Mott Transitions in Three-Orbital Hubbard Model at Fractional Band Filling

Tomoko Kita1, Takuma Ohashi2 and Norio Kawakami1

1 Department of Physics, Kyoto University, Kyoto 606-0852, Japan
2 Department of Physics, Osaka University, Toyonaka, Osaka 560-0043, Japan
E-mail: kita@scphys.kyoto-u.ac.jp

Abstract. We investigate the Mott transitions in the three-orbital Hubbard model by means of the dynamical mean field theory with continuous-time quantum Monte Carlo simulations. We obtain the phase diagram determined in the orbital level splitting versus Hubbard interaction plane in the case of two electrons per site. It is also found that the introduction of holes into the orbital selective Mott insulating phase induces the metallic state with heavy quasiparticles.

Strongly correlated electron systems with multiorbital degrees of freedom have been studied extensively. In these systems, orbital fluctuations enhanced by electron correlations induce a variety of intriguing phenomena, such as magnetic and/or orbital ordering, metal-insulator transition, etc. The orbital selective Mott transition (OSMT), where some of the orbitals become localized while the others still remain itinerant, is one of the interesting problems induced by the interplay of multiorbital effects and strong electron correlations [1, 2].

The dynamical mean field theory (DMFT) has been applied to the two-orbital Hubbard model with different bandwidths, and it has been clarified that the Hund’s coupling plays an important role in the OSMT [3–6]. Recently, the OSMT has also been addressed in the system with the same bandwidths [7, 8]. In these studies, it has been suggested that the OSMT occurs due to the difference not in bandwidths but in orbital degeneracy. The OSMT may occur in a three-orbital Hubbard model when the orbital degeneracy is lifted into doubly degenerate orbitals and a single orbital. In the doubly degenerate orbitals, a metallic state is expected to be further stabilized by orbital fluctuations than in a non-degenerate orbital, which results in separate transitions to the Mott insulating phase. However, the filling dependence of the orbital selective Mott insulator (OSMI) phase has not been sufficiently understood yet [7, 9], which may be important in real materials.

In this study, we investigate the Mott transitions in the three-orbital Hubbard model with particular focus on the filling dependence of the insulating phases in the case of two electrons per site. We clarify that the hole-doping effect on the OSMI phase induces the metallic state with the heavy quasiparticle peak.

For the purpose mentioned above, we consider the three-orbital Hubbard model defined by

\[
H = -t \sum_{\langle i,j \rangle, \alpha, \sigma} c_{i \alpha \sigma}^\dagger c_{j \alpha \sigma} + \sum_{i, \alpha, \sigma} (-\mu + \Delta_\alpha) n_{i \alpha \sigma} + U \sum_{i, \alpha} n_{i \alpha \uparrow} n_{i \alpha \downarrow} + \sum_{i, \alpha \neq \alpha', \sigma, \sigma'} (U' - \delta_{\sigma \sigma'} J) n_{i \alpha \sigma} n_{i \alpha' \sigma'},
\]

(1)
Figure 1. $\Delta$-$U$ phase diagram for the three-orbital Hubbard model with $J/U = 0.15$ and $n = 2.0$ at $T/D = 0.02$. The characteristic interaction strength of the first-order transition (crossover) is denoted by filled (open) diamonds. We only show $U_{c2}$ for the first-order transition. Solid lines are to guide the eye.

where $c_{i\alpha \sigma}^{\dagger}$ is an annihilation (creation) operator of an electron with spin $\sigma$ ($=\uparrow, \downarrow$) and orbital $\alpha$ ($= 1, 2, 3$) at the $i$th site, and $n_{i\alpha \sigma} = c_{i\alpha \sigma}^{\dagger} c_{i\alpha \sigma}$ is the number operator. Here, $t$ is the nearest-neighbor hopping integral, $\mu$ is the chemical potential, $\Delta_\alpha$ is the energy level for orbital $\alpha$. In the interaction terms, $U$ ($U'$) is the intraorbital (interorbital) Coulomb interaction, and $J$ is the Hund’s coupling. We impose the condition $U = U' + 2J$ as usual. Orbital level splitting is given by $\Delta_\alpha$ and we set $\Delta_1 = \Delta_2 = 0$, $\Delta_3 = -\Delta$ so that the energy level of doubly degenerate orbitals 1 and 2 is higher than that of the single orbital 3.

To investigate the Mott transition in this model, we use the single-site DMFT [10]. In the framework of DMFT, the lattice model is mapped onto an effective impurity model, where local electron correlations are taken into account precisely. The lattice Green’s function is obtained via a self-consistency condition imposed on the impurity problem. In this paper, we use a semicircular density of states (DOS), $\rho(\omega) = (2/\pi D)\sqrt{1 - (\omega/D)^2}$, which corresponds to the infinite-coordination Bethe lattice. We choose the energy unit as $D = 1$ (half bandwidth). To solve the effective impurity problem, we use the hybridization expansion continuous-time quantum Monte Carlo (CT-QMC) method [11, 12]. This method allows us to access the strong interaction regime in a wide range of temperature especially down to very low temperature [13–15]. Actually, calculations have been done successfully in previous DMFT + CT-QMC studies on the three-orbital Hubbard model [16–19].

