Linear spin and orbital wave theory for undoped manganites

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Abstract

We present a linear spin and orbital wave theory to account for the spin and orbital orderings observed experimentally in undoped manganite. It is found that the anisotropy of the magnetic structure is closely related to the orbital ordering, and the Jahn-Teller effect stabilizes the orbital ordering. The phase diagram and the low energy excitation spectra for both spin and orbital orderings are obtained. The calculated critical temperatures can be quantitatively comparable to the experimental data.
LaMnO$_3$ is the parent compound of colossal magnetoresistance (CMR) manganites, and has been studied both experimentally and theoretically. The compound is an insulator with layered antiferromagnetic (A-type AF) spin ordering and an orbital ordering of $e_g$ electrons. Murakami et al. has recently succeeded in detecting the orbital ordering in LaMnO$_3$ by using resonant x-ray scattering techniques with the incident photon energy tuned near the Mn K-absorption edge. The orbital order parameter decreases above the Neel temperature $T_N \sim 140 K$ and persists until $T_O \sim 780 K$. Theoretically, the problem of orbital degeneracy in a d-electron system was pioneered by Kugel and Khomskii in 1970’s and investigated extensively in recent years.

In this paper, starting from an effective Hamiltonian of the spin and orbital interactions, as well as the JT coupling between the $e_g$ electrons and the lattice distortion, we investigate the interplay among the spin, orbit and the lattice distortion. We present the phase diagram as functions of interaction parameters, and obtain the low-energy excitations of the system in different phases. It is found that special properties of the orbital operators can result in an anisotropy of the magnetic structure and an energy gap of the orbital excitations. We also estimate the critical temperatures for spin and orbital orderings as well as their dependence on the JT coupling. The calculated results are comparable to the experimental measurements.

The effective spin and orbital interactions are derived by the projection perturbation method up to the second order:

$$H_{eff}^e = J_1 \sum_{ij} (S_i \cdot S_j - 4) n_i^\alpha n_j^\alpha + J_2 \sum_{ij} (S_i \cdot S_j - 4) n_i^\alpha n_j^{\bar{\alpha}} - J_3 \sum_{ij} [S_i \cdot S_j + 6] n_i^\alpha n_j^{\bar{\alpha}},$$

(1)

where $S_i$ is the spin operator of $S = 2$. The three terms describe three processes with different intermediate states. $n_i^\alpha = d_{i\alpha}^\dagger d_{i\alpha}$ and $n_i^{\bar{\alpha}} = d_{i\bar{\alpha}}^\dagger d_{i\bar{\alpha}}$ are the particle number operators of $e_g$ electron in orbit states $|\alpha\rangle = \cos(\varphi_{\alpha}/2)|z\rangle + \sin(\varphi_{\alpha}/2)|\bar{z}\rangle$ and $|\bar{\alpha}\rangle = -\sin(\varphi_{\alpha}/2)|z\rangle + \cos(\varphi_{\alpha}/2)|\bar{z}\rangle$, respectively, with orbital states $|z\rangle \propto (3z^2 - r^2)/\sqrt{3}$ and $|\bar{z}\rangle \propto x^2 - y^2$. Here $\varphi_{\alpha}$ depends on the direction of the $(ij)$ bond by $\varphi_x = -2\pi/3,$...
\( \varphi_y = 2\pi/3 \), and \( \varphi_z = 0 \), respectively, for bond \((ij)\) parallel to the \(x\), \(y\) and \(z\) directions. The introduced \( d^\dagger_{i\alpha}, d_{i\alpha} \) and \( d^\dagger_{i\bar{\alpha}}, d_{i\bar{\alpha}} \) are operators in the orbital space, with \( d^\dagger_{i\alpha}|0\rangle = |\alpha\rangle \), \( d^\dagger_{i\bar{\alpha}}|0\rangle = |\bar{\alpha}\rangle \), they should satisfy the constraint \( n_i^\alpha + n_i^{\bar{\alpha}} = 1 \).

The JT interaction can be expressed as

\[
H_{JT} = -g \sum_{i\gamma\gamma'} d^\dagger_{i\gamma} T_{\gamma\gamma'} \cdot Q_i d_{i\gamma'} + \frac{K}{2} \sum_i Q_i^2 ,
\]

where \( T = (T_x, T_z) \) are the Pauli matrices in the orbital space with \( \gamma (\gamma') = z \) or \( \bar{z} \), and \( g \) is the coupling between the \( e_g \) electrons and the local JT lattice distortion \( Q_i = Q_i(\sin \phi_i, \cos \phi_i) \). Here we have neglected the terms for the anharmonic oscillation of JT distortion and the higher order coupling, their effect being regarded approximately as giving a preferable direction \( \phi_i \) of the JT distortion observed experimentally.

