

Magnetic ground states of a layered manganite crystal $\text{La}_{1.4}\text{Sr}_{1.6}\text{Mn}_2\text{O}_7$

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

1998 J. Phys.: Condens. Matter 10 9747

(<http://iopscience.iop.org/0953-8984/10/43/018>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 171.66.16.210

The article was downloaded on 14/05/2010 at 17:42

Please note that [terms and conditions apply](#).

Magnetic ground states of a layered manganite crystal $\text{La}_{1.4}\text{Sr}_{1.6}\text{Mn}_2\text{O}_7$

Yi Liu, L Sheng, D Y Xing[†] and Jinming Dong

National Laboratory of Solid State Microstructures and Department of Physics, Nanjing University, Nanjing 210008, People's Republic of China

Received 3 July 1998

Abstract. We extend the model Hamiltonian of cubic perovskite manganites to a layered manganite system by considering the anisotropy in charge and spin couplings. By minimizing the total free energy of the system, we have obtained the magnetic ground state of the layered manganite crystal $\text{La}_{1.4}\text{Sr}_{1.6}\text{Mn}_2\text{O}_7$ as a function of the anisotropic ratio of charge coupling, t_c/t_{ab} . It is found that while each MnO_2 bilayer has a ferromagnetic ground state, the interplane magnetic configuration changes from a ferromagnetic order to an antiferromagnetic order with decreasing t_c/t_{ab} . This result can account qualitatively for pressure-enhanced interplane magnetoresistance in layered manganite crystals.

1. Introduction

The recent discovery of colossal magnetoresistance (CMR) [1–5] in the doped manganites $\text{RE}_{1-x}\text{AE}_x\text{MnO}_3$ (RE and AE being trivalent rare earth and divalent alkaline earth ions, respectively) has stimulated a great number of efforts in understanding their unusual transport and magnetic properties [6–13]. The striking correlation between ferromagnetism and metallic conduction in the mixed-valence oxides $\text{RE}_{1-x}\text{AE}_x(\text{Mn}_{1-x}^{3+}\text{Mn}_x^{4+})\text{O}_3$ [14, 15] was explained qualitatively by Zener's double exchange (DE) model [16], which was subsequently refined by Anderson and Hasegawa [17], and by de Gennes [18]. According to this mechanism both the ferromagnetism and metallic conduction are linked to the mobility of the e_g conduction electrons. The Mn^{3+} ion has an electronic configuration of $3d^4 (t_{2g}^3 e_g^1)$ and the Mn^{4+} ion has an electronic configuration of $3d^3 (t_{2g}^3 e_g^0)$. Charge carriers are doped by substitution of RE^{3+} with AE^{2+} ions into the Mn e_g orbitals that are strongly hybridized with O 2p orbitals. These carriers become itinerant through the network of the MnO_6 octahedra, and simultaneously can mediate the ferromagnetic (FM) kinetic exchange interaction (the DE interaction) between the localized Mn t_{2g} spins ($S = 3/2$). A distinct feature is that the spin of the itinerant e_g electron and the localized spins on each Mn site tend to align parallel because the on-site Hund coupling between these spins is sufficiently large compared with the transfer integral t of itinerant electrons between the nearest-neighbour (NN) Mn sites. As a result, the amplitude for a carrier to hop from site i to j is highly affected by the relative angles between the localized spins S_i and S_j , FM order maximizing the hopping and antiferromagnetic (AF) order minimizing it. Although a great number of works have been done on the Mn oxides [6–32], their magnetic and transport properties, including the magnetic phase diagram, are not completely clear and much more needs to be done.

[†] E-mail address: dyxing@netra.nju.edu.cn.

