Berry Phase Theory of the Anomalous Hall Effect: Application to Colossal Magnetoresistance Manganites

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We show that the anomalous Hall effect (AHE) observed in colossal magnetoresistance manganites is a manifestation of Berry phase effects caused by carrier hopping in a nontrivial spin background. We determine the magnitude and temperature dependence of the Berry phase contribution to the AHE, finding that it increases rapidly in magnitude as the temperature is raised from zero through the magnetic transition temperature T_c, peaks at a temperature $T_{\max} > T_c$, and decays as a power of T, in agreement with experimental data. We suggest that our theory may be relevant to the anomalous Hall effect in conventional ferromagnets as well.

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The Anomalous Hall Effect (AHE) is a fundamental but incompletely understood aspect of the physics of metallic ferromagnets [1,2]. The Hall effect is the development of a voltage which is transverse to an applied current; the constant of proportionality is the Hall resistivity ρ_H. In nonmagnetic materials, ρ_H is proportional to the magnetic induction B and its sign is determined by the carrier charge. Many ferromagnets, however, exhibit an anomalous contribution to ρ_H which is proportional to the magnetization M; thus

$$\rho_H = R_0 B + R_s M . \qquad (1)$$

The definition of R_s implies a sample with demagnetization factor $N \cong 1$ so that M represents the spin polarization in the material and the physical dipolar magnetic field caused by the ferromagnetically aligned spins cancels. The AHE thus involves a coupling of orbital motion of electrons to the spin polarization and must involve spin-orbit coupling.

The conventional theoretical understanding of R_s is based on a skew scattering mechanism which is a third order process involving interference between spin-orbit coupling (to first order) and spin-flip scattering (to second order) [1,3,4]. In conventional ferromagnets, this theory yields values of R_s 2 orders of magnitude smaller than experimental data [3]. Also, some papers including Ref. [3] use a spin-orbit term involving coupling to the dipole fields produced by the spins which would apparently vanish for demagnetization factor $N = 1$.

Recently, several groups measured the Hall resistivity ρ_H of epitaxial films [5] and single crystals [6] of the "colossal magnetoresistance" (CMR) material $La_{0.7}Ca_{0.3}MnO_3$. These materials involve carriers derived from Mn e_g symmetry d levels which may move through the lattice but are strongly ferromagnetically coupled to localized "core spins" derived from Mn t_{2g} symmetry orbitals. The coupling is so strong that it may be taken to be infinite: a carrier on site i must have its spin parallel to the core spin on site i. The spin of the mobile carrier is thus quenched, but its amplitude to hop from site i to site j is modulated by a factor involving the relative spin states of core spins on the two sites. This physics is called "double-exchange" [7].

The Hall effect measurements found that in CMR materials ρ_H was of the form of Eq. (1) with R_0 *holelike* and R_s *electronlike*. R_s becomes evident above 100 K, increases sharply around T_c, peaks at a temperature $T_{\max} \approx T_c + 30$ K, and decreases slowly at high temperatures. R_s is proportional to the zero-field resistivity from 200 to 360 K. This cannot be explained via the conventional skew scattering theory because the quenching of the carrier spin means the required spin-flip process cannot occur. That the sign of R_s is *opposite* to R_0 and that R_s peaks *above* T_c are also surprising.

In this paper, we present a new theory for the anomalous Hall effect. It is inspired by the physics of CMR, but we suggest that a simple generalization could apply to conventional ferromagnets as well. Our mechanism is based on the observation that a carrier moving in a topologically nontrivial spin background acquires a "Berry phase" [8] which affects the motion of electrons in the same way as does the phase arising from a physical magnetic field [9] and has been argued to influence the Hall effect in high-T_c superconductors [10]. We shall show that this Berry phase can in the presence of spin-orbit coupling give rise to an AHE similar in magnitude and temperature dependence to that observed in CMR materials. This idea was advanced in an e-print [11]. The present paper treats Skyrmion physics and the high temperature phase in more detail and presents a more general treatment valid for any half-metallic ferromagnet. It supercedes Ref. [11]. After the present work was completed two reports [12] appeared presenting a discussion of the physics introduced in [11] along with new data which are argued to confirm the basic picture.

