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Anomalous Hall effect and weak localization corrections in a ferromagnet

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Abstract

In this paper, we report our results on the anomalous Hall effect. First, we summarize analytical calculations based on the Kubo formalism: explicit expressions for both skew-scattering and side-jump are derived and weak-localization corrections are discussed. Next, we present numerical calculations of the anomalous Hall resistivity based on the Dirac equation. Qualitative agreement with experiments is obtained. © 2002 Elsevier Science B.V. All rights reserved.

Keywords: Hall resistivity; Spin–orbit interaction; Kubo formalism

The anomalous Hall resistivity corresponds to the spontaneous value that takes in magnetic materials the Hall resistivity in the absence of applied magnetic field, and results from a combination of spin–orbit coupling and spin polarization. Two different mechanisms responsible for this effect are distinguished: the skew-scattering [1] and the side-jump [2], both corresponding to an asymmetric spin-dependent scattering by a potential in the presence of the spin–orbit coupling. The simplest way to calculate such an effect is to start from the Pauli equation including the spin–orbit coupling:

$$H = \frac{p^2}{2m} + V - \mu_B(\boldsymbol{\sigma}\cdot\mathbf{B}_{\rm eff}) + \frac{\hbar}{4m^2c^2}(\boldsymbol{\sigma}\times\boldsymbol{\nabla}V)\cdot\mathbf{p}, \quad (1)$$

and to use the Kubo formula for the conductivity

$$\tilde{\sigma}_{ij} = \frac{e^2\hbar}{2\pi\Omega}\mathrm{Tr}\left\langle v_i G^+(\varepsilon_F) v_j G^-(\varepsilon_F)\right\rangle_c, \quad (2)$$

where Ω is the volume of the sample, $\langle \ldots \rangle_c$ denotes the configurational average, G^+ and G^- are retarded and advanced Green's functions $G^{\pm}(\varepsilon) = (\varepsilon \pm i0 - H)^{-1}$, ε_F is the Fermi level and v_i is the i-component of the velocity which contains an additional part due to spin–orbit coupling (the so-called anomalous velocity $\mathbf{v}_{SO}$)

$$\mathbf{v} = \frac{\mathbf{p}}{m} + \mathbf{v}_{SO} = \frac{\mathbf{p}}{m} + \frac{\hbar}{4m^2c^2}(\boldsymbol{\sigma}\times\boldsymbol{\nabla}V). \quad (3)$$

The anomalous velocity inserted in Eq. (2) gives the side-jump term whereas the spin–orbit coupling contribution to Green's function (i.e., $G_0 H_{SO} G_0$ where H_{SO} is the spin–orbit coupling and G_0 the Green's function associated to the Hamiltonian in the absence of the spin–orbit coupling) inserted in Eq. (2) gives the skew-scattering term provided one goes beyond the Born approximation [1].

We present a simple application of such a method of calculation in the case of a system with a cubic symmetry and an effective magnetic field along the z-axis: thus the anomalous Hall conductivity is equal to the off-diagonal element $\tilde{\sigma}_{xy}$. We model the compound in the following way: the total volume of the sample Ω is divided into N cells of volume Ω_0. In each cell, the potential takes a constant value V with a probability distribution $P(V)$ which is characterized by its moments $\langle V^n \rangle_c = \int P(V)V^n\,dV$. A suitable choice of the energy origin yields $\langle V \rangle_c = 0$. We assume that there are no correlations in the value of the potential in different cells. In order to achieve analytical calculations, we restrict the study to the lowest order with the scattering potential and express Green's function G in terms of average Green's function $\underset{\sim}{G}$ in the relaxation time

