Chirality driven anomalous Hall effect in weak coupling regime

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Abstract

Anomalous Hall effect arising from non-trivial spin configuration (chirality) is studied based on the s-d model. Considering a weak coupling case, the interaction is treated perturbatively. Scattering by normal impurities is included. Chirality is shown to drive locally Hall current and leads to overall Hall effect if there is a finite uniform chirality. This contribution is independent of the conventional spin-orbit contribution and shows distinct low temperature behavior. In mesoscopic spin glasses, chirality-induced anomalous Hall effect is expected below the spin-glass transition temperature. Measurement of Hall coefficient would be useful in experimentally confirming the chirality ordering.
Hall effect in ferromagnetic metals has long been known to have anomalous component which does not vanish at zero external magnetic field. Theories have explained this as due to the spontaneous magnetization and spin-orbit interaction\cite{1, 2, 3}. It was also shown based on the $s$-$d$ model that the high temperature (close to the critical temperature) behavior of the anomalous Hall effect is understood in terms of the fluctuation of the magnetization coupled with spin-orbit interaction\cite{4, 5}.

Recently some manganites were found to exhibit at high temperatures abnormal behavior\cite{6, 7} which is not explainable by previous theories. This behavior was explained by Berry phase effect associated with thermally driven non-trivial background spin configuration (chirality)\cite{8, 9, 10}. Finite chirality results in a finite Berry phase and leads to Hall effect if chirality is non-vanishing as a net. In contrast to manganites, anomalous Hall coefficient in ferromagnetic pyrochlores was found to remain finite at low temperatures\cite{11, 12}. This behavior was discussed to be due to finite chirality of the ground state, which is originating from geometrical frustration\cite{13, 14, 15, 16}. Behavior which is not explained solely by chirality theories was reported recently in some Mo-based pyrochlores\cite{17, 18, 19}. These recent theories\cite{8, 9, 10, 13, 14, 15, 16} have exclusively dealt with a strong Hund-coupling limit, considering a half-metallic nature of the experimental systems. In this limit, the electron spin aligns perfectly to the local spin and feels the same Berry phase as the local spin carries, and Hall conductivity has a topological meaning\cite{20}. The weak coupling region, which would be the case of most common transition-metal magnets, has never been explored from the viewpoint of chirality.

In this paper, we study anomalous Hall effect due to chirality based on the $s$-$d$ model in the weak coupling case. Using Kubo formula and taking account of the impurity scattering, we will demonstrate that the chirality drives local Hall current in the perturbative regime. To compare with experiments, both the chirality mechanism and the conventional one due to the spin-orbit interaction (corresponding to the result by Karplus and Luttinger\cite{1, 3}) need to be taken account. We will show that the chirality contribution is independent of the conventional one, and they simply add up at lowest approximation. In order for the chirality contribution to Hall effect to be finite, there needs to be a net uniform component of the chirality. The possible effect of the spin-orbit interaction to induce a uniform component of the chirality in the presence of uniform magnetization, originally claimed to be present in the strong Hund-coupling limit\cite{8}, is examined in our weak-coupling scheme. It turns out
that the spin-orbit interaction induces a vector chirality if there is a uniform magnetization, and that this indeed results in a Hall effect in the bulk. This effect, however, would depend much on the band structure.

Our theory is applicable to a wide class of magnetic systems including canonical spin glasses, in which the conduction electron is only weakly coupled to the local spin. In spin glasses, chirality order develops at low temperature leading to the spin-glass transition\[21]. Meanwhile, the chirality order there is spatially random without a uniform component, making the experimental detection of the chirality-driven anomalous Hall effect rather difficult due to the inherent cancellation effect. Even in this case, however, average of the squared chirality remains finite in small (mesoscopic) samples\[22, 23], and enhancement of the anomalous Hall coefficient is expected below the spin-glass transition. Thus, measurement of fluctuation of Hall conductivity in mesoscopic samples may be useful in experimental confirmation of the chirality ordering. Depending on the band structure, the chirality-driven Hall effect might be observable even in bulk spin-glass samples if the sample possesses a uniform magnetization, which is induced by applied fields or is generated spontaneously (as in case of reentrant spin glasses\[24]).