A recent finding of the interplane tunnelling magnetoresistance (TMR) in layered perovskite manganites $\text{La}_{2-2x}\text{Sr}_{1+2x}\text{Mn}_2\text{O}_7$ with $x = 0.3$ and $x = 0.4$ provides a novel approach to the large MR attainable at low magnetic fields [33–35]. The layered manganite is composed of FM MnO_2 bilayers with intervening insulating $(\text{La,Sr})_2\text{O}_2$ blocks and can be viewed as an infinite array of ferromagnet/insulator/ferromagnet junctions. In such a quasi-two-dimensional system, the interplane as well as in-plane charge dynamics (and hence the MR characteristics) is expected to critically depend on the interlayer magnetic coupling between the FM MnO_2 bilayers. The degenerated e_g orbitals are split into the $d_{x^2-y^2}$ and $d_{3z^2-r^2}$ states. In the layered manganite crystal, the former extends along the sheet direction and has large t_{ab} , while the latter has small t_c , where t_{ab} and t_c are the transfer integrals of itinerant electrons between in-plane and out-of-plane NN Mn sites, respectively. Accordingly, the in-plane superexchange J_{ab} is also larger than the out-of-plane superexchange J_c . In this paper, we extend the model Hamiltonian in [21] to include the anisotropy and spin correlations between the inplane Zener carriers. Using the Hartree–Fock approximation and making numerical calculations, we obtain the magnetic coupling as a function of t_c/t_{ab} and J_c/t_{ab} in a layered manganite crystal, $\text{La}_{2-2x}\text{Sr}_{1+2x}\text{Mn}_2\text{O}_7$ ($x = 0.3$), at zero temperature. It is shown that at $x = 0.3$, while each MnO_2 bilayer always has an FM order, the interplane magnetic configuration transits from an AF order to an FM order with decreasing anisotropy (by increasing t_c/t_{ab}).

2. Theoretical description

To set up a simple model Hamiltonian of perovskite Mn oxides, only the d orbitals of Mn ions are considered by disregarding the other kinds of atoms La, O etc. The role of these atoms may be implicitly included in the parameter values in the model. An isotropic model Hamiltonian for the cubic perovskite manganites $\text{RE}_{1-x}\text{AE}_x\text{MnO}_3$ has been suggested by Inoue and Maekawa [21]. It is straightforward to extend it to an anisotropic layered structure where each plane is modelled on an MnO_2 bilayer of the layered manganite crystal and a small t_c describes the coupling between the adjacent MnO_2 bilayers separated by rock salt-type layers of $(\text{La,Sr})_2\text{O}_2$. Besides, we consider the spin correlations between the inplane carriers. The model Hamiltonian can be written as

$$H = -t_{ab} \sum_{\langle ij \rangle \sigma}^{\text{inplane}} (a_{i\sigma}^\dagger a_{j\sigma} + \text{HC}) - t_c \sum_{\langle ij \rangle \sigma}^{\text{interplane}} (a_{i\sigma}^\dagger a_{j\sigma} + \text{HC}) + \frac{U}{2} \sum_{i\sigma} n_{i\sigma} n_{i\bar{\sigma}} \\ + J_{ab} \sum_{\langle ij \rangle}^{\text{inplane}} \mathbf{S}_i \cdot \mathbf{S}_j + J_c \sum_{\langle ij \rangle}^{\text{interplane}} \mathbf{S}_i \cdot \mathbf{S}_j - J_H \sum_i \mathbf{S}_i \cdot \mathbf{s}_i - J_s \sum_{\langle ij \rangle}^{\text{inplane}} \mathbf{s}_i \cdot \mathbf{s}_j. \quad (1)$$

Here U is the on-site Coulomb repulsion between spin-up and spin-down itinerant electrons, $a_{i\sigma}^\dagger$ ($a_{i\sigma}$) is a creation (an annihilation) operator of an itinerant electron at site i with spin σ , and $n_{i\sigma} = a_{i\sigma}^\dagger a_{i\sigma}$ is the itinerant-electronic number operator. J_{ab} (>0) and J_c (>0) are the NN exchange interactions between in-plane and out-of-plane localized spins, respectively, and J_H (>0) represents the on-site Hund coupling between the itinerant electron and the localized spin. J_s (>0) stands for the spin correlation between the Zener carriers, $\mathbf{s}_i = (1/2) \sum_{\sigma\nu} (a_{i\sigma}^\dagger \boldsymbol{\tau}_{\sigma\nu} a_{i\nu})$ is the conduction-electron spin density with $\boldsymbol{\tau}$ the Pauli matrix. The introduction of the last term in equation (1) is based on the following consideration. According to the DE mechanism, the ferromagnetism of the doped Mn oxides is induced by the motion of the itinerant electrons. The superexchange interaction between the NN localized spins is antiferromagnetic, playing a counteractive role in the ferromagnetism. At

