Orbital Compass Model in a Checkerboard Lattice

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Abstract.
The orbital compass model in a checkerboard lattice is studied. There is a competition between
the interaction for the $z$ component of the orbital pseudo-spin along the
vertical/horizontal direction and the interaction for the $x$ component along the diagonal
direction in a checkerboard lattice. In a frustration point where the two interactions compete
with each other, a macroscopic number of the orbital pseudo-spin configurations are degenerated
in the classical grounds state. This degeneracy is lifted by the thermal and quantum
fluctuations and the $z$ component long range order is realized. The tricritical point appears due to the
coeexistence of the orbital frustration and the geometrical frustration.

1. Introduction
Orbital degree of freedom in the transition-metal compounds and its correlation with spin,
charge and lattice degrees of freedom are one of the central issues in the recent correlated
electron systems[1]. Essence of the orbital degree of freedom in a solid is its directional and
frustration character. Since the orbital degree of freedom represents the anisotropy of the charge
distribution, the inter-site interaction between the orbitals explicitly depends on the direction of
the bonds. When one considers an orbital configuration which minimizes the bond energy in a
direction, this configuration does not minimize the bond energy in other directions. Therefore,
all bond energies are not able to be minimized simultaneously. This is a kind of the frustration
even without geometrically frustrated lattice[3].

The inter-site interaction between the orbitals is mainly due to the superexchange-type and
the cooperative Jahn-Teller type[2]. These originate from the virtual exchange of an electron
under the Coulomb interaction and that of a Jahn-Teller phonon. The superexchange type of
the interaction is usually represented by the coupled form of the spin and orbital degrees of
freedom, although the cooperative Jahn-Teller type is written by the orbital degree of freedom
alone. One of the well known orbital model is the $e_g$ orbital model in a cubic lattice given by

$$\mathcal{H}_{e_g} = J \sum_{\langle ij \rangle} \tau_i^{l^l} \tau_j^{l^l}.$$  \hspace{1cm} (1)

We define $\tau_i^{l^l} = \cos(2\pi n_l/3) T^z_i - \sin(2\pi n_l/3) T^x_i$ where $T_i$ is the pseudo-spin operator for the
doubly degenerate $e_g$ orbital, and the numerical factor $n_l = (1, 2, 3)$ where $l = (x, y, z)$ represents
the bond direction in a cubic lattice. It is known that the classical ground states in this model
are macroscopically degenerated, and the long-range orbital order is realized by the thermal and
quantum fluctuations[4, 5]. Another well known orbital model is the orbital compass model in a square lattice defined by

\[ \mathcal{H}_{\text{compass}} = J \sum_{\langle ij \rangle_x} T^{x}_{ij} T^{x}_{ji} + J \sum_{\langle ij \rangle_z} T^{z}_{ij} T^{z}_{ji}, \]  

(2)

where \( \langle ij \rangle_x \) and \( \langle ij \rangle_z \) represent the nearest neighboring (NN) \( ij \) pair along the \( x \) and \( z \) directions in a two dimensional square lattice[2]. Only the \( x \) (\( z \)) component of the pseudo-spin is concerned in the interaction along the \( x \) (\( z \)) direction. It is known that, instead of the conventional long-range order, the directional order characterized by \( \sum_l (T^{x}_l)^2 - (T^{x}_l)^2 \) appears below a certain temperature[6].

In this paper, we study the competition and cooperation of the intrinsic orbital frustration and the geometrical frustration, by analyzing the orbital compass model in a checkerboard lattice. This model is derived from the Hubbard-type model where the doubly degenerate \( d_{xz} \) and \( d_{yz} \) orbitals are located at each site in a checkerboard lattice in the strong coupling limit. As seen in the compass model in a square lattice, there is a competition between the \( z \) component order along the horizontal/vertical directions and the \( x \) component order along the diagonal direction. The classical and quantum versions of this model are analyzed by the mean-field methods, the Monte-Carlo simulation, and the mixed method of the mean-field and the Jordan-Wigner transformation. We calculate the finite temperature phase diagram and show that, at the frustration point, the long range order is realized due to the thermal and quantum fluctuations. A competition between the different kinds of the interactions provides the tricritical point.

2. Model Hamiltonian

We consider the doubly degenerate \( d_{yz} \) and \( d_{zx} \) orbitals in a two dimensional checkerboard lattice. The two orbitals are located at each site in the lattice[7]. These orbitals are denoted by \( \sigma = \uparrow \) for \( d_{zx} \) and \( \sigma = \downarrow \) for \( d_{yz} \). We start from the Hubbard-type Hamiltonian given by

\[ \mathcal{H}_0 = \mathcal{H}_t + \mathcal{H}_U, \]  

(3)

where the electron transfer term and the on-site Coulomb interaction term are defined by

\[ \mathcal{H}_t = -\sum_{\langle ij \rangle_l} t_{ij}^{(l)\sigma\sigma'} c_{i\sigma}^\dagger c_{j\sigma'}, -\sum_{\langle ij \rangle_m} t_{ij}^{(m)\sigma\sigma'} c_{i\sigma}^\dagger c_{j\sigma'} + H.c., \]  