We consider electron on lattice whose Hamiltonian is given by

\[
H = \sum_{k\sigma} \epsilon_{k\sigma} c_{k\sigma}^\dagger c_{k\sigma} + H' + H_{\text{imp}},
\]

where \(\sigma = \pm\) denotes electron spin. Electron energy is \(\epsilon_{k\sigma} = k^2/2m - \sigma\Delta - \epsilon_F\), where \(m\) is electron mass, \(\Delta\) is a uniform polarization of conduction electron due to magnetization or external field, and \(\epsilon_F\) is the Fermi energy. The interaction with localized spin \(S_X\) (treated as classical) is represented by the exchange interaction \(H'\),

\[
H' = \frac{J}{N} \sum_{kk'} S_{k'k} (c_{k'}^\dagger \sigma_k c_k),
\]

where \(\sigma^\alpha\) \((\alpha = x, y, z)\) are Pauli matrices, and \(N\) is the total number of lattice sites. The sign of the exchange coupling \(J\) depends on the system we consider; it is positive if the interaction is the \(s-d\) exchange as in case of canonical spin glasses, and is negative if it is the Hund-coupling as in case of manganites. Configuration of \(S_X = (1/N) \sum_q e^{i\mathbf{q} X} S_q\) is fixed. We note that localized spins \(S_X\) do not necessarily occupy all \(N\) sites here: An example is a dilute magnetic alloy such as canonical spin glass\[24]. \(H'\) is assumed not to contain uniform component \(M \equiv S_{q=0}\), since it is taken into account in \(\Delta = JM\) with \(M = |M|\). The
scattering by normal impurities is represented by \( H_{\text{imp}} = (v_{\text{imp}}/N) \sum_{\boldsymbol{k} \sigma} e^{i(\boldsymbol{k} - \boldsymbol{k}')X_i} c_{\boldsymbol{k} \sigma}^\dagger c_{\boldsymbol{k}'} \), where \( n_{\text{imp}} \) is the number of nonmagnetic impurities (at sites \( X_i \)) and \( v_{\text{imp}} \) is a constant.

The electronic current is given by \( \mathbf{J} = \frac{\mathbf{e}}{m} \sum_{\boldsymbol{k} \sigma} \mathbf{k} c_{\boldsymbol{k} \sigma}^\dagger c_{\boldsymbol{k} \sigma} \). Based on Kubo formula, the anomalous Hall conductivity is obtained as \( \sigma_{xy} = \lim_{\omega \to 0} \frac{1}{\omega} \text{Im} (Q_{xy}(\omega + i0) - Q_{xy}(i0)) \) with \( Q_{xy}(i\omega_i) \equiv \frac{1}{N^2} < J_x(i\omega_i) J_y(-i\omega_i) > \), where the bracket \(< >\) denotes averaging over electrons and impurities, \( \omega_i \equiv 2\pi \ell/\beta \) being the Matsubara frequency. We treat \( H' \) perturbatively.

As is obvious, the first and second order contribution vanish since the spatial asymmetry due to current vertices \( J_x \) and \( J_y \) in the correlation function cannot be deleted. The first term which can possibly be finite is the third-order term (Fig. [4]):

\[
\sigma_{xy}^{(3)} = \frac{1}{2\pi V} \left( \frac{e}{m} \right)^2 \left( \frac{J}{N} \right)^3 \sum_{\boldsymbol{k} \boldsymbol{k}' \boldsymbol{k}''} k_x k_y' S_{\boldsymbol{k}''}^\sigma S_{\boldsymbol{k}' - \boldsymbol{k}''}^\beta S_{\boldsymbol{k}' - \boldsymbol{k}''}^\gamma \text{tr} [G_{\boldsymbol{k}}^R \sigma^\alpha G_{\boldsymbol{k}'}^R \sigma^\beta G_{\boldsymbol{k}''}^R G_{\boldsymbol{k}'}^A \sigma^\gamma G_{\boldsymbol{k}}^A] + \text{c.c.,}
\]

