Variational Monte Carlo Study of Two-Dimensional Multi-Orbital Hubbard Model on Square Lattice

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Abstract. We investigate the Mott transition in a two-dimensional two-orbital Hubbard model on a square lattice at half filling by using the variational Monte Carlo method. As a variational trial wave function, we consider Gutzwiller’s on-site correlations and nearest-neighbor doublon-holon correlations. We calculate the ground-state energy and the other physical quantities, all of which clearly signal a first-order Mott transition. We thus obtain the phase diagram at zero temperature, where we find the coexistence region of the metal and the Mott insulator. We discuss how Hund’s coupling affects the nature of the Mott transition in this system.

1. Introduction
The Mott metal-insulator transition is an interesting and important issue in condensed matter physics. In this connection, multi-orbital correlated electron systems have been investigated extensively. Prototypical examples are the orbital-selective Mott transitions in ruthenium alloys[1] and the unconventional superconductivity in iron pnictides[2]. In these multi-orbital systems, Hund’s coupling as well as inter- and intra-orbital Coulomb interactions plays important roles. To understand the effects of orbital degrees of freedom, it is necessary to study these effects by taking into account the above interactions systematically.

There have been a number of theoretical analyses of multi-orbital models in infinite dimensions by using dynamical mean field theory (DMFT)[3, 4], but those in finite dimensions[5, 6] are not so many. Here, we focus on a two-dimensional two-orbital Hubbard model and study the Mott transition by using the variational Monte Carlo (VMC) method[7]. Previous work by VMC[6] on multi-orbital systems has successfully described the Mott transition in the nonmagnetic phase by taking into account so-called doublon-holon intersite correlations. However, the calculation was restricted to the special case without Hund’s coupling. Also, the nature of the Mott transition was not clear. Here, we address this issue on the Mott transition in the multi-orbital system, and give a clear description of the first-order transition. The effects of Hund’s coupling are discussed in detail.

2. Model and Method
We consider a two-orbital correlated electron system on the square lattice at half filling given by the following Hubbard Hamiltonian,

\[ H = -t \sum_{<i,j>,\alpha\sigma} c_{i\alpha\sigma}^\dagger c_{j\alpha\sigma} + U \sum_{i\alpha} n_{i\alpha\uparrow} n_{i\alpha\downarrow} + (U' - J) \sum_{i\sigma} n_{i1\sigma} n_{i2\sigma} + U' \sum_{i\sigma} n_{i1\sigma} n_{i2\sigma} \]  

(1)
where $<ij>$ represents the nearest-neighbor pairs, $c_{iασ}(c_{iασ}^\dagger)$ annihilates (creates) an electron at $i$th site with spin $σ$ and orbital $α$, and $n_{iασ} = c_{iασ}^\dagger c_{iασ}$. Here, $t$ is the hopping integral, which is assumed to be $α$-independent, $U$ the intra-orbital Coulomb interaction, $U'$ the inter-orbital Coulomb interaction and $J$ Hund’s coupling. In this study, we impose the condition of $U = U' + 2J$ as usual. For simplicity, we employ an Ising-type Hund’s coupling not including the spin-flip and pair-hopping terms. Our main concern in this paper is to clarify the effects of orbital degeneracy and Hund’s coupling. For this purpose, the spin-flip and pair-hopping terms are less important and may not change the results qualitatively.

To apply the VMC method to the system, we introduce the Gutzwiller-type trial wave function\[8\] as,

$$\phi = \prod_i (1 - [1 - g_τ]|Γ⟩⟨Γ|_i) Φ_F$$

with the Fermi sea $Φ_F$, where $Γ$ specifies possible configurations at each site, and $g_τ$ is the corresponding variational parameter. To avoid the degeneracy of the ground state, we use the periodic (anti-periodic) boundary condition for $x$-axis ($y$-axis). It is known that a Mott transition never appears within the Gutzwiller wave function in finite dimensions, as firstly demonstrated for the single band models\[7\][9]. To treat the Mott transition, we thus perform the VMC analysis by including not only Gutzwiller’s on-site correlations but also intersite correlations, i.e. doublon-holon correlations defined as,

$$Ψ = \prod_{iα} (1 - μ_α ˆQ_{iα}) φ, \quad ˆQ_{iα} = d_{iα} \prod_τ (1 - e_{i+τ,α}) + e_{iα} \prod_τ (1 - e_{i+τ,α})$$

where $μ_α$ is the variational parameter for $α$th orbital, $d_{iα} = n_{iα}^\dagger n_{iα}$ and $e_{iα} = (1 - n_{iα})(1 - n_{iα}^\dagger)$.

The ground state energy and the other physical quantities are calculated with the variational Monte Carlo method. We can optimize the above variational parameters by using the stochastic reconfiguration method\[10, 11\]. This method makes it possible to optimize many parameters efficiently and stably, thereby allowing us to evaluate the ground-state quantities accurately. In this paper, we restrict our analysis to the paramagnetic Mott insulating state in order to compare the results with those of the previous VMC study \[6\] and the DMFT study \[4\].