Experimental measurement on \( \text{LaMnO}_3 \) indicates that the critical temperature of the orbital ordering, \( T_O \), is much higher than that of the magnetic ordering, \( T_N \). As a result, the spin and orbital degrees of freedom, which are coupled to each other in Hamiltonian (1), may be separately treated by the Hartree-Fock mean-field approach. The total Hamiltonian is reduced to \( H_{MF} = H_S + H_O + E_0 \), where \( H_S \) and \( H_O \) are the decoupled spin and orbital Hamiltonians, respectively, and \( E_0 \) is an energy constant. The spin Hamiltonian \( H_S \) is given by

\[
H_S = \sum_{(ij)} \tilde{J}_{ij} \mathbf{S}_i \cdot \mathbf{S}_j ,
\]

with the effective spin coupling depending on the orbital configuration of the two neighboring sites by

\[
\tilde{J}_{ij} = \frac{1}{2} J_1 \langle (1 + m_i^\alpha)(1 + m_j^\alpha) \rangle
+ \frac{1}{2} (J_2 - J_3) \langle 1 - m_i^\alpha m_j^\alpha \rangle + \tilde{J}_{AF} ,
\]

where \( m_i^\alpha = n_i^\alpha - n_i^{\bar{\alpha}} \) are the orbital operators, and the \( \tilde{J}_{AF} \) term comes from the magnetic superexchange between the nearest neighboring local spins. It is worthy of pointing out here that the orbital operators introduced above has unusual operator algebra, quite different
from that of the spin operators. It can be shown that they satisfy the following relations:

\((m_i^\alpha)^2 = 1, m_i^x + m_i^y + m_i^z = 0, \) and \([m_i^x, m_j^y] = [m_i^y, m_j^z] = [m_i^z, m_j^x] = \sqrt{3}(d^i_x d^i_z - d^i_z d^i_x).\)

The orbital Hamiltonian \(H_O\) can be written as

\[
H_O = \sum_{(ij)} u_{ij} m_i^\alpha m_j^\alpha - \sum_{(ij)} h_{ij} m_i^\alpha + \frac{K}{2} \sum_i Q_i^2 \\
- g \sum_i Q_i \left( m_i^z \cos \phi_i + \frac{1}{\sqrt{3}} (m_i^y - m_i^x) \sin \phi_i \right),
\]

where the effective orbital coupling \(u_{ij}\) depends on the spin configuration of the two neighboring sites by

\[
u_{ij} = \frac{1}{2} (J_1 - J_2 + J_3) \langle S_i \cdot S_j \rangle + (3J_3 - 2J_1 + 2J_2),
\]

and \(h_{ij} = -\frac{1}{2} J_1 \langle S_i \cdot S_j - 4 \rangle.\) All these coupling parameters \(\tilde{J}_{ij}, u_{ij}\) and \(h_{ij}\) in \(H_S\) and \(H_O\) are determined not only by the spin and orbital configurations of the nearest neighboring sites \(i\) and \(j\), but also by the direction of the \((ij)\) bond. For short, we denote them by \(\tilde{J}_\alpha, u_\alpha\) and \(h_\alpha\) thereafter. If there are two symmetric directions in the system, e.g., \(x\)- and \(y\)-direction, one has \(\tilde{J}_x = \tilde{J}_y, u_x = u_y,\) and \(h_x = h_y.\)

The spin Hamiltonian \(H_S\) is an anisotropic Heisenberg Hamiltonian with SU(2) symmetry. At low temperatures, the spin configuration along the \(\alpha\) direction is determined by the sign of \(J_\alpha.\) Dividing the system into two sublattices \(A\) and \(B\) according to their spin alignments, and performing the well-known Holstein-Primakoff (HP) transformation in the linear spin wave (LSW) theory, up to the quadratic terms, we diagonalize \(H_S\) as

\[
H_S = \sum_k \left[ \omega_k (\psi_k^\dagger \psi_k + \chi_k^\dagger \chi_k + 1) - 12W \right].
\]

Here \(\psi_k\) and \(\chi_k\) are the quasiparticle operators of the spin wave excitations with \(k\) the wave vectors of one sublattice. The quasiparticle spectrum is given by \(\omega_k = \sqrt{(W + P_k^-)^2 - (P_k^+)^2},\) with \(P_k^\pm = 2S \sum_\alpha \tilde{J}_\alpha \cos k_\alpha \Theta(\pm \tilde{J}_\alpha)\), and \(W = 2S \sum_\alpha |\tilde{J}_\alpha|,\) in which \(\Theta\) is the unit step function.