(3)

where \( V \) is the total volume, trace is over spin indices, and \( \alpha, \beta, \gamma \) runs over \( x, y, z \). \( G_{\boldsymbol{k}}^R (\equiv [\frac{i}{2\pi} - \epsilon_{\boldsymbol{k} \sigma}]^{-1}) \) and \( G_{\boldsymbol{k}}^A (\equiv (G_{\boldsymbol{k}}^R)^*) \) are retarded and advanced Green functions in the \( \omega \to 0 \) limit, respectively, which include lifetime due to impurities, \( \tau \equiv 2\pi \nu n_{\text{imp}} v_{\text{imp}}^2 \), \( \nu \) being the density of states per site. We consider the case where the polarization of conduction electron is small (\( \Delta \sim 0 \)). The summation over spin indices in eq. (3) is then carried out as \( \text{tr} [\sigma^\alpha \sigma^\beta \sigma^\gamma] = 2i\epsilon_{\alpha\beta\gamma} \), where \( \epsilon_{\alpha\beta\gamma} \) is the totally antisymmetric tensor. By use of the partial derivative, the Hall conductivity reduces to a compact form:

\[
\sigma_{xy}^{(3)} = \frac{N}{\pi V} \left( \frac{e}{m} \right)^2 (2\pi \nu J)^3 \tau^2 \chi_0 = (4\pi)^2 \sigma_0 J^2 \nu^2 \tau \chi_0,
\]

(4)

where \( \sigma_0 \) is the Boltzmann conductivity, \( \sigma_0 \equiv \frac{N}{2V} \left( \frac{e}{m} \right)^2 \nu k_F^2 \tau \). \( k_F \) is the Fermi wavenumber. We see that \( \sigma_{xy}^{(3)} \propto \tau^2 \propto \rho_0^{-2} \) (\( \rho_0 = \sigma_0^{-1} \) is the resistivity). The uniform chirality \( \chi_0 \) is given by

\[
\chi_0 \equiv \frac{1}{N} \sum_{X_i} \mathbf{S}_{X_1} \cdot (\mathbf{S}_{X_2} \times \mathbf{S}_{X_3})
\]

\[
\times \left[ \frac{\mathbf{a} \times \mathbf{b}}{ab} I'(a) I'(b) I(c) + \frac{\mathbf{b} \times \mathbf{c}}{bc} I(a) I'(b) I'(c) + \frac{\mathbf{c} \times \mathbf{a}}{ca} I'(a) I(b) I'(c) \right],
\]

(5)

where \( X_i \) runs over all the positions of local spins, while \( \mathbf{a} \equiv \mathbf{X}_1 - \mathbf{X}_2, \mathbf{b} \equiv \mathbf{X}_2 - \mathbf{X}_3 \) and \( \mathbf{c} \equiv \mathbf{X}_3 - \mathbf{X}_1 \) are the vectors representing sides of the triangle (\( a \equiv |\mathbf{a}| \) e.t.c.). \( I(r) \equiv \frac{1}{2\pi N \nu \tau} \sum_{\boldsymbol{k}} e^{i\boldsymbol{k} \cdot \mathbf{r}} G_{\boldsymbol{k}}^R G_{\boldsymbol{k}}^A \) and \( I'(r) = \frac{dI(r)}{dr} \). It is seen that Hall current is driven by three spins which form a finite solid angle in spin space (i.e., finite local chirality \( \chi_{123} \equiv \mathbf{S}_{X_1} \cdot (\mathbf{S}_{X_2} \times \mathbf{S}_{X_3}) \))
spanning a finite area in coordinate space (as seen from \((a \times b)_z\) etc.). Note that the factor in the square bracket in the definition of \(\chi_0\) specifies the coupling between the spin- and the coordinate-space. In the case three spins (1, 2 and 3) align right-handed in spin space \((\chi_{123} > 0)\), \(\chi_{123}\) contributes positively to \(\chi_0\) if these three spins are located anti-clockwise in real space, and is negative if they are located clockwise. In the case three spins align left-handed in spin space \((\chi_{123} < 0)\), this assignment is reversed. Noting \(I(r) = \frac{\sin k_F r}{k_F} e^{-r/2\ell}\), where \(\ell\) is elastic mean free path, contribution from largely separated three spins with the scale of \(r\) decays rapidly as \(\sim e^{-3r/2\ell}/(k_F r)^3\), and the Hall effect is dominantly driven by chiralities of spins on small triangles. Note that the large-\(r\) behavior of the weight function has resemblance to the RKKY interaction. The expression of the uniform chirality derived in our weak coupling scheme, eq. (5), contains contribution from large triangles, and is a natural extension of the conventional (and naive) definition of the chirality in terms of spins on adjacent sites only. Eqs. (4) and (5) are main results of the present paper, which gives a direct relation between the Hall conductivity and the spin configuration.