3. Results
We discuss the results of our VMC calculations. Figure 1 shows the optimized energy $E$ computed for $J = U/2$ and $J = 0$ on the $8 × 8$ lattice. The solid line with circles (squares) represents the energy for the Mott insulating state (metallic state) which exists for $U > U_{c1}$ ($U < U_{c2}$), where the corresponding critical value $U_{c1}$ ($U_{c2}$) is determined in the process of decreasing $U$ (increasing $U$). These figures show that there is the region where double minima exist in the energy profile, i.e. the coexistence region of metallic and Mott insulating states. The critical value $U_c$ for the Mott transition is determined by the crossing point of the energies of these two states. These results clearly evidence a first-order Mott transition, which is accompanied by a hysteresis. It is seen that the transition point is shifted toward the weak-interaction region when we introduce Hund’s coupling $J$, in accordance with the DMFT calculations\[4\]. This is because Hund’s coupling suppresses orbital fluctuations, and thereby prefers the insulating state. We also calculate the energy for the system of $10 × 10$ and $12 × 12$ square lattice for $J = 1/2U$ in order to clarify the finite size effect. We find almost the same results as in the $8 × 8$ lattice. For example, the coexistence phase appears in the $U$ region of $[3.5, 4.5]$ approximately for the $8 × 8$, $10 × 10$ and $12 × 12$ systems, respectively. This indicates that the finite size effect is not so large for our systems larger than the $8 × 8$ lattice.

To corroborate the realization of the Mott transition, we calculate other physical quantities. First, we discuss the momentum distribution defined by $n_k = \frac{1}{4} \sum_{ασ} < c_{kασ}^\dagger c_{kασ} >$. In Fig. 2(a),
Figure 1. Optimized energy as a function of $U$: (a) $J = U/2$ and (b) $J = 0$. The solid line with squares (circles) represents the metallic (Mott insulating) state. The first-order transition is clearly observed for $J = U/2$, while $U_c$ is very close to $U_c$ for $J = 0$. We have used the relation $U = U' + 2J$.

Figure 2. (a) Momentum distribution function and (b) Spin structure factor in the case of $J = U/2$. Inset in (b) shows the square of the local spin moment.

we show the momentum distribution for $J = U/2$. In the metallic state, a clear discontinuity exists at the Fermi level, and it suddenly disappears when the system enters the Mott insulating phase. This confirms that the first-order metal-insulator transition indeed occurs. We also consider the spin structure factor defined by $S_1(\vec{q}) = \frac{1}{N_s} \sum_{ij} e^{i\vec{q} \cdot (\vec{r}_i - \vec{r}_j)} < S_z^i S_z^j >$, where $N_s$ is the number of the sites. In Fig. 2(b), $S_1(\vec{q})$ is plotted as a function of $U$ under the condition $J = U/2$. The spin structure factor $S_1(\vec{q})$ at the AF nesting vector $\vec{q} = (\pi, \pi)$ has a sharp peak, in particular, in the insulating phase. In the inset of Fig. 2, the square of the local spin moment defined by $S_{\alpha}^z = \sum_{i} (n_{\alpha i} - n_{\alpha i})/2$ is plotted. It is seen that Hund’s coupling forms the $S = 1$ spin, and the resulting effective spins have a tendency toward the antiferromagnetic order especially in the insulating region.

We evaluate the ground state energy for various choices of the parameters and thus determine the phase diagram, which is shown in Fig. 3. Including the effects of Hund’s coupling $J$, we clearly identify the coexistence region and the hysteresis associated with the Mott transition. It is not easy to discuss the nature of Mott transition in the single-orbital system [9], also in the multi-orbital system without $J$ [6]. In this work, we can describe the first-order transition quite well. It is seen that the metallic phase becomes more stable along the line of $U = U'$ (i.e. $J = 0$) because of enhanced orbital fluctuations. The introduction of Hund’s coupling suppresses the
orbital fluctuations, thereby making the metallic region smaller. These results are consistent with the DMFT calculation.

4. Summary
We have investigated a two-dimensional two-orbital Hubbard model on a square lattice at half filling by using the VMC method with particular emphasis on the effect of Hund’s coupling. For the variational wave functions, we have considered Gutzwiller’s on-site correlations and nearest-neighbor doublon-holon correlations. We have demonstrated that a first-order Mott transition occurs in the model, which is accompanied by the coexistence region with a hysteresis. It has been found that in the absence of Hund’s coupling, the coexistence region is very tiny, making it difficult to figure out the nature of the Mott transition. This difficulty is what we encountered in the previous study on the multi-orbital model with $U = U'$ [6]. We have confirmed that Hund’s coupling has a tendency to stabilize the Mott insulating state, in accordance with the DMFT study. Our discussions in this paper have been focused on the paramagnetic Mott transition in order to compare the results with the previous ones. A more detailed VMC analysis of multi-orbital systems is in progress, which incorporates possible spin/orbital orderings. The results will be reported elsewhere.

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