The orbital Hamiltonian \(H_O\) looks quite like \(H_S,\) where the orbital operator may be regarded as an isospin operator. But the absence of the SU(2) symmetry in \(H_O\) and the
abnormal algebra of orbital operators make the orbital operators quite different from the spin operators. For example, orbital F-type arrangement is not an eigenstate of $H_O$, and in case of orbital AF configuration, on orbital sublattice $\tilde{A}$ or $\tilde{B}$ there are only several preferable orbital alignments at which the ground-state energy of the system reaches its minimum, unlike in an AF spin system where all the spin orientations on a sublattice are energy-degenerate. In this case, the orbital state at site $i$ can be generally expressed as

$$|i\rangle = \cos(\theta/2)|z\rangle + \sin(\theta/2)|\tilde{z}\rangle \quad \text{with} \quad \sigma = + \text{ for } i \in \tilde{A} \text{ and } - \text{ for } \tilde{B},$$

respectively. From the symmetry of $h_x = h_y$ and relation $m_{ix} + m_{iy} + m_{iz} = 0$, the second term on the right-hand side of Eq. (5) can be rewritten in a more intuitive form

$$H_z = -\varepsilon_z \sum_i m_i^z,$$

with $\varepsilon_z = h_z - h_x$. This anisotropic Hamiltonian arises from anisotropy of electronic hopping integrals in orbital space as well as unusual algebra of orbital operators. Both $u_\alpha$ and $h_\alpha$ are anisotropic and depend on the spin configurations along the $\alpha$ direction, as shown in their expressions below Eq. (5). Since $J_1 - J_2 + J_3$ is always positive,$^{13}$ we have $u_z < u_x$ and $\varepsilon_z > 0$ for the A-type AF spin configuration; $u_x > u_z$ and $\varepsilon_z < 0$ for the C-type AF one; and $u_x = u_z$ and $\varepsilon_z = 0$ for the ferromagnetic (F) one. The static JT distortions $Q_i$ are approximately treated as classical variables and assumed to be different in the two sublattices, i.e., $Q_i \equiv Q_\sigma$ and $\phi_i \equiv \phi_\sigma$ with $\sigma = + (-)$ for $i \in \tilde{A} (\tilde{B})$. From x-ray diffraction experiments, it has been confirmed that the MnO$_6$ octahedron is elongated along the $x$ or $y$ direction, and the octahedrons are alternatively aligned in the $x$-$y$ plane,$^8$ which corresponds to $\phi_+ = 2\pi/3$ and $\phi_- = -2\pi/3$ in the present formula. Similar to the treatment of the spin degrees of freedom, we perform the HP transformation for localized orbital operators.$^8$ To the lowest order, $H_O$ can be diagonalized as

$$H_O = \sum_{k\sigma} \varepsilon_{k\sigma} \xi_{k\sigma}^\dagger \xi_{k\sigma} + \frac{1}{2} \sum_{k\sigma} (\varepsilon_{k\sigma} - P_\sigma) + E_C.$$

Here $\xi_{k\sigma}^\dagger$ and $\xi_{k\sigma}$ are the quasiparticle operators of the orbital excitations, the second term stands for the quantum fluctuation energy where
\[ P_\sigma = -\sum_\alpha 4u_\alpha \cos \theta^\alpha_+ \cos \theta^\alpha_- + 2\varepsilon_z \cos \theta_\sigma 
+ \frac{2g^2}{K} \cos^2(\theta_\sigma - \phi_\sigma) . \]

with \( \theta^\sigma_\alpha = \theta_\sigma - \varphi_\alpha \), and \( E_C \) is the classical grand-state energy. The expression for \( E_C \) depends on the orbital configuration. For both G- and C-type AF configurations, it is given by

\[ E_C/N = \sum_\alpha u_\alpha \cos \theta^\alpha_+ \cos \theta^\alpha_- - \frac{1}{2} \sum_\sigma [\varepsilon_z \cos \theta_\sigma + gQ_\sigma \cos(\theta_\sigma - \phi_\sigma) - \frac{K}{2} Q^2_\sigma], \]

with \( N \) the number of the sites. In principle, \( \theta_\sigma \) and \( Q_\sigma \) in Eq.(8) should be determined by minimizing the total ground state energy of the system. In the present case, the quantum fluctuations in \( H_S \) and \( H_O \) are small, and so the ground-state energy can be approximately replaced by \( E_C \). It is found that besides the same ground-state energy \( E_C \), there is the same excitation spectrum for the C- and G-type AF orbital configurations, yielding