Conventional theories of anomalous Hall effect is based on the spin-orbit interaction, \(H_{so} \equiv i\lambda \sum_{kk'}(k' \times k) \cdot (c_{k'}^{\dagger} \sigma \sigma_{c_k})\), where \(\lambda\) is the spin-orbit coupling constant\[1,2,3\]. Thus we have also analyzed the contribution of \(H_{so}\) on the same footing as that of \(H'\) performing a double power series expansion. At the lowest (first) order, the contribution of \(H_{so}\) is made up of so-called skew scattering and side-jump ones\[25\], which are calculated as \(\sigma_{so}^{xy} = -\lambda M (A' \tau + B)\)[26]. Here \(A'\) and \(B\) are constants independent of \(\tau\), each term corresponding to skew scattering and side-jump processes, respectively. We note that \(A'\) and \(B\) are positive in the present single band approximation, but their signs actually depend on the band structure in real materials. At the lowest order, spin-orbit \((\sigma_{so}^{xy})\) and chirality (eq. (4)) contributions are independent, and the total Hall conductivity is simply their sum. These can mix as higher order corrections, but we neglect such small contributions. The total Hall resistivity, \(\rho_{xy} = \sigma_{xy} \rho_0^2\), then behaves as

\[
\rho_{xy} \simeq -\lambda M (A' \rho_0 + B \rho_0^2) + CJ^3 \chi_0, \tag{6}
\]

where \(A = A' \rho_0 \tau\) is independent of \(\tau\), while \(C = \frac{1}{2} A' \frac{2k}{N} (\frac{m}{k_F})^2 > 0\) in our single band approximation. The sign of chirality contribution depends on whether the coupling is of the \(s-d\) type \((J > 0)\) or of the Hund type \((J < 0)\). It is seen that the three terms in eq. (6) depend differently on the impurity concentration. The chirality contribution is dominant
in the clean regime and at low temperatures. It should be noted that the analysis in the strong Hund-coupling case which does not consider impurities yields $\rho_{xy} \propto \rho_0^2 \chi^{13}$. These different dependences on $\rho_0$, which indicate different behavior as a function of temperature, would be useful in interpreting the experimental results.

The chirality contribution to Hall coefficient is finite only if there is a net uniform chirality, $\chi_0 \neq 0$. Finite net chirality, however, may not be very easy to realize on regular lattices with simple nearest-neighbor exchange interaction, since the chirality on adjacent plaquettes usually tends to cancel each other due to symmetry$^{13, 27}$. One possible mechanism to realize a finite net chirality has been proposed in Ref. $^8$, where it was argued in the strong coupling case that the spin-orbit interaction induced a net chirality in the presence of magnetization as $\chi_0^{so} = -\alpha \lambda M$ ($\alpha$ is a positive constant). Inspired by this observation, we have examined whether such a mechanism works in the present weak coupling case. To examine the possible coupling between the uniform chirality and the magnetization $M$, we look into the expectation value (effective Hamiltonian) of the spin-orbit interaction, $\langle H_{so} \rangle$, where $\langle >$ denotes the thermal averaging over electrons, treating $H'$ as perturbation. We identify two types of terms as possible candidates. One is the term linear in $M$ for small $M$ and comes from the third-order contribution in $H'$,