We begin our analysis by writing down the double exchange model for electrons hopping on a lattice, coupled ferromagnetically by atomic exchange J_H to core spins S_c and subject to a spin-orbit coupling H_{so} and to other interactions represented by $\cdots$. Repeated indices are summed.

$$H = -t\sum_{\langle ij\rangle}(d^\dagger_{i\alpha}d_{j\alpha} + \text{H.c.}) - \mu\sum_{\langle ij\rangle}d^\dagger_{i\alpha}d_{j\alpha} - J_H\sum_i \vec{S}_{ic}\cdot d^\dagger_{i\alpha}\vec{\sigma}_{\alpha\beta}d_{i\beta} + H_{so} + \dots \quad (2)$$

The orbital indices of the two e_g orbitals are suppressed in Eq. (2) because they are not essential in this paper [13]. H_{so} in Eq. (2) arises from the fundamental spin-orbit coupling $H_{so} \sim (\vec{k}\times\vec{\sigma})\cdot\vec{\nabla}V_c$ (V_c is the crystalline potential and $\vec{\sigma}$ are the Pauli spin matrices). The projection of H_{so} onto tight binding bands leads to many terms [4]; the one of relevance here is

$$H_{so} = i\,\frac{\lambda_{so}}{4}\sum_i \epsilon^{abc}\sigma^a_{\alpha\beta}(d^\dagger_{i+\hat{b},\alpha} - d^\dagger_{i-\hat{b},\alpha}) \times (d_{i+\hat{c},\beta} - d_{i-\hat{c},\beta})\,. \quad (3)$$

The crucial physics of the manganites is a strong Hunds coupling $J_H \gg t$. In the following, we study the $J_H/t \to \infty$ limit and comment on the $J_H < t$ case in the conclusion. It is convenient to parametrize $\vec{S}_{ic}$ by polar angles θ_i, ϕ_i and to express the electron operator as

$$d_{i\alpha} = d_i z_{i\alpha}, \qquad z_{i\alpha} = |\vec{n}_i\rangle = \begin{pmatrix}\cos\frac{\theta_i}{2}\\ \sin\frac{\theta_i}{2}e^{i\phi_i}\end{pmatrix}, \quad (4)$$

where $z_{i\alpha}$ is the SU(2) coherent spin state along $\vec{n}_i = z^\dagger_{i\alpha}\vec{\sigma}_{\alpha\beta}z_{i\beta}$.

Using Eq. (4), in the presence of an external magnetic field $\vec{H} = \nabla\times\vec{A}$, we can write the action

$$S = \int_0^\beta d\tau\left\{\sum_i in_c a_0 + \sum_i d^\dagger_i(\partial_\tau - ia_0 - \mu)d_i - t\sum_{i\hat{\delta}}\left(\frac{1+\vec{n}_i\cdot\vec{n}_j}{2}\right)^{1/2}[e^{ia(a_{i\hat{\delta}}+\frac{e}{\hbar c}A_{i\hat{\delta}})}d^\dagger_i d_{i+\hat{\delta}} + \text{H.c.}] - g\mu_B\vec{H}\cdot\sum_i\vec{n}_i\left(S_{ic} + \frac{1}{2}d^\dagger_i d_i\right)\right\} + H_{so}\,, \quad (5)$$

where $n_c = 2S_c$ and μ is the chemical potential fixing the electron density $\langle d^\dagger_i d_i\rangle = n_{el}$. a is the lattice constant, $a_0 = iz^\dagger\partial_\tau z$, and $a_{i,\hat{\delta}}$ (defined below) are the internal gauge fields generated by the spin configurations.

The term involving t shows explicitly how the electron hopping is affected by the nearest neighbor spin overlap factor $z^\dagger_{i\alpha}z_{j\alpha} = \langle\vec{n}_i\,|\,\vec{n}_j\rangle = e^{i\Phi(\vec{n}_i,\vec{n}_j)/2}(\frac{1+\vec{n}_i\cdot\vec{n}_j}{2})^{1/2}$. The phase factor $\Phi(\vec{n}_i,\vec{n}_{i+\hat{\delta}}) = aa_{i\hat{\delta}}$ is the solid angle subtended by the three unit vectors $\vec{n}_i, \vec{n}_{i+\hat{\delta}}$ and $\hat{z}$ on the unit sphere. In the continuum $a_{i,\delta} \to z^\dagger\partial_\delta z \equiv \vec{a}\cdot\hat{\delta}$, which defines $\vec{a}$. $a_{i,\delta}$ affects the motion of a electron just as does an external electromagnetic field [9]. A time dependent $\vec{a}$ was shown by Noziéres and Lewiner [4] to lead to a time dependent AHE when the magnetization precessed. Here we show a static $\vec{a}$ leads to a static AHE when topologically nontrivial spin configurations are considered, by using Eq. (5) to calculate R_s. We study the low, high, and critical temperature regimes separately.

