SUPPRESSION OF FERROMAGNETIC ORDERING IN THE ANISOTROPIC DOUBLE-EXCHANGE MODEL: A MONTE CARLO STUDY *

Hongsuk Yi and Sansang Lee

Supercomputing Center, Korea Institute of Science and Technology Information
Yuseong, P.O. Box 122, Daejeon 305-600, Korea

(Received July 10, 2002)

We report a detailed Monte Carlo study of the magnetic properties of double exchange model in the highly anisotropic hopping integral t_c/t_{ab} regime. We find that the resistivity upturns at low temperature is related to the suppression of ferromagnetic arrangement, accompanied by strong spin fluctuations. This anomalous magnetic behavior comes from the competition between the reduced interlayer double exchange coupling and the thermal frustration of the ordered two dimensional ferromagnetic layer, which leads to a mixture of ferromagnetic and antiferromagnetic clusters.

PACS numbers: 75.50.Cc, 75.30.Et, 75.30.–m, 72.10.–d

1. Introduction

Cubic perovskite manganese oxides has stimulated considerable interest because of their colossal magnetoresistance (CMR) effects, showing an extremely large change in resistance in response to applied magnetic field. But for immediate technological applications to switching device to be viable, great improvements are required in the development of new CMR materials operating at low field. One of the convincing candidates for the low-field CMR materials is the so called Ruddlesden-Popper series, achieved by building series of intergrowths of multiple perovskite slabs. Particularly the $n = 2$ member of $(La, Sr)_{n+1}Mn_nO_{3n+1}$ has drawn a lot of attention due to its unique two dimensional (2D) structural nature [1]. The most notable feature of these materials is the occurrence of a large tunneling magnetoresistance (TMR) below T_c [2]. Recently Kimura *et al.* has observed a remarkable enhancement of interplane TMR, reflecting the field-induced

* Presented at the International Conference on Strongly Correlated Electron Systems, (SCES 02), Cracow, Poland, July 10–13, 2002.

dimensional crossover of the charge-transport [3]. These nontrivial spin and charge dynamics may be crucial to understand the unusual TMR effects observed in the layered manganites.

2. Theoretical description and Monte Carlo results

The anisotropic double exchange (DEX) model Hamiltonian can be written as [4]

$$\mathcal{H} = -\sum_{\langle ij\rangle} t_{ij}^{ab}\left(c_j^+ c_i + c_i^+ c_j\right) - \sum_{\langle ll'\rangle} t_{ll'}^{c}\left(c_l^+ c_{l'} + c_{l'}^+ c_l\right) - h\sum_i S_i^z, \quad (1)$$

where $\langle ij\rangle$ and $\langle ll'\rangle$ indicate the nearest neighbor pairs of intraplane and interplane sites respectively, and h is an external magnetic field. The effective hopping integral can be written as $t_{ij}^{ab} = t_{ab}\cos(\theta_{ij}^{ab}/2)$ and $t_{ll'}^{c} = t_c\cos(\theta_{ll'}^{c}/2)$ where θ_{ij}^{ab} and $\theta_{ll'}^{c}$ are the relative angle between nearest neighbor Mn^{4+} ions in the intraplane and interplane, respectively. Monte Carlo calculation [5] has been performed mostly on $6 \times 6 \times 6$ lattices with periodic boundary conditions. Unless stated otherwise, we take $t_{ab} = 1$ (we set $t = t_{ab}$) as the unit of energy, and $t_c = 0.2t$.

Fig. 1(a) shows the calculated magnetization $M = \langle\sum_i S_i^z\rangle$ as a function of temperature for the zero magnetic field and $h = 0.01t$ which corresponds

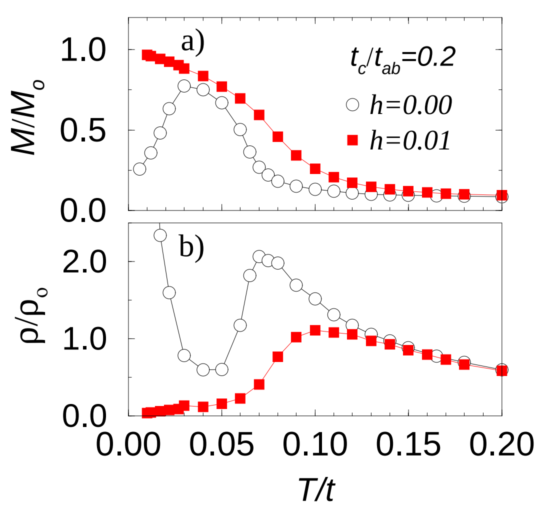

Fig. 1. The temperature dependence of magnetization (a) and resistivity (b) for the highly anisotropic ratio of hopping integral $t_c/t_{ab} = 0.2$.

to about 5 T if we take $t = 0.2$ eV. With decreasing temperature, the zero-field magnetization increases to a maximum near $T^* = 0.03t$ and then drastically decrease below T^*. The applied magnetic field greatly enhances the magnetization, and eventually reaches to the saturated value of $M/M_{\rm o}$ at low temperature. This unusual magnetic order with incomplete saturation is strongly correlated with the spin disorder scattering.