$$H_{so}^{(3)} = 2\lambda \left( \frac{J}{N} \right)^3 \sum_{x} \mathbf{S}_x \cdot (\mathbf{S}_{x_2} \times \mathbf{S}_{x_3}) [(\mathbf{x}_1 - \mathbf{x}) \times (\mathbf{x}_3 - \mathbf{x})]_z$$

$$\times \frac{1}{\beta} \sum_{\omega_n} g_{\omega_n}(|\mathbf{x} - \mathbf{x}_1|) g_{\omega_n}(a) g_{\omega_n}(b) \Delta'_{\omega_n}(|\mathbf{x}_3 - \mathbf{x}|),$$

where $\mathbf{x}$ denotes the site at which the spin-orbit interaction acts ($a$ and $b$ are defined after eq. $^8$), and the uniform magnetization is assumed to be in $z$-direction. The thermal Green functions are defined here as $g_{\omega_n}(r) \equiv \frac{1}{2}(G_{\omega_n} + G_{\omega_n} -); \Delta_{\omega_n}(r) \equiv (G_{\omega_n} + G_{\omega_n} -)$, where $G_{\omega_n}(X) = \sum_k e^{-i\mathbf{k} \mathbf{x}} [i(\omega_n - \text{sgn}(\omega_n)) - \epsilon_k + \Delta]^{-1}$, and $G'(r) \equiv \frac{dG}{dr}$. Note that $\Delta_{\omega_n}$ is proportional to $\Delta$, and hence to $M$, for $\Delta/\epsilon_F \ll 1$. It is seen that $H_{so}^{(3)}$ apparently describes the coupling between the uniform magnetization and the local chirality, but without referring to the spatial spin configuration. In fact, since the factor of $(|\mathbf{x}_1 - \mathbf{x}| \times (\mathbf{x}_3 - \mathbf{x}))_z$ specifies only the angles between the two spins $S_{\mathbf{x}_1}$ and $S_{\mathbf{x}_3}$ when looked from the position $\mathbf{x}$ irrespective of spatial configuration of $S_{\mathbf{x}_2}$, $H_{so}^{(3)}$ does not contain the component inducing the uniform chirality $\chi_0$.

The other term is quadratic in $M$ for small $M$ and comes from the second-order contri-
In the presence of uniform magnetization $M$, the Fourier transform of the electron part becomes
\[
H_{so}^{(2)x} = -2\lambda \left( \frac{J}{N} \right)^2 \sum_{x \in X_0} \langle S_{x_1} \times S_{x_2} \rangle_z \left[ (X_1 - x) \times (X_2 - x) \right]_z \times \frac{1}{|X_1 - x||X_2 - x|} \sum_{\omega_n} \Delta'_{\omega_n}(|X_1 - x|)g_{\omega_n}(|X_1 - X_2|) \Delta'_{\omega_n}(|X_2 - x|).
\]

In the presence of uniform magnetization $M$, $z$-component of the vector chirality, defined by two spins as $C_{12} \equiv \langle S_{x_1} \times S_{x_2} \rangle$, plays essentially the same role as the scalar chirality ($\chi_{123} \simeq MC_{12}^z$). Then, eq. (8) above describes the coupling between the vector chirality and the magnetization via the spin-orbit interaction. After summation over the thermal distribution in $H$, where $\chi_{123} \simeq MC_{12}^z$, then, a finite contribution is expected to remain in general. Thus, this term could serve as a “symmetry-breaking field” $(H_{so}^{(2)x} \propto M^2 \sum_x C_{12}^z \propto M\chi_0)$ inducing a uniform chirality, which results in a Hall effect in the bulk.