(4)

and

\[ \mathcal{H}_U = U \sum_i n_{i\uparrow} n_{i\downarrow}, \]  

(5)

respectively. Here, \( c_i \) and \( n_i (\equiv c_i^\dagger c_i) \) represent the annihilation operator and the number operator of a spin-less fermion at site \( i \), respectively. In the electron transfer term \( \mathcal{H}_t \), the first term represents the electron hopping along the \([10]\) and \([01]\) directions in the checkerboard lattice and \( t_{ij}^{(l)\sigma\sigma'} \) is the intensity between the NN sites \( i \) and \( j \) along the direction \( l = (x, y) \). The second term in \( \mathcal{H}_t \) represents the electron transfer along the \([11]\) and \([1\bar{1}]\) directions and \( t_{ij}^{(m)\sigma\sigma'} \) is its intensity along \( m = (xy, x\bar{y}) \). The symbols \( \sum_{\langle ij \rangle_l} \) and \( \sum_{\langle ij \rangle_m} \) represent the summation for the NN \( ij \) pairs along the direction \( l \), and that for the next NN \( ij \) pair along \( m \), respectively. Since the \( d_{zx} \) and \( d_{yz} \) orbitals have the transfer integrals along the \( x \) and \( y \) directions, the matrix elements in the basis of \( d_{zx}, d_{yz} \) are given by \( t_0^{(x)} = -t_0(1 + \sigma^z)/2 \) and \( t_0^{(y)} = -t_0(1 - \sigma^z)/2 \) where \( \sigma \) are the Pauli matrices. On the other hand, the electron transfer along the \([11]\) \( ([1\bar{1}]\)) direction is finite between the \( d_{yz} + d_{zx} \ (d_{zx} - d_{yz}) \) orbitals. Therefore, the matrix elements of the transfer integrals in these directions are given by \( t_1^{(xy)} = -t_1(1 + \sigma^z)/2 \) and \( t_0^{(xy)} = -t_1(1 - \sigma^z)/2 \).
In the strong coupling limit of $U \gg t_0, t_1$ at half filling, the effective Hamiltonian for the Hubbard-type model is obtained by the perturbational calculation. The result is given by

$$H = -J_z \sum_{\langle ij \rangle}^\dagger S_i^z S_j^z - J_x \sum_{\langle ij \rangle} S_i^x S_j^x$$  \hspace{1cm} (6)

where we introduce the pseudo-spin operator for the orbital degree of freedom defined by $S_i = (1/2) \sum_{\sigma \sigma'} c_i^\dagger \sigma \sigma' c_i \sigma'$ and the symbols $\sum_{\langle ij \rangle}$ and $\sum_{\langle ij \rangle}$ represent the summation for the NN $ij$ pairs, and those for the next NN pairs, respectively. The exchange constants are given by $J_z(x) = -2t_0^2 / U$ which are negative. However, these signs are not essential, since the signs are reversed by rotation of the pseudo-spins in one of the sublattices in the checkerboard lattice with respect to the $S_y$ axis. We define a ratio of the two interaction as $J \equiv J_x / (2J_z)$. In this Hamiltonian, the $z$-component of the pseudo-spin operators is concerned in the interaction along the $[10]$ and $[01]$ directions. On the other hand, the $x$ component appears in the interaction along $[11]$ and $[1 \bar{1}]$ directions. Therefore, this is recognized as an orbital compass model defined in the checkerboard lattice.

We analyze the classical and quantum versions of the orbital compass model in a checkerboard lattice. In the classical and quantum models, the pseudo-spins are treated as the classical vectors in the $S_x - S_z$ plane, and the quantum spin operators of an amplitude of $1/2$, respectively.

3. Results of Calculation

First we show the numerical results of the classical version of the compass model. It is obvious that in the limits of $J = 0$ and $J \to \infty$, the system corresponds to the Ising model in a square lattice, and an independent set of the Ising models in a one-dimensional chain, respectively. In the mean-field approximation at zero temperature, there are two phases as a function of the interaction ratio $J$. In the region of $J < 1$, the ferromagnetic long-range order of the $z$ component is realized. On the other hand, in the region of $J > 1$, the ferromagnetic order of the $x$ component is stabilized. It is worth noting that in this region, since each one-dimensional chains are independent, reverse of all spins in any chains along the $[11]$ and $[1 \bar{1}]$ directions does not change the mean-field energy. Thus, a macroscopic number of the mean-field ground state exists in the region of $J > 1$. At the frustration point $J = 1$, the two interactions compete with each other. The mean field solutions have a rotational symmetry in the two dimensional $S^x - S^z$ plane. Since this is not seen in the Hamiltonian, this high symmetry in the mean-field solution is accidental. From now on, the point $J = 1$ is termed a frustration point.
In Fig. 2, the finite temperature phase diagram obtained by the classical Monte-Carlo simulation is presented. A two-dimensional $20^2 \times 40^2$ site cluster with the periodic boundary condition is used. We adopt the Wang-Landau algorithm[8] where $2 \times 10^8$ MC steps is used for standard measurements. The phase diagram is obtained by the correlation functions and the specific heat. As expected, in the region of $J < 1$, the $S^z$ Ising order is realized. The transition temperature gradually decreases with increasing $J$. At the point of $J = 1$, where the classical ground state is not determined uniquely, the two dimensional order of the $S^z$ component is stabilized at finite temperature. This is a kind of the order by thermal fluctuation mechanism. As results the reentrant feature of the two-dimensional order appears around the frustration point.