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approximation. Neglecting weak-localization corrections, the diagonal conductivity is then given by the Einstein relation and for the off-diagonal conductivity, we get

$$\tilde{\sigma}_{xy}^{\mathrm{SS}} = -\frac{\pi m^2 \lambda^2}{6\hbar^2} \frac{\langle V^3 \rangle_{\mathrm{c}}}{\langle V^2 \rangle_{\mathrm{c}}} \Big(\mathcal{N}_{\uparrow} \Omega_0 \tilde{\sigma}_{xx}^{\uparrow} (v_{\mathrm{F}}^{\uparrow})^2 - \mathcal{N}_{\downarrow} \Omega_0 \tilde{\sigma}_{xx}^{\downarrow} (v_{\mathrm{F}}^{\downarrow})^2 \Big) \quad (4)$$

for the skew-scattering, and

$$\tilde{\sigma}_{xy}^{\mathrm{SJ}} = -e^2 \mathcal{N}_{\uparrow} \frac{2\delta^{\uparrow} v_{\mathrm{F}}^{\uparrow}}{3} + e^2 \mathcal{N}_{\downarrow} \frac{2\delta^{\downarrow} v_{\mathrm{F}}^{\downarrow}}{3} \quad (5)$$

for the side-jump, respectively (detailed calculations are presented in Ref. [3]). We have introduced the lengths $\lambda = \hbar/mc$ and $\delta^{\uparrow(\downarrow)} = \hbar v_F^{\uparrow(\downarrow)}/4mc^2$. $\mathcal{N}_{\uparrow(\downarrow)}$, $v_F^{\uparrow(\downarrow)}$ and $\tilde{\sigma}_{xx}^{\uparrow(\downarrow)}$ are respectively, the density of states per unit volume Ω_0, the velocity at Fermi energy and the diagonal conductivity, each for up and down spins. In contrast to $\tilde{\sigma}_{xx}$ and $\tilde{\sigma}_{xy}^{\mathrm{SS}}$, $\tilde{\sigma}_{xy}^{\mathrm{SJ}}$ does not depend on disorder. The Feynmam diagrams associated with these mechanisms are depicted in Fig. 1. A simple illustration of these results can be given in the case of a binary alloy $\mathrm{A}_x\mathrm{B}_{1-x}$ for which we have $\langle V^2 \rangle_{\mathrm{c}} = x(1-x)(\varepsilon_{\mathrm{A}} - \varepsilon_{\mathrm{B}})^2$ and $\langle V^3 \rangle_{\mathrm{c}} = x(1-x)(1-2x)(\varepsilon_{\mathrm{A}} - \varepsilon_{\mathrm{B}})^3$ where $\varepsilon_{\mathrm{A(B)}}$ is the value that takes the potential on side A(B). As a consequence, the anomalous Hall resistivity for skew-scattering is equal to $\tilde{\rho}_{\mathrm{H}}^{\mathrm{SS}} \simeq \tilde{\sigma}_{xy}^{\mathrm{SS}}/\tilde{\sigma}_{xx}^2 \propto (x - 3x^2)$ and for side-jump to $\tilde{\rho}_{\mathrm{H}}^{\mathrm{SJ}} \simeq \tilde{\sigma}_{xy}^{\mathrm{SJ}}/\tilde{\sigma}_{xx}^2 \propto x^2$ which is in agreement with the empirical relation $\tilde{\rho}_{\mathrm{H}} = a\tilde{\rho}_{xx} + b\tilde{\rho}_{xx}^2$ but in disagreement with the common belief that the quadratic term arises only from the side-jump.

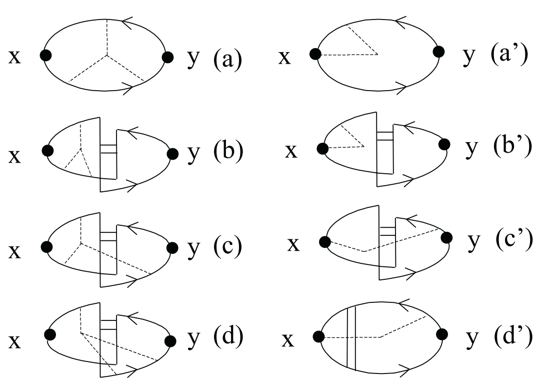

Fig. 1. Feynman diagrams for the anomalous Hall effect: (a) corresponds to the skew-scattering; (a') to the side-jump; (b), (c) and (d) are the Cooperons corrections to the skew-scattering; (b') and (c') to the side-jump; (d') is the Diffusons correction to the side-jump. The curve lines represent average Green's functions, the dashed lines correspond to the potential (including the spin–orbit coupling) and the double straight lines correspond to the ladder part. Symmetrical diagrams have also to be considered.