$x = 0$, there is neither motion of itinerant electrons nor the DE-induced ferromagnetism. In this case, however, on each MnO_2 plane perpendicular to the crystal c -axis, the magnetic moments on Mn sites are aligned, even though the moment direction alternates from plane to plane, which is called the type-A AF configuration. It follows that besides the DE-induced FM interaction, there exists a direct in-plane FM coupling between the $3d_{x^2-y^2}$ orbitals of e_g electrons on the NN Mn sites, which can be described by the last term of equation (1). As the e_g electrons are decreased with doping, this coupling becomes gradually weak. At $x = 1$, there is no e_g electron and so this direct FM coupling as well as the DE-induced FM coupling vanishes, resulting in a three-dimensional (type-G) AF configuration of the localized spins.

We apply the Hartree–Fock approximation to Hamiltonian (1) and compare the free energies of the spiral (SP) and canted (CN) states, the FM, A-type AF and G-type AF states being their special cases. In our coordinate system, the direction of the localized spin on site i is denoted by its spherical coordinate $(\pi/2, \varphi_i)$. The relative angle between the spins on two NN sites i and j is $\varphi_{ij} = \varphi_i - \varphi_j$. For either SP or CN states, their absolute values are assumed to be $|\varphi_{ij}| = 2\theta_{ab}$ for the NN sites i and j on the same x - y plane and $|\varphi_{ij}| = 2\theta_c$ for them on adjacent x - y planes. The sign of φ_{ij} is determined not only by the relative position between sites i and j , but also by the spin configuration of the system. In an SP state, $\varphi_{ij} > 0$ for $\mathbf{R}_{ij} = \mathbf{R}_i - \mathbf{R}_j = \mathbf{a}, \mathbf{b}$ or \mathbf{c} ; $\varphi_{ij} < 0$ for $\mathbf{R}_{ij} = -\mathbf{a}, -\mathbf{b}$ or $-\mathbf{c}$, where \mathbf{a}, \mathbf{b} and \mathbf{c} are the basis vectors along the x, y and z directions, respectively. For a CN state, we divide all the sites into two sublattices so that all the NN sites of each site in sublattice A belong to sublattice B, and *vice versa*. The sign of φ_{ij} in the CN state rely on whether site i is in sublattice A or B, i.e. $\varphi_{ij} > 0$ for $i \in \text{A}$ and $\varphi_{ij} < 0$ for $i \in \text{B}$. Obviously, both SP and CN states become the FM state for $\theta_{ab} = \theta_c = 0$, the type-G AF state for $\theta_{ab} = \theta_c = \pi/2$, and type-A AF state for $\theta_{ab} = 0$ and $\theta_c = \pi/2$, respectively.

If directly decoupling the Hund coupling term in equation (1) by the Hartree–Fock approximation, we will have a term $s_i \cdot \langle \mathbf{S}_i \rangle$, which depends explicitly on the orientation of $\langle \mathbf{S}_i \rangle$. This is not convenient for further calculation, because the orientation of $\langle \mathbf{S}_i \rangle$ varies from site to site. Instead of a fixed spin quantization axis, we use a set of local spin quantization axes by taking the quantization axis at site i along $\langle \mathbf{S}_i \rangle$. Rotation of spin quantization axes from the original fixed one to the local ones is equivalent to the following unitary transformation

$$\begin{aligned} a_{i\uparrow} &= e^{-i\varphi_i/2}(c_{i\uparrow} + c_{i\downarrow})/\sqrt{2} \\ a_{i\downarrow} &= e^{i\varphi_i/2}(c_{i\uparrow} - c_{i\downarrow})/\sqrt{2}. \end{aligned} \quad (2)$$

By using the transformation above and the Hartree–Fock approximation, the Hamiltonian can be reduced to $H = H_d + H_s + E_0$, where H_d is the Hamiltonian of the localized spins H_s is the Hamiltonian of the itinerant electrons and E_0 is a constant term. They are given by

$$H_d = \sum_i \langle \mathbf{L}_i \rangle \cdot \mathbf{S}_i \quad (3)$$

$$\begin{aligned} H_s = - \left\{ t_{ab} \sum_{(ij)\sigma}^{\text{inplane}} [\cos(\varphi_{ij}/2)c_{i\sigma}^\dagger c_{j\sigma} + i \sin(\varphi_{ij}/2)c_{i\sigma}^\dagger c_{j\bar{\sigma}}] \right. \\ \left. + t_c \sum_{(ij)\sigma}^{\text{interplane}} [\cos(\varphi_{ij}/2)c_{i\sigma}^\dagger c_{j\sigma} + i \sin(\varphi_{ij}/2)c_{i\sigma}^\dagger c_{j\bar{\sigma}}] \right\} + \sum_{i\sigma} v_\sigma c_{i\sigma}^\dagger c_{i\sigma} \end{aligned} \quad (4)$$