The low temperature regime.—Here the core spins are slowly varying on the lattice scale and the system is metallic, so we can take the continuum limit, treat the core spins classically, and obtain

$$S = \beta\int d^dx\left[\frac{\rho_s}{2}(\partial_i\vec{n})^2 - M_0\vec{H}\cdot\vec{n}\right] + S_{el} + H_{so}\,, \quad (6)$$

where $\rho_s \sim tn_{el}a^{2-d}$ is the spin stiffness, $M_0 = g\mu_B[S_c + \frac{1}{2}n_{el}]a^{-d}$ is the magnetization, and S_{el} is the action of spinless fermions moving in the band structure defined by t in Eq. (2) and coupled to a gauge field $\vec{a} + \frac{2\pi}{\Phi_0}\vec{A}$, to spin fluctuations and to other interactions not explicitly written. It is important to stress that in the CMR case considered here, the core spins and electrons are independent fields and the internal gauge field is simply a representation of topologically nontrivial configuration of the core spins instead of an *independent* field. However, in high T_c-cuprates, the gauge fields are *independent* fields related to spin-charge separation [9].

Taking the continuum limit of Eq. (3) and neglecting terms involving electron currents yield

$$H_{so} = i\lambda_{so}n_{el}a^2\int d^dx\,\epsilon^{abc}(\partial_b + ia_b) \times z^\dagger_\alpha\sigma^a_{\alpha,\beta}(\partial_c - ia_c)z_\beta\,. \quad (7)$$

Integrating the conduction electrons out of Eq. (6) and evaluating H_{so} using Eqs. (4) and (7) yields

$$S = \beta\hbar\int d^dx\left[\frac{\rho_s}{2}(\partial_i\vec{n})^2 - M_0\vec{H}\cdot\vec{n} + \frac{\chi_F}{2}\left(\frac{2\pi}{\Phi_0}\vec{H} + \vec{b}\right)^2\right] + \lambda_{so}\frac{n_{e]}}{2a}\int d^dx\,\vec{n}\cdot\vec{b}\,, \quad (8)$$

where $\chi_F \sim \tan^{1/3}_{el}$ is the electron diamagnetic susceptibility, $\Phi_0 = \frac{hc}{e} = 4.1358\times10^{-7}$ G $\cdot$ cm^2 is the fundamental flux quantum, and $\vec{b} = \vec{\partial}\times\vec{a} = \frac{1}{4}\epsilon_{ijk}\vec{n}\cdot(\partial_j\vec{n}\times\partial_k\vec{n})$ is the internal magnetic field arising from $\vec{a}$.

A nonzero $\vec{b}$ arises from topologically nontrivial spin configurations. In two spatial dimensions, these are the Skyrmions [14] which are important in quantum Hall ferromagnets [15]. In three dimensions, the objects are Skyrmion strings (dipoles) which begin at monopoles and end at antimonopoles [14]. In the ordered phase, these have finite creation energies and are exponentially suppressed at low T but can proliferate near T_c. Their behavior has been studied numerically [16].

It is known that at zero external magnetic field, the core energy of a dipole separated by distance d is $E_c = 4\pi\rho_s d$ (i.e., string tension $\sim\rho_s$). To relate E_c to experimental parameters we note that according to the numerical analysis of Ref. [16], $T_c = 1.45\rho_s a$, while in the experiment of Ref. [5] $T_c = 265$ K. We find the core energy for a dipole separated by a lattice constant a is $E_c = 2295$ K. Following Ref. [15], we find only a 2%–3% increase of E_c in an external magnetic field $H = 10$ T; therefore, we can simply neglect the core energy dependence of H. The core energy E_c is *independent* of the angle ϕ which defines the global orientation of the XY spin component. This U(1) invariance implies the existence of a family of very soft twist modes. Dilatation modes have a small energy gap but are also likely to be thermally excited. These soft modes mean that at $T > 0$ each Skyrmion carries a large entropy.

