Spatial Fluctuations in Two-Orbital Hubbard Model

Tomoko Kita¹, Takuma Ohashi², and Sei-ichiro Suga¹,³

¹ Department of Applied Physics, Osaka University, Suita, Osaka 565-0871, Japan
² Department of Physics, Osaka University, Toyonaka, Osaka 560-0043, Japan
³ Department of Materials Science and Chemistry, University of Hyogo, Himeji, Hyogo 671-2280, Japan
E-mail: kita@tp.ap.eng.osaka-u.ac.jp

Abstract. We study spin and orbital correlations in the two-orbital Hubbard model with the different bandwidths at quarter filling by means of the cellular dynamical mean field theory combined with the noncrossing approximation. We demonstrate that the ferromagnetic-antiferro-orbital insulating state is stabilized in the system with the same bandwidth and the antiferromagnetic-ferro-orbital insulating state appears when the difference of the bandwidth is quite large. In the intermediate region, we find that the competition between the two states occurs and this competition gives rise to the heavy Fermi-liquid metallic state.

Strongly correlated electron systems with orbital degrees of freedom have attracted much attention. One of novel orbital dependent physics is the orbital-selective Mott transition [1–3]. In Ca₂₋ₓSrₓRuO₄, a localized spin in the metallic state has been experimentally observed. The heavy fermion behavior observed in the transition metal oxide LiV₂O₄ [4–7] has also activated the intensive studies of the multiorbital systems.

The dynamical mean field theory (DMFT) [8] is the powerful framework to treat the strong electron correlations. The DMFT studies have made considerable progress in understanding the Mott transition, magnetic properties, etc. in the multiorbital strongly correlated systems [2, 3, 9–13]. However, this method is justified for infinite dimensional systems and does not treat the spatially extended correlations. Very recently, nontrivial momentum-dependent dynamics, which is extremely relevant to the spatial correlation effects, have been observed in Ca₂₋ₓSrₓRuO₄ [14, 15]. Therefore, it is desirable to investigate the strong correlation effects in multiorbital systems using an extended method which incorporates spatial fluctuations of spin and orbital.

In this paper, we investigate the two-orbital Hubbard model on the square lattice by means of the cellular dynamical mean field theory (CDMFT) combined with the noncrossing approximation (NCA) [16–18]. In our previous work [19], we have studied the effects of the Hund’s coupling at quarter filling. It has been clarified that the strong Hund’s coupling enhances the antiferro-orbital fluctuations, which give rise to insulating behavior. On the other hand, for weak Hund’s coupling, the Fermi-liquid metallic state is stabilized down to low temperatures. In the present study, we investigate the effects of the difference of the bandwidths between the two orbitals. We demonstrate that it causes the competition between the antiferromagnetic-ferro-orbital (AFM-FO) and ferromagnetic-antiferro-orbital (FM-AFO) states, which gives rise to the heavy Fermi-liquid metallic state.

We consider the two-orbital Hubbard model on the two-dimensional square lattice, 

\[ H = \sum_{\langle i,j \rangle, \alpha \sigma} (-t_{ij} - \delta_{ij} \mu) c_{i \alpha \sigma}^\dagger c_{j \alpha \sigma} + U \sum_{i \alpha} n_{i \alpha \uparrow} n_{i \alpha \downarrow} \]
Figure 1. Temperature dependence of the density of states for $U/t = 4.0$, $J/t = 0.4$. The top (a), middle (b) and bottom (c) panels show the density of states for $R = 1.0$, $R = 0.7$ and $R = 0.3$, respectively. In the middle and bottom panels, the left one is for the orbital 1 (the wider band) and the right one is for the orbital 2 (the narrower one).

\[ T/t = 0.20 \quad T/t = 0.10 \quad T/t = 0.05 \]

\[ \sum_{i \sigma \sigma'} (U' - \delta_{\sigma \sigma'} J) n_{i \sigma} n_{i \sigma'} - J \sum_i \left( c_{i11}^\dagger c_{i11} c_{i22}^\dagger c_{i22} + c_{i11}^\dagger c_{i11} c_{i21}^\dagger c_{i21} + \text{H.c.} \right), \quad (1) \]

where $c_{i \alpha \sigma}^{(\dagger)}$ is an annihilation (creation) operator with spin $\sigma (=\uparrow, \downarrow)$ and orbital $\alpha (=1, 2)$ at the $i$th site, and $n_{i \alpha \sigma} = c_{i \alpha \sigma}^\dagger c_{i \alpha \sigma}$ is a number operator. Here, $t_\alpha$ denotes the nearest-neighbor hopping integral in orbital $\alpha$, $\mu$ the chemical potential, $U(U')$ the intra-orbital (inter-orbital) Coulomb interaction and $J$ the Hund’s coupling including the spin-flip and pair-hopping terms. We impose the condition $U = U' + 2J$, which is obtained by symmetry arguments. In this study, we fix the filling at $n = \sum_{\alpha, \sigma} \langle n_{i \alpha \sigma} \rangle = 1$ (quarter filling). We introduce the ratio of the bandwidths $R = t_2/t_1$ and take $t_1 = t$ as the unit of energy. In order to investigate the effects of nonlocal fluctuations of spin and orbital near the Mott transition, we use CDMFT, a cluster extension of DMFT. In CDMFT, the original lattice is regarded as a superlattice consisting of clusters, which is then mapped onto an effective cluster model via a standard DMFT procedure.
We use a two-site two-orbital cluster model coupled to the self-consistently determined medium, which is solved by NCA.