In the model (1), it is known that the OSMT occurs when the electron filling per site is fixed at $n = 2.0$ [7, 8, 20]. Figure 1 shows the $\Delta$-$U$ phase diagram for $J/U = 0.15$ and $n = 2.0$ at low temperature $T/D = 0.02$. Note that for small Hund’s coupling, e.g., $J/U = 0.05$, we have shown that the OSMI phase does not appear down to $T/D = 0.02$ at $n = 2.0$ in Ref. [20]. Therefore, we here choose a typical strength of Hund’s coupling $J/U = 0.15$ which stabilizes the OSMI phase. In the phase diagram, the critical interaction of the first-order transition (crossover) is denoted by filled (open) diamonds, which is determined by the $U$-dependence of the double occupancy; the first order transition point is defined as the position where the double occupancy jumps and the crossover point is defined as the inflection point in the double occupancy curve. The crossover behavior is due to the finite-temperature effects and all the phase boundaries shown.
Figure 3. Electron number in the upper orbitals 1 and 2, $n_1 + n_2$ (top panel), and in the lower orbital 3, $n_3$ (bottom panel), as a function of doping $\delta$. Other parameters are set as $J/U = 0.15$, $\Delta/D = 0.8$ and $T/D = 0.02$.

Figure 4. Density of states for the upper orbital 1 and the lower orbital 3 for several values of Coulomb interaction $U$ and hole-doping $\delta$. Other parameters are set as $J/U = 0.15$, $\Delta/D = 0.8$ and $T/D = 0.02$.

in the figure should be of first order at zero temperature. In the strong interaction regime, two kinds of insulators appear. One is the Mott insulator (MI) and the other is the correlated band insulator (BI). In a small $\Delta$ region, the Hund’s coupling dominates the effect of $\Delta$, inducing the MI with the electron number in each orbital $(n_1 + n_2, n_3) = (1, 1)$, where $n_\alpha$ denotes the electron number in orbital $\alpha$. For a large $\Delta$ region, another insulating phase is stabilized, which is adiabatically connected to a BI specified by $(n_1 + n_2, n_3) = (0, 2)$. This insulating phase is referred to as the correlated BI. It is seen that the OSMI phase emerges in the MI region with intermediate interactions. For finite $\Delta$ ($0.2 < \Delta/D < 1.5$), we find that the transition (or crossover) occurs twice. The Mott transition in the lower orbital occurs first at the smaller interaction, where the upper orbital is still metallic. This discrepancy in critical interaction strengths is due to the difference in orbital degeneracy.

To see how the quasiparticles evolve with changing temperature, we show the orbital-dependent DOS. We calculate the DOS in orbital $\alpha$, $\rho_\alpha(\omega)$, by applying the maximum entropy method [21] to the imaginary-time QMC data. In Fig. 2, we show $\rho_\alpha(\omega)$ for several choices of $T$ in three phases, the metal, the OSMI, and the MI. In the metallic phase (Fig. 2 (a)), the peaks around the Fermi level appear in both orbitals when temperature decreases. It is seen that at low temperature, the DOS for both orbitals form quasiparticle states around the Mott transition. With increasing $U$, the system enters the OSMI phase, as shown in Fig. 2 (b). The DOS for the lower orbital 3 opens a gap at low temperature while the DOS for the upper orbital 1 is still metallic with the quasiparticle peak. In the MI phase (Fig. 2 (c)), the DOS for both orbitals open gaps.

We discuss the hole-doping effect to clarify the stability of the OSMI phase and the quasiparticle behavior. Here, we introduce the parameter $\delta = 2.0 - n$. In Fig. 3, we show the electron number in each orbital as a function of $\delta$. It is seen that the electron number in the upper orbitals $n_1 + n_2$ decreases with increasing $\delta$ for all $U$. On the other hand, in the lower orbital, $n_3$ remains 1 in the insulating phases ($U/D \geq 2.8$) for small $\delta$; most of the holes are doped in the upper orbitals due to correlation effects. In Fig. 4, we also show the orbital-
dependent DOS to clarify the quasiparticle behavior. For $U/D = 2.8$, the undoped system is in the OSMI phase, as shown in the bottom panel of Fig. 2 (b). With increasing $\delta$, the quasiparticle peaks in the upper orbitals (1 and 2) are suppressed, which is caused by the gradual decrease of $n_1 + n_2$. In the lower orbital 3, we find the filling-control Mott transition. The orbital 3 keeps insulating for small $\delta$ and becomes metallic at not infinitesimal but finite critical doping. As shown in Fig. 4 (b), $\rho_3(\omega)$ is insulating for $\delta = 0.3$ and becomes metallic for $\delta = 0.7$. In this metallic phase, the heavy quasiparticle state is formed and sharp peak appears. These results are consistent with the behavior of the particle number. For $U/D = 3.8$, where the system is in the MI phase for $\delta = 0$, the gap in the upper orbital closes for infinitesimal doping, because $n_1 + n_2$ decreases and the filling becomes incommensurate one. On the other hand, the lower orbital 3 remains insulating for $\delta \leq 0.7$. Therefore, in the strong $U$ regime, the system changes from the MI to the OSMI with hole doping.

In summary, we have studied the Mott transitions in the three-orbital Hubbard model with particular focus on the filling dependence of insulating states at $n = 2.0$. We have clarified that the OSMI phase appears in the doped system by doping holes into the MI phase at $n = 2.0$. It has also been found that the hole-doping effect on the OSMI phase at $n = 2.0$ induces the transition to the metal with the formation of the heavy quasiparticle state near the filling-control Mott transition.

**Acknowledgments**

The authors thank S. Sakai and K. Inaba for valuable discussions. This research is granted by the Japan Society for the Promotion of Science (JSPS) through the “Funding Program for World-Leading Innovative R&D on Science and Technology (FIRST Program)”, initiated by the Council for Science and Technology Policy (CSTP). T.O. is supported by the Grant-in-Aid for Scientific Research [Grant nos. 21740232, 20104010] and the Next Generation Super Computing Project “Nanoscience Program” from the MEXT of Japan. N.K. is supported by the Grant-in-Aid for Scientific Research [Grant nos. 21540359, 20102008].

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