In the absence of spin-orbit coupling, dipoles are randomly oriented, leading to vanishing average $\vec{b}$. In the presence of spin-orbit coupling and a nonzero magnetization, the dipoles are preferentially oriented, leading to a nonzero average $\vec{b}$. To see this we rewrite Eq. (8) in terms of the polarization $\vec{P} = Q\vec{l}$, where $Q = \pm 1$ is the charge of a monopole and $\vec{l}$ is the vector connecting the monopole to antimonopole which are the two end points of the dipole. We find, for $\vec{M}$ parallel to $\mathbf{z}$

$$M_\lambda \int dz \int dx\, dy\, b_z = M_\lambda \int dz\, Q_z = \frac{\lambda_{so} n_{el}}{a} \frac{\vec{M} a^3}{g\mu_B} \cdot \vec{P}, \qquad (9)$$

where $M_\lambda = \frac{\lambda_{so} n_{el}}{a} \frac{Ma^3}{g\mu_B}$.

At low T numerics Ref. [16] shows that the monopole and antimonopole are very dilute and are tightly bound into dipoles of size of one lattice constant. We thus can treat them as independent classical particles. The density ($n_\pm$) of (anti-) Skyrmions is

$$n_\pm = \alpha e^{-\beta(E_c \pm \lambda M Q a)}, \qquad (10)$$

where α is the entropy per dipole. Reference [16] finds $\alpha \sim 320$. We believe this large factor comes from the twist and dilatation modes mentioned above.

The average z direction internal magnetic field $\langle b_z \rangle = -Q(n_+ - n_-)/a^2$ is thus

$$\langle b_z \rangle = -\alpha \frac{Q}{a^2} e^{-\frac{E_c}{k_B T}} \sinh\left(\frac{Q\lambda_{so} n_{el} M a^3}{k_B T g \mu_B}\right). \qquad (11)$$

An internal field b produces the same change in the phase of an electron as would be produced by a physical field of magnitude $\frac{\Phi_0}{2\pi}|\vec{b}|$. The equivalent physical field is large because the appropriate dimensionless coupling (fine structure constant) for the internal field is 1, rather than the 1/137 relevant for physical fields.

The internal magnetic field produces a Hall effect in the usual way. Writing the Hall resistivity as $\rho_H = \frac{1}{n_{eff} ec}(H + \frac{\Phi_0}{2\pi}\langle b \rangle)$, and linearizing the sinh, we find

$$\frac{R_s}{R_0} = -\alpha \frac{\Phi_0}{2\pi} \frac{\lambda_{so} Q^2}{k_B T} \frac{a n_{el}}{g\mu_B} e^{-\frac{E_c}{k_B T}}. \qquad (12)$$

$Q = 1$ is the charge of a monopole and $a = 3.92$ Å is the lattice constant of $La_{1-x}Ca_xMnO_3$. At $T = 200$ K, the experimental value [5] is $\frac{R_s}{R_0} = -13.6$, implying $\frac{\lambda_{so}}{k_B T} = 2.5 \times 10^{-2}$ so $\lambda_{so} \sim 5$ K which justifies the linearization used in Eq. (12). Because the on-site spin-orbit interaction is quenched by the cubic crystal field, λ_{so} is dominated by interion hopping and is difficult to determine, but a rough estimate can be obtained by combining the dimensionless coupling appropriate for d orbitals $(\frac{Ze^2}{2mc^2 r_d})$ ($r_d \sim 0.5$ Å is the d-orbital size) with the band kinetic energy $\frac{\hbar^2}{2ma^2}$ yielding $\lambda_{so} \sim 2$ K.

The sign of R_s relative to R_0 depends on the sign of the spin-orbit coupling. The physically reasonable sign (usual precession of charge around field of core spin) leads to an internal field b which acts to cancel the applied field, implying opposite signs for R_s and R_o.

