Skyrmion Strings and Anomalous Hall Effect in Double Exchange Systems.

M.J. Calderón and L. Brey
Instituto de Ciencia de Materiales de Madrid, CSIC, 28049 Cantoblanco, Madrid, Spain.
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We perform Monte Carlo simulations to obtain quantitative results for the anomalous Hall resistance, $R_A$, observed in colossal magnetoresistance manganites. $R_A$ arises from the interaction between the spin magnetization and topological defects via spin-orbit coupling. We study these defects and how they are affected by the spin-orbit coupling within the framework of the double exchange model. The obtained anomalous Hall resistance is, in sign, order of magnitude and shape, in agreement with experimental data.

Doped perovskite manganites have attracted much attention lately, since they show the so called colossal magnetoresistance [1]. These materials undergo a ferromagnetic-paramagnetic transition accompanied by a skew scattering theory [9]. Recently, it was proposed to couple the defects orientation with the $M$ tensors. We compute the number of topological defects as in order to obtain a quantitative form of $R$ that in skew scattering theory [9].

These effects can not be explained with the conventional mechanism [2] plays a major role to explain this magnetic transition. In the DE picture, the carriers moving through the lattice are strongly ferromagnetically coupled to the $Mn$ core spins and this produces a modulation of the hopping amplitude between neighboring $Mn$ ions.

The Hall resistivity $\rho_H$ in ferromagnets has two contributions [3], one proportional to the magnetic field $H$, and the other to the spin magnetization $M$: $\rho_H=R_OH+R_AM$. $R_O$ and $R_A$ denote the ordinary (O) and the anomalous (A) Hall resistances (HR). The existence of $R_A$ requires a coupling of orbital motion of electrons to $M$, and the AHE is usually explained in terms of skew scattering due to spin-orbit (s-o) interaction [4].

Several groups [5, 8] have measured $\rho_H$ of the doped $Mn$ oxide $La_{0.7}Ca_{0.3}MnO_3$ for different temperatures ($T$). These experiments found that $R_O$ and $R_A$ have opposite sign, that $R_A$ is much bigger than $R_O$, that $R_A$ peaks at a $T$ above $T_c$, and decreases slowly at higher $T$. These effects can not be explained with the conventional skew scattering theory [6]. Recently, it was proposed [7, 11] that in $Mn$ oxides $R_A$ arises from the interaction of $M$ with non trivial spin textures (topological charges) via s-o coupling. The number of topological charges in the three-dimensional (3D) Heisenberg model increases exponentially with $T$ [12] and Ye et al. [11] extrapolated these results to DE materials obtaining a rapid increase of $R_A$ at low $T$. For $T>T_c$, although in 3D there is not a theory of topological defects, Ye et al. were able to estimate the overall shape of $R_A$.

In this work we perform Monte Carlo simulations in order to obtain a quantitative form of $R_A$ in DE systems. We compute the number of topological defects as a function of $T$ and, by introducing s-o interaction, we couple the defects orientation with $M$. In this way we obtain an AHR which has the same sign, shape and order of magnitude as found experimentally [5].

Hamiltonian. The electronic and magnetic properties of the $Mn$ oxides are described by the DE Hamiltonian,

$$\hat{H} = -t \sum_{i \neq j, \sigma} e^{i\delta A_{i,j} \hat{\sigma}} d_{i,\sigma}^\dagger d_{j,\sigma}$$

$$- J_H \sum_{i,\sigma,\sigma'} d_{i,\sigma}^\dagger \sigma \sigma' d_{i,\sigma'} S_i + \hat{H}_{so} + \hat{H}_z , \quad (1)$$

here $d_{i,\sigma}^\dagger$ creates an electron at site $i$ and with spin $\sigma$, $t$ is the hopping amplitude between nearest-neighbor sites, $J_H$ is the Hund’s rule coupling energy, $S_i$ is the core spin at site $i$ and $\hat{H}_{so}$ is the spin-orbit (s-o) interaction. In the tight binding approximation, the effect of $H$ is to modify the hopping matrix element by introducing the phase $a \hat{A}_{i,j} \bar{A}_{i,j}$, where $a$ is the lattice parameter, $j=i+\delta$ and $A$ is the vector potential corresponding to $H$. The last term in the Hamiltonian is the Zeeman coupling $\hat{H}_z = g_i \mu_B \sum_i \vec{S}_i$. We assume that the $Mn$ ions form a perfect cubic lattice.