$$\begin{aligned}
E_0 = & -NUn_\uparrow n_\downarrow - J_{ab} \sum_{\langle ij \rangle}^{\text{inplane}} \langle \mathbf{S}_i \rangle \cdot \langle \mathbf{S}_j \rangle - J_c \sum_{\langle ij \rangle}^{\text{interplane}} \langle \mathbf{S}_i \rangle \cdot \langle \mathbf{S}_j \rangle \\
& + J_H \sum_i \langle \mathbf{S}_i \rangle \cdot \langle \mathbf{s}_i \rangle + J_s \sum_{\langle ij \rangle}^{\text{inplane}} \langle \mathbf{s}_i \rangle \cdot \langle \mathbf{s}_j \rangle.
\end{aligned} \quad (5)$$

Here $\mathbf{L}_i = 2J_{ab} \sum_{j \neq i}^{\text{inplane}} \mathbf{S}_j + 2J_c \sum_{j \neq i}^{\text{interplane}} \mathbf{S}_j - J_H \mathbf{s}_i$, and $v_\sigma = Un_\sigma - \beta_\sigma J_H |\langle \mathbf{S}_i \rangle|/2 - 2J_s \sum_{j \neq i}^{\text{inplane}} |\langle \mathbf{s}_j \rangle| \cos(2\theta_{ab})$ in which $\beta_\uparrow = -\beta_\downarrow = 1$ and $n_\sigma = \langle c_{i\sigma}^\dagger c_{i\sigma} \rangle$ is the density of the electrons with spin σ . We have assumed that both J_H and U are large enough, so that \mathbf{s}_i and \mathbf{S}_i are always aligned parallel and on-site double-occupancy of e_g electrons is prohibited. Under this approximation, we have $|\langle \mathbf{S}_i \rangle| = S = 3/2$ and $|\langle \mathbf{s}_i \rangle| = (1-x)/2$.

We next diagonalize Hamiltonian H_s by considering the SP and CN states, respectively. For the SP state, by the aid of the Fourier transformation, equation (4) becomes

$$H_s^{SP} = \sum_{k\sigma} [(v_\sigma + \epsilon'_k) c_{k\sigma}^\dagger c_{k\sigma} - \epsilon''_k c_{k\sigma}^\dagger c_{k\bar{\sigma}}]. \quad (6)$$

Here, $\epsilon_{k'} = -2t_{ab} \cos \theta_{ab} (\cos k_x a + \cos k_y b) - 2t_c \cos \theta_c \cos k_z c$, $\epsilon''_k = 2t_{ab} \sin \theta_{ab} (\sin k_x a + \sin k_y b) + 2t_c \sin \theta_c \sin k_z c$. Introducing further new operators $d_{k\uparrow}$ and $d_{k\downarrow}$ in terms of the relations

$$\begin{aligned}
c_{k\uparrow} &= [U_+(\xi) d_{k\uparrow} + (\epsilon''_k / |\epsilon''_k|) U_-(\xi) d_{k\downarrow}] / \sqrt{2} \\
c_{k\downarrow} &= [(\epsilon''_k / |\epsilon''_k|) U_-(\xi) d_{k\uparrow} - U_+(\xi) d_{k\downarrow}] / \sqrt{2}
\end{aligned} \quad (7)$$

with $\xi = (1/2) \tan^{-1}[\Delta_E / |\epsilon''_k|]$ and $U_\pm(\xi) = |\sin \xi \pm \cos \xi| / \sqrt{2}$, the Hamiltonian is diagonalized as

$$H_s^{SP} = \sum_{\mathbf{k}} [E_-^{SP}(\mathbf{k}) d_{k\uparrow}^\dagger d_{k\uparrow} + E_+^{SP}(\mathbf{k}) d_{k\downarrow}^\dagger d_{k\downarrow}] \quad (8)$$

where

$$E_\pm^{SP}(\mathbf{k}) = v_0 - \epsilon'_k \pm \sqrt{(\Delta_E^2 + \epsilon''_k^2)} \quad (9)$$

with $v_0 = (v_\uparrow + v_\downarrow)/2$ being the normalized on-site potential and $\Delta_E = (v_\uparrow - v_\downarrow)/2$ being the effective field proportional to the strength of the Hund coupling.