Within this approach, the weak-localization corrections to the anomalous Hall effect can also be calculated. We have considered both Cooperons and Diffusons (see Fig. 1). The results are the following [4]: (i) the Cooperons diagrams for the side-jump cancel exactly each other whereas the Diffusons diagrams give a negligible contribution (of order $(\hbar/\varepsilon_{\mathrm{F}}\tau)^4$ where τ is the relaxation time), (ii) the Cooperons diagrams for the skew-scattering give a non-zero contribution which includes both spin up and spin down channels. As a consequence, the weak-localization corrections to the anomalous Hall resistivity $\Delta\tilde{\rho}_{\mathrm{H}}/\tilde{\rho}_{\mathrm{H}}^0 \simeq \Delta\tilde{\sigma}_{xy}/\tilde{\sigma}_{xy}^0 - 2\Delta\tilde{\sigma}_{xx}/\tilde{\sigma}_{xx}^0$ exhibit a strikingly different behavior as compared to the normal Hall resistivity for which weak-localization corrections vanish by an exact cancellation of the diagonal and off-diagonal parts [5]. Due to the presence of two spin channels, such a cancellation can never take place in the case of the anomalous Hall resistivity.

The analytical expressions (4) and (5) have been obtained in the weak-scattering limit and using the free electron approximation. In order to get a more realistic description of the anomalous Hall effect, we have performed numerical calculations starting from a tight-binding description and using the coherent potential approximation in order to treat disorder. Green's function is then expressed in term of the t-matrix and average Green's function: $G = \underline{G} + \underline{G}T\underline{G}$. As a consequence, the conductivity (2) can be split, in the case of a configuration-independent velocity, into two different parts:

$$\tilde{\sigma}_{ij} = \frac{e^2\hbar}{2\pi\Omega} \mathrm{Tr}\big[v_i^+(\varepsilon_{\mathrm{F}}) v_j \underline{G}^-(\varepsilon_{\mathrm{F}})\big] + \frac{e^2\hbar}{2\pi\Omega} \mathrm{Tr}\big[v_i \underline{G}^+(\varepsilon_{\mathrm{F}}) \Gamma_j(\varepsilon_{\mathrm{F}}) \underline{G}^-(\varepsilon_{\mathrm{F}})\big], \quad (6)$$

where Γ_j is the vertex function equal to $\langle T^+ \underline{G}^+ v_j \underline{G}^- T^- \rangle_c$. This formulation is very useful since it allows the exact determination of the vertex corrections in the ladder approximation. However, because of the presence of the spin–orbit coupling, the velocity is no longer configuration-independent (see Eq. (3)) and it is then not possible to take it out of the configuration average $\langle \ldots \rangle_c$ like it is done in Eq. (6). A means to avoid this problem is to start, rather than from the Pauli equation, from the Dirac equation:

$$H = c(\boldsymbol{\alpha} \cdot \mathbf{p}) + \beta mc^2 + V - \mu_{\mathrm{B}}\beta(\boldsymbol{\sigma} \cdot \mathbf{B}_{\mathrm{eff}}), \quad (7)$$

where $\boldsymbol{\alpha}$ and β correspond to the standard Dirac matrices. Indeed, in this description, the velocity operator is simply equal to $c\boldsymbol{\alpha}$ and then is configuration-independent.