In the presence of the spin disorder scattering via DEX interaction [6], we phenomenologically assumed that the fluctuation of the carriers arising from fluctuating random potential can be written as [4]

$$\rho \approx \frac{\langle \sum_{i,R,\delta_1,\delta_2} t_{i,i+\delta_1} t_{i+R,i+R+\delta_2} \rangle - \langle \sum_{i,\delta_1} t_{i,i+\delta_1} \rangle^2}{\langle \sum_{i,\delta_1} t_{i,i+\delta_1} \rangle^2}\,, \tag{2}$$

where $\vec{R}$ represents sites on three dimensional (3D) lattice and any of the vectors $\hat{x}$, $\hat{y}$, and $\hat{z}$ connecting a site to one of the nearest neighbors denote as $\vec{\delta}_1$ and $\vec{\delta}_2$. It is worth noting that Eq. (2) is a generalization of the result by Kubo and Ohata [7] where only the shortest hopping correlation of scattering, *i.e.*, $\vec{R} = 0$, is taken into account.

Fig. 1(b) shows the T-dependence of ρ/ρ_o. A sharp drop of zero-field resistivity is observed near $T_{\rm c} \approx 0.07$ due to the robust 3D ferromagnetic spin alignment via the DEX mechanism, and a sharp upturn in ρ occurs near T^*. This reentrant insulating phase is strongly correlated with the observed unusual magnetic arrangement at low temperature regimes. Upon applying magnetic field, this upturn drops sharply, resulting in a very high magnetoresistance ($\Delta\rho/\rho \equiv (\rho(0) - \rho(h))/\rho(0)$) which is 99% at $T = 0.012t$.

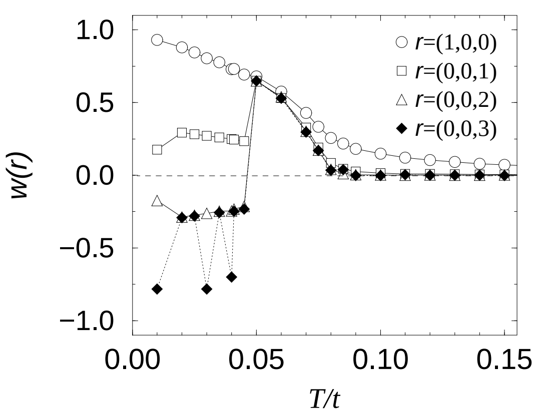

Fig. 2. The temperature dependence of spin-spin correlation function $w(r) = 1/N \sum_i \vec{S}_i \cdot \vec{S}_{i+r}$ for four values of $\vec{r}$ in the highly anisotropic regime of $t_c/t_{ab} = 0.2$.

To study this unusual magnetic properties, we consider spin-spin correlations among the classical spins defined as $w(r) \equiv \frac{1}{N}\sum_i \vec{S}_i \cdot \vec{S}_{i+r}$. Figure 2 shows $w(r)$ *vs* T for several values of lattice sites $\vec{r}$ and $t_c = 0.2$. The planer correlation for $\vec{r} = (1,0,0)$ is robust even for the low temperature limit. Below $T < 0.05t$, however, the robust ferromagnetic correlation along the c-axis is drastically reduced for $\vec{r} = (0,0,1)$ and the weak antiferromagnetic correlation is enhanced for $\vec{r} = (0,0,3)$, reflecting the magnetic domain structure.

3. Discussion and summary

The upturn behavior found in this study under the external field is well related to the low field TMR effects observed in the layered manganites [2]. Our results suggest that the ferromagnetic exchange coupling between the adjacent bilayers can be weakened due to the reduced dimensionality which makes the charge dynamics more two-dimensional but highly diffusive. Such a 2D-like conduction is controlled by the anisotropic hopping integral of $t^c_{ll'} = t_c \cos(\theta^c_{ll'}/2)$ where the e_g carriers cannot hop between the adjacent ferromagnetic layers if the relative angle $\theta^c_{ll'}$ between the adjacent t_{2g} spins closely reaches to π. In the real materials [2, 3] however, each decoupled ferromagnetic domain can be aligned by the externally applied field, reflecting the field-induced dimensional crossover from the quasi two dimensional magnetic domain structure to three dimensional long-range ferromagnetism.

REFERENCES

[1] T. Fukumura, H. Sugawara, T. Hasegawa, K. Tanaka, H. Sakaki, T. Kimura, Y. Tokura, *Science* **284**, 1969 (1999).

[2] Y. Moritomo, A. Asamitsu, H. Kuwaharaa, Y. Tokura, *Nature* **380**, 141 (1996).

[3] T. Kimura, Y. Tomioka, H. Kuwahara, A. Asamitsu, M. Tamura, Y. Tokura, *Science* **274**, 1698 (1996); T. Kimura, A. Asamitsu, Y. Tomioka, Y. Tokura, *Phys. Rev. Lett.* **79**, 3720 (1997).

[4] H. Yi, N. H. Hur, J. Yu, J. Phys. C **12**, 5453 (2000); H. Yi, J. Yu, N. H. Hur, J. Kor, *Phys. Soc.* **37**, 114 (2000).

[5] S. Yunoki, J. Hu, A. Malvezzi, A. Moreo, N. Furukawa, E. Dagotto, *Phys. Rev. Lett.* **80**, 845 (1998); H. Yi, J. Yu, *Phys. Rev.* **B58**, 11 123 (1998).

[6] C. Zener, *Phys. Rev.* **82**, 403 (1951): P. W. Anderson, H. Hasegawa, *Phys. Rev.* **100**, 675 (1955).

[7] K. Kubo, N. Ohata, *J. Phys. Soc. Jpn.* **33**, 21 (1972).