For the CN state with two sublattices, the Fourier transformation of equation (4) yields

$$H_s^{CN} = \sum_{k\sigma} [(v_\sigma + \epsilon'_k) c_{k\sigma}^\dagger c_{k\sigma} + i\epsilon'''_k c_{k\sigma}^\dagger c_{\tilde{k}\bar{\sigma}}] \quad (10)$$

where $\tilde{\mathbf{k}}$ is the reduced wavevector corresponding to $\mathbf{k} + \mathbf{k}_0$ with $\mathbf{k}_0 = \sum_{l=1}^3 \hat{\mathbf{b}}_l/2$, $\hat{\mathbf{b}}_l$ being the basis vectors of the three-dimensional reciprocal lattice, and $\epsilon'''_k = -2t_{ab} \sin \theta_{ab} (\cos k_x a + \cos k_y b) - 2t_c \sin \theta_c \cos k_z c$. It is easy to see that $\epsilon'''_{\tilde{k}} = -\epsilon'''_k$. In equation (10), the coupled electronic states with momentum \mathbf{k} and $\tilde{\mathbf{k}}$ as well as opposite spins can be decoupled by using the unitary transformation

$$\begin{aligned}
c_{k\uparrow} &= [U_+(\chi) d_{k\uparrow} + i(\epsilon'''_k / |\epsilon'''_k|) U_-(\chi) d_{\tilde{k}\downarrow}] / \sqrt{2} \\
c_{\tilde{k}\downarrow} &= [i(\epsilon'''_k / |\epsilon'''_k|) U_-(\chi) d_{k\uparrow} + U_+(\chi) d_{\tilde{k}\downarrow}] / \sqrt{2}
\end{aligned} \quad (11)$$

with $\chi = (1/2) \tan^{-1}[(\Delta_E + \epsilon'_k) / |\epsilon'''_k|]$, and $U_\pm(\chi) = |\sin \chi \pm \cos \chi| / \sqrt{2}$. The Hamiltonian is diagonalized as

$$H_s^{CN} = \sum_{\mathbf{k}} [E_-^{CN}(\mathbf{k}) d_{k\uparrow}^\dagger d_{k\uparrow} + E_+^{CN}(\mathbf{k}) d_{\tilde{k}\downarrow}^\dagger d_{\tilde{k}\downarrow}] \quad (12)$$

where

$$E_{\pm}^{CN}(\mathbf{k}) = v_0 \pm \sqrt{\Delta_E^2 + \epsilon_{\mathbf{k}}^2 \pm 2\Delta_E \epsilon'_{\mathbf{k}}} \quad (13)$$

with $\epsilon_{\mathbf{k}} = -2t_{ab}(\cos k_x a + \cos k_y b) - 2t_c \cos k_z c$. The eigenvalues of AF and FM states are easily obtained in the limits of $\theta_{ab} = \theta_c = 0$ and $\theta_{ab} = \theta_c = \pi/2$, respectively.

The average of e_g electron number per Mn site is equal to $(1-x)$, i.e. $n_{\uparrow} + n_{\downarrow} = 1-x$. At zero temperature the total free energy per site is given by

$$F(\theta_{ab}, \theta_c) = [4J_{ab}S^2 + J_s(1-x)^2] \cos(2\theta_{ab}) + 2J_c S^2 \cos(2\theta_c) + \frac{1}{N} \sum_{\mathbf{k}} [E_- f(E_-) + E_+ f(E_+)]. \quad (14)$$

Here the first part is the free energy of the localized spins, and the second part is that of the itinerant electrons, in which N is the total number of the Mn sites and \mathbf{k} is the wavevectors. $f(\epsilon)$ is the Fermi–Dirac distribution function and equal to a unit step function $\Theta(\mu - \epsilon)$ at $T = 0$, where the chemical potential μ is determined from the condition

$$1-x = \frac{1}{N} \sum_{\mathbf{k}} [f(E_-) + f(E_+)]. \quad (15)$$

From equations (14) and (15), the total free energies of the SP and CN states for various θ_{ab} and θ_c can be calculated. By comparing them, one finds the ground state corresponding to a minimal free energy. For fixed $x = 0.3$, the interplane magnetic order of the layered manganite crystals is evaluated as a function of t_c/t_{ab} and $J_{ab}S^2$. Magnetic phase diagrams in the $J_{ab}-x$ and J_c-x planes can be also obtained by the same calculations.