In the limit of infinite $J_H$, the electron spin at site $i$ should be parallel to $S_i$, and $H$ becomes [5]

$$\hat{H} = -t \sum_{i \neq j} \frac{\cos \theta_{i,j}}{2} c_{(i,j)2} c_{(j,i)2}^* \delta_{A_{i,j}} c_{j} + \hat{H}_{so} + \hat{H}_z . \quad (2)$$

Now $c_{i,j}^\dagger$ creates an electron at site $i$ with spin parallel to $S_i$, $m_i=S_i/S$ and $\cos \theta_{i,j}=m_i \cdot m_j$. The first term in Eq.(2) describes the motion of electrons in a background of core spins. The electron hopping is affected by the nearest neighbor spin overlap, $\cos(\theta_{i,j}/2)$, being the kinetic energy minimum when all core spins are parallel. This is the DE mechanism for the existence of a ferromagnetic metallic ground state in $Mn$ doped oxides. When the orientation of the electron spin is moved around a close loop the quantum system picks up a Berry’s phase [13] proportional to the solid angle enclosed by the tip of the spin on the unit sphere. $\phi(i,j)$ is the Berry’s phase defined mathematically as the solid angle subtended by the unit vectors $m_i$, $m_j$ and $\hat{z}$ on the unit sphere.

The phase $\phi(i,j)$ in the Hamiltonian affects the motion of electrons in the same way as does the phase arising from a physical magnetic field. $\phi(i,j)$ is related with internal gauge fields generated by non trivial spin textures, which appears in the system when increasing $T$. In absence of s-o coupling the phases $\phi(i,j)$ are random and
the net internal gauge field is zero. In the presence of s-o coupling there is a privilege orientation for the spin textures and a non zero average internal gauge field appear.

In the following we study, as a function of $T$, the appearance of topological defects in the DE model. Once the spin textures are characterized, we study the effect that the s-o coupling has on the defects and we analyze their contribution to the Hall effect.

**Topological defects in the DE model.** The temperature induces fluctuations in the ferromagnetic state of the core spins and at $T > T_c$ the system becomes paramagnetic. Typically $T_c \sim 300K$ and this $T$ is much smaller that the electron Fermi energy, $t \sim 0.1eV$, therefore we consider that the conduction electrons temperature is zero.

In first order in the electron wave function the temperature dependence of the magnetic properties is described by the classical action \cite{14},

$$S = \beta t \langle c_i^\dagger c_j \rangle_0 \sum_{i \neq j} \cos \frac{\theta_{ij}}{2} e^{i\phi_{(i,j)}/2} + \bar{H}_z ,$$  \hspace{1cm} \text{(3)}

where $\langle \_ \_\_ \rangle_0$ means expectation value at $T = 0$.

The system described by Eq.(3) is expected to behave with $T$ similarly to the Heisenberg model. In particular, at low $T$, we expect the occurrence of point singularities as those occurring in the 3D Heisenberg model \cite{13}. These points singularities are called topologically stable because no local fluctuations in a uniform system can produce them. The defects are classified \cite{13} by the topological charge, $Q$, which represents the number of times and the sense in which spins on a closed surface surrounding the defect cover the surface of a unit sphere in spin space. An example of topological defects with $Q = +1(-1)$ occurs at a position from where all the spins point radially outward (inward).

In order to locate the topological charges in the lattice model we follow the prescription of Berg and Liisher \cite{15}. For each unit cube of the lattice we divide each of its six faces into two triangles. The three unit-normalized spins at the corners of a triangle $l$ define a signed area $A_l$ on the unit sphere. The topological charge enclosed by the unit cube is given by

$$Q = \frac{1}{4\pi} \sum_{l=1}^{12} A_l .$$  \hspace{1cm} \text{(4)}

This definition of $Q$ ensures that, when using periodic boundary conditions, the total topological charge in the system is zero. $Q$ in each cube is an integer number, and the magnitude of nonzero charges is almost always equal to unity. Only at rather high temperatures a few defects with $|Q| \geq 2$ are found.

$Q$ can be interpreted as the number of magnetic monopoles enclosed by the unit cube. The quantities $A_l/\phi_0/4\pi$ represent the magnetic flux piercing the triangle $l$. Here $\phi_0 = hc/e$ is the magnetic flux quantum.

Following this analogy we assign at each point of the lattice, $i$, a three dimensional internal magnetic field $b_i$.

The phase $\phi(i,j)$ can be written in the form,

$$\phi(i,j) = \frac{e}{hc} a_{i,j} ,$$  \hspace{1cm} \text{(5)}

where $b = \nabla \times a$. Here it is clear that the $b$ associated with a spin texture affects the motion of an electron just as does an external magnetic field.