The system we consider is a ferromagnetic binary alloy $\mathrm{A}_x\mathrm{B}_{1-x}$ with an effective magnetic field along the z-axis. First, we have expressed Eq. (7) in the tight-binding approximation for a cubic symmetry, next the

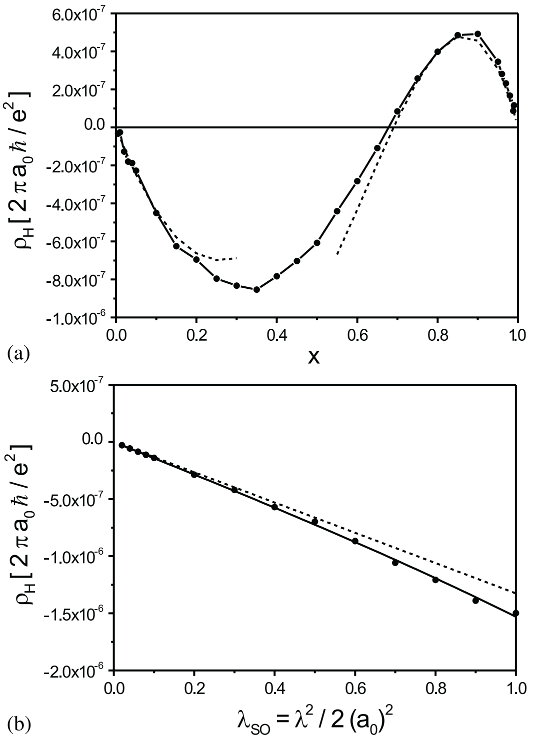

Fig. 2. Variation of the anomalous Hall resistivity as a function (a) of the concentration for a spin–orbit coupling $\lambda_{SO} = 0.5$ and as a function (b) of the spin–orbit coupling for a concentration $x = 0.2$. The other parameters are $\varepsilon_F/t = 0.2$, $\varepsilon_A/t = 0.1$ and $\varepsilon_B/t = 0$ where $t = \hbar^2/2ma_0^2$ (a_0 is the unit cell parameter) and $\Delta\varepsilon_A/t = \Delta\varepsilon_B/t = 0.05$ where $\pm\Delta\varepsilon_{A(B)}/2$ is the value that takes the exchange coupling $-\mu_B\sigma_z B_{\rm eff}$ on site A(B). The full lines with full circle symbols correspond to the numerical calculations and the dashed lines correspond to the analytical results given by Eqs. (4) and (5).

self-energy has been numerical calculated by the means of an iteration procedure and used to calculate average Green's function and the vertex corrections that we insert in Eq. (6) in order to get the conductivity tensor. Variations of the anomalous Hall resistivity $\tilde{\rho}_H \simeq \tilde{\sigma}_{xy}/\tilde{\sigma}_{xx}^2$ as a function of concentration of disorder and spin–orbit coupling are depicted in Fig. 2. We obtain a change of sign of the anomalous Hall resisitivity for a particular value of the concentration which corresponds to an exact cancellation of the skew-scattering and the side-jump contributions. Such a change of sign has been observed experimentally in PdCo and PdNi alloys [6]. The variation of the anomalous Hall resistivity with spin–orbit coupling is consistent with the Onsager relation since the numerical curve can be very well fitted when one consider only odd powers with respect to the spin–orbit coupling. A very good agreement with analytical expressions which apply in the weak-scattering limit (close to $x = 0$ and 1) and in the weak-relativistic limit ($\lambda_{SO} \simeq 0$) is obtained.

To summarize, we have performed both analytical and numerical calculations concerning the anomalous Hall effect. Explicit expressions of the skew-scattering and side-jump conductivities have been derived, which allows the clarification of the influence of the potential on each mechanism: whereas the skew-scattering conductivity varies on the third order of the potential, the side-jump conductivity does not depend on it. Contrary to what happens for the normal Hall resistivity, the weak-localization corrections to the anomalous Hall resistivity do not vanish because of the presence of two different spin channels. Numerical results obtained in the case of a ferromagnetic binary alloy are in qualitative agreement with measurements in the sense that they show a change of sign of the anomalous Hall resistivity.

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