Even in the case the chirality does not contain uniform component, $\chi_0$ could still be finite if the system size is sufficiently small. Let us consider the case of spin glasses in zero external field, in which the chirality is randomly ordered. The number of triangles which contribute to $\sigma_{xy}$ is given roughly as $N_\chi \simeq Nn_m^3(\ell/a_0)^4$ ($n_m$ is the concentration of localized spins, and $a_0$ is lattice constant). Hence, the sum of random chirality is $\chi_0 \propto \frac{1}{\sqrt{N}}n_m^{3/2}(\ell/a_0)^2$. Although this quantity decays as $\propto 1/\sqrt{N}$, we expect that detection of Hall effect may be possible by high-sensitivity-measurements on mesoscopic samples. This chirality-driven Hall effect of random sign in mesoscopic spin glasses would be measurable [22, 23] by looking at the sample-dependent or thermal-cycle-dependent fluctuations, $\delta\sigma_{xy} \equiv \sigma_{xy} - [\sigma_{xy}]_s$ ([$\cdot$]$_s$ denotes average over spin configurations), whose squared average is given as
\[
\left[ \sqrt{[\delta\sigma_{xy}]^2}_s \right]/\sigma_0 = (4\pi)^2F^2\nu^2/\sqrt{2}\chi^2_s, \quad \sqrt{[\chi^2}_s \equiv \frac{1}{N} \sum_{ijk} (\chi_{ijk} F_{ijk})^2 \right]^{1/2} \propto \frac{1}{\sqrt{N}}n_m^3(\ell/a_0)^4.
\]

In the 70’s, anomalous Hall effect in spin glasses was experimentally investigated [24, 25]. It was found that the Hall resistivity of canonical spin glasses, i.e., dilute magnetic alloys such
as AuFe and AgMn, measured in weak applied fields were negative and exhibited a cusp-like anomaly around the spin-glass transition temperature whose behavior was quite similar to that of the magnetic susceptibility, \( \chi_m \); i.e., \( \rho_{xy}/H \propto -\chi_m \). Although this behavior can be explained by the standard spin-orbit contribution (the first two terms in eq. (6)), it could also be explainable by the contribution of a uniform chirality induced by \( H_{so}^{(2)} \) described above. In order to experimentally resolve the spin-orbit contribution of Karplus-Luttinger type from the spin-orbit induced chirality contribution, one might possibly examine the dependence on \( \rho_0 \) (Eq. (7)), or measure the response to external magnetic fields applied in various directions. In this connection, reentrant spin-glass systems, which exhibit successive phase transitions, first from para to ferro and then from ferro to spin glass at lower temperature, would be of much interest. In the ferromagnetic regime, only the conventional spin-orbit mechanism is expected to work, while in reentrant spin-glass regime, the chirality contribution sets in due to the spin canting giving rise to distinct contribution at lower temperatures.

To summarize, we have demonstrated based on the s-d model in the weak coupling regime that a topologically nontrivial spin configuration (chirality) induces Hall current. The chirality-driven Hall effect as a bulk appears if uniform component of the chirality is finite. This contribution is independent of the conventional contribution from the spin-orbit coupling exhibiting different dependence on resistivity from the spin-orbit contribution and other predictions based on chirality mechanism. If chirality is ordered randomly, as in spin glasses below the spin-glass transition temperature, sample-to-sample or thermal-cycle-dependent fluctuations of Hall conductivity in mesoscopic samples is expected to show an anomalous enhancement. Without a direct method of magnetic detection of the chirality available so far, measurement of (fluctuation of) Hall conductivity would be powerful tool in experimental confirmation of the chirality ordering.

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FIG. 1: Three spin contribution to $\sigma_{xy}$.

The interaction with the local spin, $S$, is denoted by a shaded small circles. The two processes are complex conjugate to each other. Other contributions vanish due to symmetry.