Ferromagnetism and orbital order in the two-orbital Hubbard model

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Abstract. We investigate spin and orbital states of the two-orbital Hubbard model on a square lattice by using a variational Monte Carlo method at quarter-filling, i.e., the electron number per site is one. As a variational wave function, we consider a Gutzwiller projected wave function of a mean-field type wave function for a staggered spin and/or orbital ordered state. Then, we evaluate expectation value of energy for the variational wave functions by using the Monte Carlo method and determine the ground state. In the strong Coulomb interaction region, the ground state is the perfect ferromagnetic state with antiferro-orbital (AF-orbital) order. By decreasing the interaction, we find that the disordered state becomes the ground state. Although we have also considered the paramagnetic state with AF-orbital order, i.e., purely orbital ordered state, and partial ferromagnetic states with and without AF-orbital order, they do not become the ground state.

1. Introduction
It has been recognized that orbital degree of freedom is important for magnetism in some materials, such as colossal magneto-resistance and complex ordered phases of manganites [1,2], and exotic magnetism in f-electron systems [2,3]. The orbital degree of freedom plays an important role in particular for realization of ferromagnetism. In two orbital models at quarter-filling, i.e., the electron number per site is one, a perfect ferromagnetic state realizes with antiferro-orbital (AF-orbital) order in the strong coupling limit [4]. On the other hand, in the intermediate coupling regime, it is not obvious whether the inclusion of the orbital degree of freedom is enough for the stabilization of ferromagnetism. In addition, it is interesting whether the perfect ferromagnetic state is continuously connected to the paramagnetic state through partial ferromagnetic states or the ground state changes abruptly from the perfect ferromagnetic state to the paramagnetic state at a certain interaction strength.

In this study, in order to unveil the ground state property in a system with the orbital degree of freedom in weak coupling to strong coupling cases, we study spin and orbital states of the two-orbital Hubbard model by using a variational Monte Carlo method at quarter-filling. A similar model has been studied by the variational Monte Carlo method for states without orbital order, and it has been found that staggered orbital correlation enhances in a ferromagnetic state in a strong coupling region [5]. In the strong Coulomb interaction limit, the ground state should be the ferromagnetic state with AF-orbital order, and in the weak coupling case, the ground state
is the disordered state. In this study, in addition to these two states, we consider a purely AF-orbital ordered state without magnetic order, a purely magnetic ordered state without orbital order, and partial ferromagnetic state with and without AF-orbital order.

2. Model and Method
The two-orbital Hubbard model is given by the following Hamiltonian:

\[
H = \sum_{k\tau\sigma} \epsilon_k c_{k\tau\sigma}^{\dagger} c_{k\tau\sigma} + U \sum_{i,\tau} n_{i\tau\uparrow} n_{i\tau\downarrow} + U' \sum_i n_{i1} n_{i2} \\
+ J \sum_{i,\sigma,\sigma'} c_{i1\sigma}^{\dagger} c_{i2\sigma'} c_{i1\sigma'} c_{i2\sigma} + J' \sum_{i,\tau \neq \tau'} c_{i\tau\uparrow}^{\dagger} c_{i\tau'\downarrow}^{\dagger} c_{i\tau'} c_{i\tau\downarrow},
\]

where \( c_{i\tau\sigma} \) is the annihilation operator of the electron at site \( i \) with orbital \( \tau (=1 \text{ or } 2) \) and spin \( \sigma (=\uparrow \text{ or } \downarrow) \), \( c_{k\tau\sigma} \) is the Fourier transform of it, \( n_{i\tau\sigma} = c_{i\tau\sigma}^{\dagger} c_{i\tau\sigma} \), and \( n_i = \sum_{\tau,\sigma} n_{i\tau\sigma} \). We consider the nearest neighbor hopping and the dispersion is given by \( \epsilon_k = -2t(\cos k_x + \cos k_y) \). We set the lattice constant unity. The coupling constants \( U, U', J, \) and \( J' \) denote the intra-orbital Coulomb, inter-orbital Coulomb, exchange, and pair-hopping interactions, respectively.

We evaluate expectation value of energy for variational wave functions by using the Monte Carlo method. We consider a Gutzwiller-projected wave function of a mean-field type wave function as a variational wave function [5, 6, 7]. In this study, we consider staggered order of spin and/or orbital states for the mean-field type wave function. The variational wave function is given by

\[
|\Psi\rangle = P_G|\Phi\rangle,
\]

where \( P_G \) is the Gutzwiller projection operator defined in Ref [7]. The mean-field type wave function \( |\Phi\rangle \) is given by

\[
|\Phi\rangle = \prod_{k\tau\sigma \tau'} b_{k\tau\sigma}^{(m)\dagger} |0\rangle,
\]

where \( |0\rangle \) is the vacuum. The quasiparticles occupy \( N_\sigma \) states for each spin \( \sigma \) from the lowest quasiparticle energy state, where \( N_\sigma \) is the number of electrons with spin \( \sigma \). The number of parameters in the Gutzwiller projection can be reduced from sixteen to ten by considering symmetry [7], and we can further reduce the number of the parameters to seven when we fix \( N_\sigma \). The energy of the quasiparticle in the ordered state is given by

\[
\lambda_k^{(m)} = m \sqrt{\Delta_{\tau\sigma}^2 + \epsilon_k^2}.
\]

