(0)} - \sqrt{B_-(0)}) \right] \tag{5}$$

with

$$\gamma = (3g\mu_B B/8eD(B_{so} - 3B_s^t))^2.$$

The characteristic fields B_{so} , B_s^z and B_s^t are also associated, according to equation (3), with the corresponding spin-orbit and spin-scattering relaxation rates.

The field dependence through the average of S^z of the characteristic fields B_s^z and B_s^t for magnetic scattering can be written as

$$B_s^z = B_s \langle (S^z)^2 \rangle / S(S+1)$$

and

$$B_s^t = B_s \frac{\langle S^z \rangle}{2S(S+1)} \frac{\alpha/2}{\sinh^2(\alpha/2)}$$

where $B_s = (2\pi N(E_F)/4eD)c\Omega J^2 S(S+1)$ and α is given by equation (2).

For zero applied field these parameters are identical

$$B_s^z(0) = B_s^t(0) = \frac{1}{3}B_s.$$

When the applied field B increases up to magnetic saturation the spin-flip contribution becomes frozen and we have

$$B_s^z(\infty) = B_s S/(S+1) \quad B_s^t(\infty) = 0.$$

It is also interesting to note that the non-spin-flip magnetic scattering does not contribute to dephasing if there are no spin-mixing interactions. In fact, if spin-orbit scattering is absent ($B_{so} = 0$, very light atoms) and the spin-flip scattering is frozen ($B_s^t = 0$) either by applying a large magnetic field or in the case of Ising-like magnetic impurities (see also [9]), we get $B_+ = B_-$ in equation (5) and then $\Delta\rho_{WL}$ only depends on $B' = B_i$.

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