In a system with a uniform magnetization at the surface, the interaction between a positive and a negative defect is finite and in the continuous Heisenberg model increases linearly with separation. \cite{14} Defects with opposite charges are closely bound in pairs at low $T$. These pairs of defects are Skyrmion \cite{17,18} strings (dipoles) which begin at a monopole ($Q=1$) and end at an antimonopole ($Q=-1$). The Skyrmions are characterized by a dipole $P$ joining $Q=-1$, and $Q=+1$,

$$P = \frac{a^2}{\phi_0} \sum_i b_i .$$  \hspace{1cm} \text{(6)}

By performing Monte Carlo simulations on the classical variables $m$, \cite{14}, we have studied the dependence on $T$ of the number of defects in the system. With the definition of $Q$, the number of positive and negative defects is the same and the important quantity is the average defect pair density $\langle n \rangle$. In Fig. 1 we plot $\langle n \rangle$ as a function of $T$ for a DE system of size $16 \times 16 \times 16$. We have checked that our results are free of finite size effects. In the same figure we plot $m(T)$. In the DE system $T_c \sim 1.06 t(c_i^\dagger c_j \rangle_0$. The results correspond to $g\mu_b H=0$ and $g\mu_b H=0.067T_c$ ($H \sim 10$ Tesla).

![FIG. 1. Plot of the logarithm of the average defect pair density as a function of the inverse temperature for a system of size $16 \times 16 \times 16$. The dashed lines are linear fits to the data below $T_c$. Their slope is the core energy $E_c = 7.05T_c$.](image-url)

We have studied correlation between defects. For $T < T_c$ the $Q=+1$ and $Q=-1$ defects are strongly cou-
For $T < T_c$ the increase of the system size does not change the overall shape.

\[ (n) = \alpha e^{-\beta E_c} . \]  

Here $E_c$ and $\alpha$ are, respectively, the core energy and the entropy of the Skyrmions. Numerically we have obtained $E_c = 7.05 T_c$. This value is slightly smaller than the value obtained for the Heisenberg model \( E_{Heis} \approx 8.7 T_c \). At $T > T_c$ the number of defects increases sharply and it becomes very difficult to pair up defects with opposite charges in an unambiguous way. The core energy practically does not depend on $H$, this result is in agreement with the obtained for pure two-dimensional Skyrmions \cite{19}. The entropy $\alpha$ is related with the degeneracy of the Skyrmions in the orientation of $P$ and with thermally activated twist and dilatation soft modes. We have obtained that for $H=0$, $\alpha = 51$. Note that $\alpha_{Heis} \approx 320$ \cite{12}.

For finite $H$ the six $(1,0,0)$ directions keep being degenerated, but some of the twist soft modes becomes more gaped and the value of the entropy is reduced.

By performing calculations in a system constrained to get a unique Skyrmion with a given dipole $P$, we have calculated the energy of isolated Skyrmions. In this way we have checked that in the absence of s-o coupling the energy of the Skyrmion only depend on the absolute value of $P$ and not on its orientation. We have obtained that the core energy of a Skyrmion with $P=(1,0,0)$ is $E_{(1,0,0)}^c = 7.05 T_c$, with $P=(1,1,0)$ is $E_{(1,1,0)}^c = 8.65 T_c$ and for $P=(1,1,1)$ is $E_{(1,1,1)}^c = 10.11 T_c$. The dependence of the energy on $P$ confirm the strong confinement energy of the topological defect \cite{10}. The increase of the Skyrmion energy with $P$, implies that for $T < T_c$ the only relevant pairs are those with $P=1$.

In the case of zero s-o coupling, the Skyrmion core energy does not depend on the direction of $P$ and the average internal gauge magnetic field is zero, $\langle b \rangle = 0$. The s-o coupling privileges an orientation of the Skyrmions and it results in a finite value of $\langle b \rangle$.

**Spin-orbit interaction.** The s-o coupling has two contributions, the interaction of the spin of the carriers with the ion electric field, and the magnetic interaction between the carriers with the core spins $S_i$. In the $J_H \rightarrow \infty$ limit, both contributions have the same form \cite{10} and, \[ \hat{H}_{so} = \lambda_{so} x a^2 \phi_0 S \sum_i m_i \cdot b_i , \]  

where $x$ is the carriers concentration. For $\lambda_{so} \neq 0$ and $m \neq 0$, the Skyrmions are preferentially oriented. If $\hat{H} \parallel \hat{z}$, $m \parallel \hat{z}$ and a net $z$ component of $\langle b \rangle$ results.