The high temperature regime.—Here $k_B T_c, g\mu_B H, \ll k_B T \ll J_H$, so the core spins vary on the lattice scale; the continuum action Eq. (8) does *not* apply. It is easiest simply to calculate the average of the z component of the gauge invariant internal flux $\Phi^z_\triangle = \epsilon^{abc} n^a_{i+\hat{x}} n^b_i n^c_{i+\hat{y}}$ through a triangle of adjacent sites $i + \hat{x}, i, i + \hat{y}$ to leading order in $\lambda_{so}/k_B T$ using the lattice action Eq. (5), finding (χ is the spin susceptibility)

$$\Phi_{\triangle^z} \sim \frac{\lambda_{so}\chi H}{k_B T} \sum_\alpha \langle d^\dagger_{i+\hat{x},\alpha} d_{i+\hat{y},\alpha} \rangle. \qquad (13)$$

Further, at high T the $La_{1-x}Ca_xMnO_3$ materials of main experimental interest are in a highly resistive "polaron hopping" regime which we model by assuming $t \ll k_b T$. In the original lattice model with only nearest neighbor hopping the fermion expectation value is of second order in $t/k_B T$ and may be computed, leading to

$$\frac{R_s}{R_0} = -\frac{\lambda_{so}}{k_B T} \left(\frac{t}{k_B T}\right)^2 n_{el}(1 - n_{el})(1 - 2n_{el}) C_3, \qquad (14)$$

where C_3 is a constant of order unity. (Recall R_s is the term in the Hall resistance proportional to $M \sim \chi H$.)

The difficulty of unambiguously extracting the term in the Hall conductivity proportional to the spin susceptibility increases as T is increased further above T_c, so a detailed study of the high-T R_s is probably not waranted.

The critical regime.—For T near T_c, a theory of the topological defects has not been constructed, because in the 3D Heisenberg model, there is *no* decoupling between spin-wave fluctuations and the topological defects, so spin

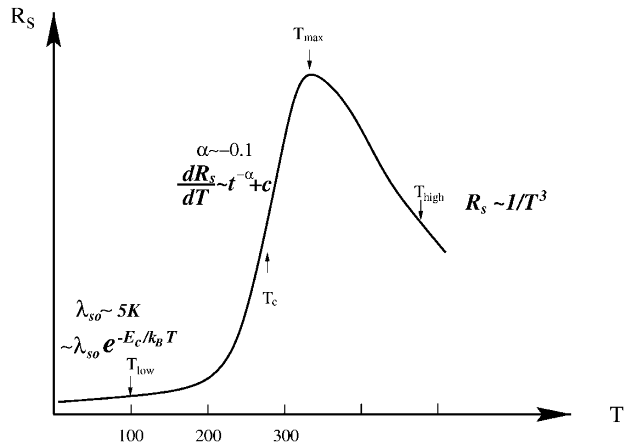

FIG. 1. Calculated temperature dependence of anomalous Hall coefficient.

waves cannot simply be integrated out. Reference [16] simulated the behavior of the topological defects near T_c at zero external magnetic field. The dipole density n was found to increase sharply as T passes through T_c; there is a derivative discontinuity at T_c which is controlled by the specific heat exponent α [16] (as is also the case for the resistivity). The singularity at T_c may be difficult to observe: it is cut off by the field needed to observe an AHE at $T > T_c$ and obscured by the dependence of the AHE on the field and temperature dependence of $\vec{M}$.

From the low temperature and critical regime calculations, we find R_s increases as T is increased, and $dR_s/dT > 0$ at T_c. The high temperature expansion yields a $dR_s/dT < 0$. Therefore, R_s has a maximum at some $T_{\max} > T_c$. The decrease for $T > T_{\max}$ has two causes—strong thermal spin fluctuations disrupt the local correlations needed to produce a $\vec{b}$ and also the fermion correlator in Eq. (13) decreases. Our knowledge of CMR materials is insufficient to allow a quantitative theory of the region near $T_{\max}$.

To summarize, we have constructed a new theory of the anomalous Hall effect in CMR manganites. Our results are shown in Fig. 1 and account naturally for the order of magnitude, the sign (relative to the conventional Hall effect), and the peak at $T > T_c$ found experimentally [5,6]. Our results for R_s have the same qualitative behavior as (and identical critical behavior to) the longitudinal resistivity, but we have no argument for the very close correspondence found experimentally [5].

This paper has assumed a large J_H limit, so the conduction band is completely spin polarized. An extension to the smaller J_H limit, with a partially polarized conduction band would be of interest in connection with the AHE in conventional magnets. In this case, conventional skew scattering would also contribute and indeed would dominate at low T because it varies as a power of T. Recently, a very large AHE was found in Co oxides [17]. These materials involve additional physics, including high-spin/low-spin transitions and inhomogeneous states, whose incorporation in our theory would be of interest.

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