The creation operators of quasiparticles are given by

\[
\begin{align*}
\hat{u}_{k\tau\sigma}^{(-)} &= u_{k\tau\sigma} c_{k\tau\sigma}^{\dagger} + \text{sgn}(\Delta_{\tau\sigma}) v_{k\tau\sigma} c_{k+Q\tau\sigma}^{\dagger}, \\
\hat{v}_{k\tau\sigma}^{(+)} &= -\text{sgn}(\Delta_{\tau\sigma}) u_{k\tau\sigma} c_{k\tau\sigma}^{\dagger} + u_{k\tau\sigma} c_{k+Q\tau\sigma}^{\dagger},
\end{align*}
\]

where \( Q = (\pi, \pi) \) is the ordering vector considered in this study and

\[
\begin{align*}
u_{k\tau\sigma} &= \left( 1 - \frac{\epsilon_k}{\sqrt{\Delta_{\tau\sigma}^2 + \epsilon_k^2}} \right) / 2, \\
u_{k\tau\sigma} &= \left( 1 + \frac{\epsilon_k}{\sqrt{\Delta_{\tau\sigma}^2 + \epsilon_k^2}} \right) / 2.
\end{align*}
\]
The quasiparticle gap in the ordered state is given by

\[ \Delta_{\tau \sigma} = \Delta_c + \Delta_s (\delta_{\sigma\uparrow} - \delta_{\sigma\downarrow}) + \Delta_o (\delta_{\tau 1} - \delta_{\tau 2}) + \Delta_{so} (\delta_{\sigma\uparrow} - \delta_{\sigma\downarrow})(\delta_{\tau 1} - \delta_{\tau 2}), \]  

where \( \Delta_c, \Delta_s, \Delta_o, \) and \( \Delta_{so} \) denote the gap for charge, spin, orbital, and spin-orbital ordered states, respectively. We evaluate the expectation value of energy for the variational wave function by using the Monte Carlo method, and optimize these gap parameters and the Gutzwiller parameters to minimize energy. We can also evaluate energy by fixing some parameters, for example, we set all the gap parameters zero for the disordered phase. In addition to states without magnetization, we also consider states with finite magnetization \( m = (N_\uparrow - N_\downarrow)/(N_\uparrow + N_\downarrow) \).

3. Result

Figure 1 shows energy \( E \) per site as functions of \( U \) of several states for \( J = 0, J = 0.1U, J = 0.2U, \) and \( J = 0.3U \) on a \( 12 \times 12 \) lattice. We have used the relations \( U = U' + J + J' \) and \( J = J' \). Note that at \( J = 0 \), the orbital space is equivalent to the spin space and we can exchange them, for example, the ferromagnetic AF-orbital state is equivalent to antiferro-spin ferro-orbital state. At \( J \neq 0 \), the orbital space is not equivalent to the spin space, and the ground state is uniquely determined except for trivial degeneracy, e.g., the degeneracy due to

![Figure 1](image-url)

**Figure 1.** Energy as functions of the Coulomb interaction obtained with several variational functions (a) for \( J = 0 \), (b) for \( J = 0.1U \), (c) for \( J = 0.2U \), and (d) for \( J = 0.3U \). Dash-dotted line, dotted line, dashed line, and solid line represent energy of Hartree-Fock wave functions for \( m = 1 \) para-orbital, \( m = 1 \) AF-orbital, \( m = 0.5 \) para-orbital, and \( m = 0 \) para-orbital, respectively.
the rotational symmetry in the spin space. The lines are the Hartree-Fock energy, i.e., without the Gutzwiller projection.

We find that the paramagnetic ($m = 0$) orbital-disordered (para-orbital) state has the lowest energy for $U < U_c$, where $U_c \simeq 10t - 15t$. For $U > U_c$, the perfect ferromagnetic ($m = 1$) AF-orbital state becomes the ground state. When the Coulomb interaction becomes large, electrons tend to occupy the same spin state to avoid the large energy loss by the Coulomb interaction even though the kinetic energy becomes large. In the perfect ferromagnetic state, the model reduces to the single-orbital Hubbard model at half-filling with Coulomb interaction $U_{\text{eff}} = U' - J$ if we regard the spin of the single-orbital Hubbard model as orbital. Thus, in the perfect ferromagnetic state, orbital-AF order occurs to reduce energy. The obtained critical value $U_c$ from the disordered state to the ferromagnetic state is not so large. If we do not consider the orbital order, $U_c$ becomes larger. The critical value $U_c$ increases as $J$ is increased. By increasing $J$, the effective interaction $U_{\text{eff}}$ between different orbitals becomes weak, and a larger value of the Coulomb interaction is necessary for the appearance of the ferromagnetic state.

Although we have also calculated energy for the purely AF-orbital state with $m = 0$ and for partial ferromagnetic states, e.g., $m = 0.5$ shown in figure 1 with and without AF-orbital order, energy for them does not become the lowest. This fact indicates that the ferromagnetism and the AF-orbital order stabilize each other and occur simultaneously in the ground state at quarter-filling. Note that the absence of a partial ferromagnetic state at quarter-filling has also been found in one dimension [8] and in infinite dimensions [9].

4. Summary
We have studied ground state of the two-orbital Hubbard model on a square lattice at quarter-filling within the variational wave functions. For the variational wave functions, we have considered Gutzwiller projected functions of spin and/or orbital ordered states. We have found that in the strong coupling region, the ground state is the perfect ferromagnetic state with AF-orbital order. In the weak coupling region, the ground state is the disordered state. We have also found that, at quarter-filling, other states do not become the ground state even in the intermediate coupling region.

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