The observed $S^z$ order at finite temperature in $J > 1$ is explained by the density of excited state in the ordered state as follows. The low-energy excitations in the $S^z$ ordered state are mainly governed by the one-dimensional like $S^x$ fluctuation. This is the larger density of excited state than that in the $S^x$ mean-field ordered state where the two-dimensional $S^z$ fluctuation dominates the low energy excitation. As a result, the large entropy stabilizes the $S^z$ order at finite temperature. This is not contradict to the fact mentioned previously that there is a macroscopic number of the mean-field ground-state for the $S^x$ ordered state. This degeneracy originates from the inter-chain configuration of the one-dimensional $S^x$ order and does not contribute to the entropy in the thermodynamic limit.

With increasing of $J$ furthermore, temperature dependence of the specific heat shows a broad peak which corresponds to the cross over where the spin correlation develops in the one-dimensional chain as well known in the one-dimensional Ising model. This is plotted by the broken line in Fig. 2. One noticeable point in the phase diagram is that the order of the phase transition of the $S^z$ component is changed from the first order to the second one with decreasing temperature. Thus, the tricritical point exists in the connecting point of the first and second order phase transition lines.

In particular, the first order phase transition line is identified by the Wang-Landau method in the MC simulation. In this method, the free energy is obtained as a function of energy. Near
Figure 3. (Color online) Finite temperature phase diagram in the quantum version of the orbital compass model in a checkerboard lattice obtained by the mixed method of the mean-field approximation and the Jordan-Wigner transformation. The broken line shows a cross over line where the one-dimensional pseudo-spin correlation develops. A circle represents the tricritical point. Inset shows a detailed phase transition lines around the tricritical point.

In the phase transition line, there are double minima in the free energy function. By changing the temperature, the free energy at one of the minima becomes lower than that at another minimum. This is a direct evidence of the first order phase transition at low temperature around $J = 1$.

Next we show the results in the quantum version of the orbital compass model in the checkerboard lattice. We analyze this model by utilizing the spin wave approximation, the exact diagonalization method based on the Lanczos procedure, and the mixed method of the Jordan-Wigner transformation and the mean-field approximation. Here we introduce the last method and its results. In this method, the interaction between the one-dimensional chain is treated by the mean-field approximation. In a chain, the Ising interaction between the $S^x$ component under the mean-field is treated exactly. The effective Hamiltonian is given by

$$H/(2J_z) = -J \sum_{(ij)} S^x_i S^x_j - h \sum_i S^z_i + L \langle S^z \rangle^2,$$

where the effective field is defined by $h = 2 \langle S^z \rangle$, and $L$ is a size of the chain. This is the one-dimensional Ising model under the transverse magnetic field, and is solved by using the Jordan-Wigner transformation.

The phase diagram in the quantum version of the orbital compass model is shown in Fig 3. This phase diagram is obtained by the free energy calculation in the above mixed method of the mean-field approximation and the Jordan-Wigner transformation. We have checked that the qualitative results are reproduced by the quantum Monte-Carlo simulation [9]. The cross over behavior of the one-dimensional $S^x$ correlation is also consistent with the prediction form the generalized Elitzur's theorem [10].

Even at $T = 0$ and $J = 1$, the $S^z$ long range order is realized. This is the order by quantum fluctuation mechanism. The reentrant feature of the phase boundary around $J = 1$ is survived in the quantum calculation. The tricritical point represented by the circle in Fig. 3 is also confirmed by a direct calculation of the free energy. Origin of this tricritical point is interpreted
by the following facts: 1) the phase transition for the two-dimensional square lattice expected in $J \ll 1$ is the second order, and 2) the quantum phase transition between the $S^z$ Ising order and the $S^x$ one at $T = 0$ is the first order. Therefore, there is a tricritical point at the connecting point of the first and second order phase transition lines. This is a consequence of the orbital frustration and the geometrically frustration effect.

4. Summary
In summary, the orbital compass model in a checkerboard lattice is studied. The intrinsic orbital frustration and the geometrical frustration coexist. There is a competition between the interactions between $S^z$ along the vertical/horizontal direction and $S^x$ along the diagonal direction. The two interactions compete with each other at $J = 1$ where a macroscopic number of the classical pseudo-spin configurations are degenerated. This degeneracy is lifted by the thermal and quantum fluctuations and the $S^z$ Ising order is realized. The tricritical point appears due to the coexistence of the orbital frustration and the geometrical frustration.

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