3. Numerical results

At low temperatures of $k_B T \ll \Delta_E$, only the lower energy branch $E_-(\mathbf{k})$ is occupied by the carriers. So we can neglect the higher branch $E_+(\mathbf{k})$ in calculating the free energy of the itinerant electrons. Then equations (14) and (15) are reduced to

$$F(\theta_{ab}, \theta_c) = [4J_{ab}S^2 + J_s(1-x)^2] \cos(2\theta_{ab}) + 2J_c S^2 \cos(2\theta_c) + \frac{1}{N} \sum_{\mathbf{k}} [E_- f(E_-)] \quad (16)$$

and

$$1-x = \frac{1}{N} \sum_{\mathbf{k}} f(E_-) \quad (17)$$

with

$$E_-^{SP}(\mathbf{k}) = v_0 - \epsilon'_{\mathbf{k}} - \sqrt{\Delta_E^2 + \epsilon_{\mathbf{k}}'^2} \quad (18)$$

$$E_-^{CN}(\mathbf{k}) = v_0 - \sqrt{\Delta_E^2 + \epsilon_{\mathbf{k}}^2 - 2\Delta_E \epsilon'_{\mathbf{k}}}. \quad (19)$$

In the following numerical calculations, all energies are taken in unit of t_{ab} . We first choose to vary t_c and J_c , the other parameters being fixed as $x = 0.3$, $\Delta_E = 10$, $J_s = 0.3$ and $J_{ab}/J_c = 4$. For a given point on the t_c – J_c plane, substituting equations (18) and (19) into equation (17), we can obtain the chemical potentials as functions of θ_{ab} and θ_c for the SP and CN states, respectively. Then, from equation (16), together with equations (18) and (19), the free energies $F_{SP}(\theta_{ab}, \theta_c)$ and $F_{CN}(\theta_{ab}, \theta_c)$ can be obtained, their minimum corresponding to the magnetic configuration (θ_{ab}, θ_c) in either SP or CN state for the given

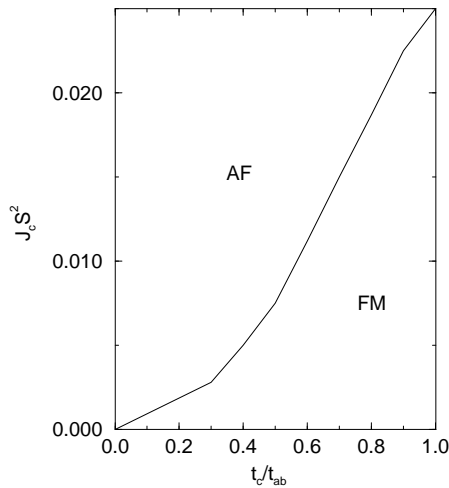


Figure 1. Interplane magnetic configuration of $\text{La}_{1.4}\text{Sr}_{1.6}\text{Mn}_2\text{O}_7$ in the t_c - J_c plane.