\[ \varepsilon_{k\sigma} = \sqrt{\frac{1}{2}\{P^2_+ + P^2_- + \sigma[(P^2_+ - P^2_-)^2 + 16P_+P_-C_{2k}^2]^{1/2}\}}, \]

where \( C_k = \sum_\alpha 2u_\alpha \sin \theta^\alpha_- \sin \theta^\alpha_+ k_\alpha \). This degeneracy of C- and G-type AF orbital configurations agrees to Mizokawa and Fujimori’s result.\(^1\)\(^6\) Independent of the magnetic structure, such a degeneracy suggests the possibility of a mixed C- and G-type AF orbital configuration in the system, i.e, neighboring orbital states along the \( z \) direction may be either “parallel” or “antiparallel”. In the absence of the Coulomb interactions, a C-type AF orbital structure may have lower energy.\(^9\)

The JT coupling plays an important role in determining the orbital ordering. In the absence of the JT coupling and in the small limit of \( \varepsilon_z \), the \( e_g \) electrons may occupy two “antiparallel” states in the two sublattices: \((|z\rangle \pm |\bar{z}\rangle)/\sqrt{2} (\theta_+ = -\theta_- = \pi/2) \) for \( u_z < u_x \); \(|z\rangle \) and \(|\bar{z}\rangle (\theta_+ = 0, \theta_- = -\pi) \) for \( u_z > u_x \). Such symmetric “antiparallel” states will be broken by the uniform crystal field appeared in Eq. (7). Furthermore, the JT distortions also lead to an effective anisotropic crystal field acting on the two sublattices. To distinguish it from the uniform crystal field \( \varepsilon_z \), we call it the JT field. The JT field, whose strength increases with the coupling constant \( g \), tends to align the orbital states in the two sublattices towards \(|y\rangle (\theta_+ = 2\pi/3) \) and \(|x\rangle (\theta_- = -2\pi/3) \), respectively.
The orbital ordering is described by the average value of operators \( m_\sigma^\alpha \). From the orbital spectrum, it can be shown that

\[
\langle m_\sigma^\alpha \rangle = M_\sigma \cos \theta_\sigma^\alpha ,
\]

with \( \sigma = + ( - ) \) for \( i \in \tilde{A} ( \tilde{B} ) \), where

\[
M_\sigma = 1 - \sum_{\sigma'} \int \frac{d^3k}{(2\pi)^3} \frac{2P_\sigma C_k^2}{\varepsilon_{k\sigma'}[4P_+P_-C_k^2+(P_\sigma^2-\varepsilon_{k\sigma'}^2)^2]} \times \left( \frac{2(P_\sigma^2+\varepsilon_{k\sigma'}^2)}{e^{3\varepsilon_{k\sigma'}}-1} + (P_\sigma - \varepsilon_{k\sigma'})^2 \right) .
\]

The second term on the right-hand side of Eq. (10) comes from the quantum and thermal fluctuations. To keep a good approximation, this term must be small at low temperatures.

We now discuss the ground state of the system. First, it is impossible to realize an isotropic orbital ordering. Since \( m_x^i + m_y^i + m_z^i = 0 \), if \( \langle m_x^i \rangle = \langle m_y^i \rangle = \langle m_z^i \rangle \), they must be equal to zero and there is no any orbital ordering. From Eq. (4), it then follows that the anisotropy in \( \langle m_\sigma^\alpha \rangle \) will lead to anisotropic \( \tilde{J}_\alpha \). At zero temperature, \( M_\sigma = 1 \) and \( \langle m_\sigma^\alpha \rangle = \cos \theta_\sigma^\alpha \) if the quantum fluctuation in Eq. (9) is neglected. Taking into account the symmetry requirement of \( \langle m_x^i + m_y^j \rangle = \langle m_y^i + m_y^i \rangle \), we get two possible relations: (I) \( \theta_+ + \theta_- = 0 \) or (II) \( \theta_+ - \theta_- = \pi \). As the quantum fluctuation is taken into account, relation (I) keeps unchanged, while relation (II) is satisfied only approximately. In both cases, we have \( \tilde{J}_x = \tilde{J}_y \neq \tilde{J}_z \) from Eq. (4), provided the small quantum fluctuations are neglected. Since the magnetic structure at zero temperature is determined by the sign of \( \tilde{J}_\alpha \), the same sign of \( \tilde{J}_\alpha \), regardless of anisotropic magnitude of them, will lead to a F or G-type AF spin configuration, while different signs of \( \tilde{J}_x \) and \( \tilde{J}_z \) will result in a A- or C-type spin configuration. Our calculations show that the ground-state magnetic structure is very sensitive to the on-site Coulomb interactions. Even though the magnetic superexchange \( \tilde{J}_{AF} \) is fixed and the JT coupling is absent (\( g = 0 \)), an evolution of spin configuration in the order of \( F \rightarrow A \rightarrow C \rightarrow G \) can be obtained with increasing the Coulomb interactions, as shown in Fig. 1(a). It is found that spin configurations A and G satisfy relation (I), and spin configuration C satisfies relation (II). Figure 1(b) shows that an increasing JT coupling narrows gradually the C-type AF
region. This is because the JT coupling tends to align the orbital states along $|x\rangle$ and $|y\rangle$, and so raises the effective ferromagnetic coupling in the $x$-$y$ plane and the AF coupling in the $z$ direction, making the C-type AF spin configuration unstable.