We have included the s-o interaction in the Monte Carlo simulation and we have obtained that $\langle b_z \rangle$ is linear with $\lambda_{so}$ in all range of $T$. In Fig. 2 we plot for a system of size $12 \times 12 \times 12$, $\phi_z = \langle b_z \rangle a^2 / \phi_0$ as a function of $T$. For $T < T_c$ our results are free of finite size effects. For $T > T_c$ the increase of the system size does not change the overall shape.

![Plot of $\phi_z$ as a function of $T$ for a system of size $12 \times 12 \times 12$ and $g \mu_B H = 0.067 T_c$. The interaction of the spin magnetization and topological defects via spin-orbit coupling has been included. The dashed line corresponds to an independent Skyrmions picture (see Eq. [10]).](image)

It is interesting to analyze the results for $\phi_z$ as a function of the density of defects $\langle n \rangle$. The main effect of the s-o coupling is to privilege the appearance of Skyrmions polarized parallel to $m$, $\langle n_- \rangle$, with respect to Skyrmions with $P$ antiparallel to $m$, $\langle n_+ \rangle$. This asymmetry produce a $z$-component of the internal gauge field, $\langle b_z \rangle = \phi_0 / a^2 (\langle n_- \rangle - \langle n_+ \rangle)$. Assuming that the Skyrmions are independent, \[ \langle n_- \rangle - \langle n_+ \rangle = \frac{1}{3} \langle n \rangle \sinh (\varepsilon_0 / T) , \]  

where \[ \varepsilon_0 = \lambda_{so} x / 2 \]  

is the s-o energy interaction of a Skyrmion with $P = (0,0,1)$ and $\hat{m}(T)$ is the spin polarization inside the Skyrmion. Finally, within the independent Skyrmions picture, after linearizing Eq. [10], \[ \phi_z^{ind} = \frac{\langle n \rangle \lambda_{so}}{6 T} \hat{m}(T) . \]  

$\hat{m}(T)$ is expected to be a function of $m(T)$. By comparing the expression for $\phi_z^{ind}$ with the Monte Carlo results, Fig. 2, we obtain that for $T \leq T_c$, $\hat{m}(T) = m(T) / 5$. That means that the spin polarization inside the Skyrmions is five times smaller that the average spin polarization. It is interesting to note how the independent Skyrmions picture describes not just the low temperature regimen, but also the trends of $\langle b_z \rangle$ at $T \geq T_c$. The sign of $\phi_z$ depends on the sign of $\lambda_{so}$. Physically we expect that the motion of the electrons leads to an
Anomalous Hall effect. The Hall resistivity can be written as $\rho_H = (H + (b))/nec$. Comparing this expression with the definition of $R_A$ we obtain

$$R_A/R_0 = -\frac{a^3}{g\mu B} m .$$

(12)

By using the appropriate parameters, we plot in Fig. 3 $R_A/R_0$ for $La_0.7Ca_{0.3}MnO_3$. We take $T_c \sim 270K$ [12], we use $\lambda_{so}=5K$ [8] and $g\mu B H = 0.067T_c$.

Fig.3 is the main result of our calculation. We obtain an AHR which i) is negative, ii) increases exponentially and becomes evident at $T \sim T_c/2$, iii) at temperatures close to $T_c$, is around 20 times bigger than the ordinary Hall resistance, and iv) has a maximum at temperatures slightly higher ($\sim 30K$) than $T_c$. The subsequent decrease is due to thermal fluctuations that destroy the directional order of the Skyrmions. If we take into account the fact that the conductance at $T > T_c$ is mainly due to polaron hopping, an extra factor of $1/T^2$ is expected [10] leading to a steeper decrease. Our results are in good agreement with the data obtained experimentally [16]. We have checked that these results do not depend significantly on the magnetic field applied.

In addition, we have found, by diagonalizing the electron Hamiltonian, that there is not significant electronic charge associated to the Skyrmions [19]. This is in contrast to the quantum Hall ferromagnetic systems where charge associated to the Skyrmions [20]. This is in agreement with the definition of $\lambda_{so}$.

The Skyrmions we have studied appear when increasing the topological and electrical charge are equivalent [19]. In contrast to the quantum Hall ferromagnetic systems where the Skyrmions are present in the system [20].

In closing, we have computed the anomalous Hall resistance in colossal magnetoresistance manganites. We have obtained, as a function of temperature, the average value of Skyrmions for the double-exchange model. By introducing a spin-orbit interaction, we obtain a coupling between the Skyrmions orientation and the magnetization which results in the appearance of an anomalous Hall resistance. The sign, order of magnitude and shape of the obtained anomalous Hall resistance are in agreement with the experimental information.

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