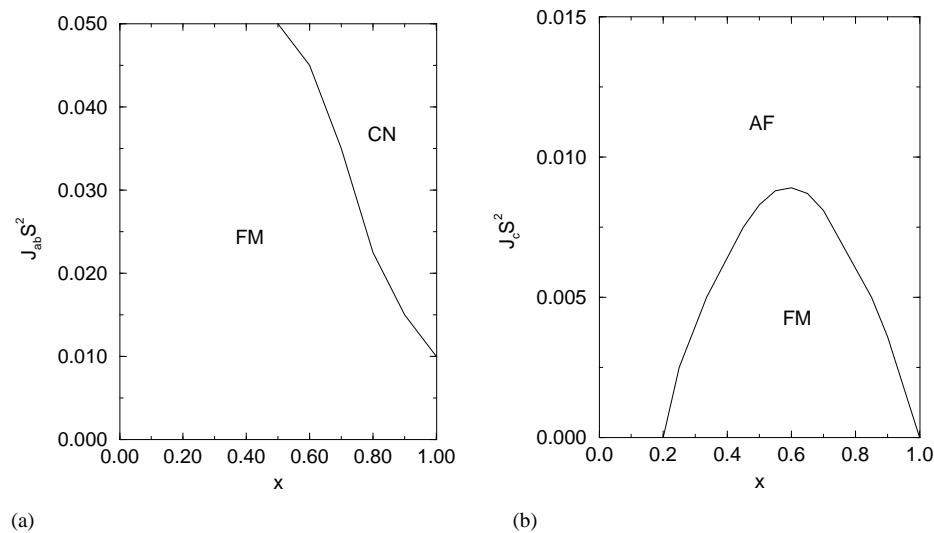


Figure 2. Inplane (a) and interplane (b) magnetic configurations of $\text{La}_{2-2x}\text{Sr}_{1+2x}\text{Mn}_2\text{O}_7$ in the x - J_{ab} and x - J_c planes, respectively.

t_c and J_c . Repeated calculations by varying t_c and J_c can yield a magnetic phase diagram in the t_c - J_c plane.

It is found that at $x = 0.3$ and $T = 0$, the inplane magnetic order is always FM ($\theta_{ab} = 0$) provided that J_{ab} is taken as reasonable values. The interplane magnetic order is a function of t_c and $J_c S^2$, as shown in figure 1. For a given J_c , in the small t_c region there is an AF configuration along the c -axis direction. As t_c is increased beyond a critical value, the AF order is replaced by a FM order. The calculated result in figure 1 can account qualitatively for the transport measurements under pressure in $\text{La}_{2-2x}\text{Sr}_{1+2x}\text{Mn}_2\text{O}_7$ ($x = 0.3$) [35]. They show that the interplane TMR is greatly enhanced by the application of pressure. This behaviour can be understood by the following argument. It was shown that the applied

pressure can weaken the interplane charge and spin coupling [36]. According to figure 1, a decrease of t_c may result in a crossover from the interplane FM alignment to the AF alignment. Thus, the suppression of the interplane coupling, by applying pressure, may produce AF static order between the adjacent MnO_2 bilayers, causing the increase of the resistivity at zero magnetic field and so the increase of the TMR [37].

We next calculate the magnetic phase diagram in the x - J_{ab} and x - J_c planes by taking $t_c = 0.25$. The calculated results for inplane and interplane magnetic configurations are shown in figure 2(a) and 2(b), respectively. There are an inplane FM order and an interplane AF order for small x . With increasing x , the interplane AF order changes into the FM order. As x is close to 1, there are an inplane CN order and an interplane AF order. In the inplane CN region, with the increase of x , the canted angle increases from $2\theta_{ab} = 0$ (FM order) and arrives at $2\theta_{ab} = \pi$ (AF order) at $x = 1$, which is a continuous crossover from the FM to AF order.

4. Summary

We have developed a model Hamiltonian of a layered manganite system. It includes not only the anisotropic transfers of the itinerant electrons, the on-site Hund coupling and the Coulomb repulsion and the anisotropic superexchange coupling between localized spins, but also the spin coupling between the inplane itinerant electrons. Minimizing the total free energy with the aid of numerical calculations, we have obtained the magnetic ground state of the layered manganite crystal $\text{La}_{1.4}\text{Sr}_{1.6}\text{Mn}_2\text{O}_7$ as a function of the interplane charge and spin couplings (t_c and J_c). It is shown that at $x = 0.3$, while the inplane ground state is FM, the interplane magnetic configuration changes from the AF order to the FM order with increasing t_c , which can account qualitatively for the pressure-enhanced interplane magnetoresistance observed in layered manganite crystals.

Acknowledgments

This work is supported by the National Natural Science Foundation and the Doctoral Foundation of the State Education Committee of China.