We next discuss the orbital excitation spectra. Owing to the absence of SU(2) symmetry in the orbital Hamiltonian, an orbital excitation spectrum usually has an energy gap. For A-, C- and G-type AF spin configurations, there is always an energy gap in the orbital spectrum, regardless whether or not the JT coupling is taken into account (not shown here). However, if the JT coupling is absent, gapless orbital spectra may appear for the F spin configuration. Furthermore, if relation (II) is satisfied, the orbital spectrum has a two-dimensional form: $\varepsilon_{k\sigma} = 6u_x\sqrt{1 + \sigma(\cos k_x + \cos k_y)/2}$. For such a two-dimensional spectrum, quantum and thermal fluctuations, characterized by the second term of $M_\sigma$ in Eq. (10), will completely destroy long-range orbital ordering at finite temperatures, resulting in an orbital-liquid state similar to that obtained by Ishihara et al. The orbital excitation gap can be widened by the JT field acting on the orbital states. It is very similar to an anisotropic magnetic crystal field on the spin states in an AF Heisenberg Hamiltonian. Quantum fluctuations are greatly suppressed by this JT field, making the orbital ordering stable.

At finite temperatures, $\langle S_i^z \rangle$ and $M_\sigma$ in Eq. (9) serve as the spin and orbital order parameters, respectively. Both of them decrease with increasing the temperature, and $\langle S_i^z \rangle$ ($M_\sigma$) vanishes as the temperature is increased beyond the critical temperature $T_N$ ($T_O$). One may evaluate $\langle S_i^z \rangle$ and $M_\sigma$ from a self-consistent equation for $\langle S_i^z \rangle$ and Eq. (10). In our calculation, parameters $J_1$, $J_2$ and $J_3$ are taken from the Racah parameters and $t = 0.41$ eV. The system is found to have an A-type AF spin configuration at low temperatures. In Fig. 2 we plot the variation of $T_N$ and $T_O$ as functions of the strength of the JT coupling. Both $T_N$ and $T_O$ increase with the JT coupling, but there are different physical origins. The increase of $T_N$ is attributed to an enhancement of the effective magnetic coupling $\tilde{J}_x$ and $\tilde{J}_y$ caused by the JT field. On the other hand, the increase of $T_O$ stems from the fact that a stronger JT field will widen the energy gap of the orbital excitation spectrum, and so a higher temperature is required to excite orbital quasiparticles to break the long-range orbital
ordering. According to experimental data and theoretical analysis, $g$ is of the same order of magnitude as $t$ and $K$ is greater than $g$ by a factor of ten to hundred, so that $g^2/K$ is the order of $0.01t \sim 0.1t$. According to Fig. 2, to fit with $T_O = 780K$ measured by the experiment, the strength of JT coupling should be $g^2/K = 0.045t$, at which the calculated $T_N = 146K$ is very close to the experimental value of $T_N = 140K$. The present calculation may overestimate the critical temperatures due to neglecting the frequency-softened effect for the excitation spectrum at high temperatures, and so the required strength of JT coupling may be greater than the evaluated magnitude.

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FIGURES

FIG. 1. Phase diagram at zero temperature in the absence (a) and presence (b) of the JT field. The parameters used are $\tilde{J}_{AF} = 0.006$ and $J_H = 4/3$ with $t$ the unit of energy. The relation $U = U' + 2J$ has been used and $U = 20$ fixed in (b).

FIG. 2. Critical temperatures $T_N$ and $T_O$ as functions of $g^2/Kt$. 