References

- [1] Kusters R M, Singleton J, Keen D A, McGreevy R and Hayes W 1989 *Physica B* **155** 362
- [2] von Helmolt R, Wecker J, Holzapfel B, Schultz L and Samwer K 1993 *Phys. Rev. Lett.* **71** 2331
- [3] Jin S, Tiefel T H, McCormack M, Fastnacht R, Ramesh R and Chen L H 1994 *Science* **264** 413
- [4] Tokura Y, Urushibara A, Moritomo Y, Arima T, Asamitsu A, Kido G and Furukawa N 1994 *J. Phys. Soc. Japan* **63** 3931
- [5] Asamitsu A, Moritomo Y, Tomloka Y, Arima T and Tokura Y 1995 *Nature* **373** 407
- [6] Coey J M D, Viret M, Ranno L and Ounadjela K 1995 *Phys. Rev. Lett.* **75** 3910
- [7] Satpathy S, Popvić Z S and Vukajlović F R 1996 *Phys. Rev. Lett.* **76** 960
- [8] Pickett W E and Singh D J 1996 *Phys. Rev. B* **53** 1146
- [9] Varma C M 1996 *Phys. Rev. B* **54** 7328
- [10] Okimoto Y, Katsufuji T, Ishikawa T, Arima T and Tokura Y 1997 *Phys. Rev. B* **55** 4206
- [11] Kawano H, Kajimoto R, Yoshizawa H, Tomioka Y, Kuwahara H and Tokura Y 1997 *Phys. Rev. Lett.* **78** 4253
- [12] Riera J, Hallberg K and Dagotto E 1997 *Phys. Rev. Lett.* **79** 713
- [13] Youn S J and Min B I 1997 *Phys. Rev. B* **56** 12046
- [14] Jonker G H and Van Santen J H 1950 *Physica* **16** 337
- [15] Van Santen J H and Jonker G H 1950 *Physica* **16** 599

- [16] Zener C 1951 *Phys. Rev.* **82** 403
- [17] Anderson P W and Hasegawa H 1955 *Phys. Rev.* **100** 675
- [18] de Gennes P-G 1960 *Phys. Rev.* **118** 141
- [19] Wollen E O and Koehler W C 1955 *Phys. Rev.* **100** 545
- [20] Goodenough J B 1955 *Phys. Rev.* **100** 564
- [21] Inoue J and Maekawa S 1995 *Phys. Rev. Lett.* **74** 3407
- [22] Tomioka Y, Asamitsu A, Moritomo Y, Kuwahara H and Tokura Y 1995 *Phys. Rev. Lett.* **74** 5108
- [23] Schiffer P, Ramirez A P, Bao W and Cheong S-W 1995 *Phys. Rev. Lett.* **75** 3336
- [24] Radaelli P G, Cox D E, Marezio M, Cheong S-W, Schiffer P E and Ramirez A P 1995 *Phys. Rev. Lett.* **75** 4488
- [25] Chen C H and Cheong S-W 1996 *Phys. Rev. Lett.* **76** 4042
- [26] Martin M C, Shirane G, Endoh Y, Hirota K, Moritomo Y and Tokura Y 1996 *Phys. Rev. B* **53** 14285
- [27] Müller-Hartmann E and Dagotto E 1996 *Phys. Rev. B* **54** R6819
- [28] Kawano H, Kajimoto R, Yoshizawa H, Tomioka Y, Kuwahara H and Tokura Y 1997 *Phys. Rev. Lett.* **78** 4253
- [29] Sheng L, Xing D Y, Sheng D N and Ting C S 1997 *Phys. Rev. Lett.* **79** 1710
Sheng L, Xing D Y, Sheng D N and Ting C S 1997 *Phys. Rev. B* **56** R7053
- [30] Mishra S K, Satpathy S, Aryasetiawan F and Gunnarsson O 1997 *Phys. Rev. B* **55** 2725
- [31] Ishihara S, Inoue J and Maekawa S 1997 *Phys. Rev. B* **55** 8280
- [32] Guo Z B, Huang H, Ding W P and Du Y W 1997 *Phys. Rev. B* **56** 10789
- [33] Kimura T, Tomioka Y, Kuwahara H, Asamitsu A, Tamura M and Tokura Y 1996 *Science* **274** 1698
- [34] Moritomo Y, Maruyama Y, Akimoto T and Nakamura A 1997 *Phys. Rev. B* **56** R7057
- [35] Kimura T, Asamitsu A, Tomioka Y and Tokura Y 1997 *Phys. Rev. Lett.* **79** 3720
- [36] Ishihara S, Okamoto S and Maekawa S 1998 *J. Phys. Soc. Japan* **66** 2965
- [37] Julliere M 1975 *Phys. Lett.* **54A** 225