We first investigate the effects of the difference of the bandwidths on spin and orbital fluctuations in the two-orbital Hubbard model at quarter filling. Fig. 1 shows the density of states (DOS) for $R = 1.0$ (the same bandwidths), $R = 0.7$ and $R = 0.3$, respectively. For $R = 1.0$, a dip evolves at very low temperatures. Therefore, the ground state for $R = 1.0$ is expected to be an insulator. Also for very small $R (= 0.3)$, DOS at the Fermi level in both 1 and 2 orbitals monotonically decrease with lowering $T$ and the system tends to be an insulator at low temperatures. On the other hand, for intermediate $R (= 0.7)$, the temperature dependence of DOS is quite different from the above two cases. We find that the quasiparticle peak evolves with lowering $T$ and the metallic state persists down to very low temperatures.

To clarify the behavior of DOS, we next investigate the electron number in each orbital. In Fig. 2, we show the temperature dependence of the electron number in orbital 1, $n_1 = \sum_{\sigma} \langle n_{1\sigma} \rangle$. For $R = 1.0$, the electron number in orbital 1 is the same as that in the orbital 2, namely $n_1 = n_2 = 0.5$. As $R$ decreases, $n_1$ increases and $n_2$ decreases. This indicates that electrons in the narrower band 2 move to the wider band 1 because of the kinetic energy gain. This tendency becomes stronger at lower temperatures. In the small $R$ region ($R = 0.3$), $n_1$ approaches 1 with lowering $T$ and $n_2$ goes to zero. These features are consistent with the results in the one-dimensional system and in the strong-coupling limit [20]. We thus find that the difference of the bandwidths causes the orbital polarization due to naturally expected energy gain. Note that for intermediate $R (= 0.7)$, $n_1$ approaches neither 1 nor 0.5 with lowering $T$. In this case, any correlations of spin and orbital do not evolve, which gives rise to the nontrivial metallic behavior (shown in Fig. 1 (b)), as discussed momentarily below.

The orbital polarization drastically changes the spin and orbital correlations. In Fig. 3, we show the nearest-neighbor correlation functions of spin $(S_i^z S_{i+1}^z)$ and orbital $(\tau_i^z \tau_{i+1}^z)$ as a function of $R$. Here, spin and orbital operators are defined as $S_i^z = \sum_\sigma (n_{i\sigma\uparrow} - n_{i\sigma\downarrow})/2$ and $\tau_i^z = \sum_\sigma (n_{i\sigma\uparrow} - n_{i\sigma\downarrow})/2$, respectively. As discussed in our previous study [19], with the same bandwidths ($R = 1.0$), the Hund’s coupling $J$ enhances the FM-AFO correlations and these correlations induce the dip in DOS around the Fermi level as shown in Fig. 1 (a). The dip develops as $T$ decreases and a real gap opens at very low temperatures. We note that $S_i^z S_{i+1}^z$
is positive and the spin correlations are FM for larger $U$, although $\langle S_i^z S_{i+1}^z \rangle$ is negative for $U/t = 4.0$. As $R$ decreases, the spin correlation function $\langle S_i^z S_{i+1}^z \rangle$ decreases and the AFM correlations develop. The orbital correlation function $\langle \tau_i^z \tau_{i+1}^z \rangle$ increases with decreasing $R$ and changes its sign at $R \sim 0.45$ ($R \sim 0.35$) for $J/t = 0.4$ ($J/t = 0.6$), which indicates that the orbital correlations change from AFO to FO. We thus find that the AFM-FO state is stabilized in the small $R$ region. The insulating behavior of DOS for $R = 0.3$ shown in Fig. 1 (c) is due to the AFM fluctuations. As above discussed, in the small $R$ region, most electrons occupy the orbital 1 and the orbital 2 is nearly empty. In the orbital 1, electrons are antiferromagnetically correlated with each other, which is a similar situation to the single-band Hubbard model at half filling. Therefore, we conclude that the AFM correlations in the wider band induces the insulating behavior in the small $R$ region. On the other hand, in the intermediate $R$, the competition between FM-AFO and AFM-FO states occurs and both AFM and AFO correlations are weak. This competition induces nontrivial fluctuations of spin and orbital, which give rise to the heavy quasiparticle peak in DOS (shown in Fig. 1 (b)). Within the framework of CDMFT, these fluctuations are due to the degeneracy of the ground state in the isolated cluster. This degeneracy causes the Kondo effect in the effective cluster model of CDMFT and the Kondo-like quasiparticle peak appears in DOS. This is a similar situation in the frustrated Hubbard models [21, 22]. Therefore, we conclude that the competition between FM-AFO and AFM-FO states induces the heavy Fermi-liquid behavior in the intermediate $R$ region.

In summary, we have studied the two-orbital Hubbard model at quarter filling, particularly focusing on the effects of the difference of the bandwidths between the two orbitals. We have shown that the FM-AFO insulating state is stabilized in the system with the same bandwidth. When the difference of the bandwidth is quite large, the AFM-FO insulating state appears. We have found the competition between AFM-FO and FM-AFO states in the intermediate region, which gives rise to the heavy Fermi-liquid metallic state.

This work has been supported by the Japan Society for the Promotion of Science and also by a Grant-in-Aid from the Ministry of Education, Science, Sports and Culture of Japan (No. 21740232, No. 20540390).

References

[1] Nakatsuji S et al., 2003 Phys. Rev. Lett. 90 137202
[2] Koga A, Kawakami N, Rice T M and Sigrist M 2004 Phys. Rev. Lett. 92 216402
[3] Koga A, Inaba K and Kawakami N 2005 Prog. Theor. Phys. Suppl. 160 253
[4] Kondo S et al., 1997 Phys. Rev. Lett. 78 3729
[5] Jönsson P E, Takenaka K, Niihara K, SasaT A, Sugai S and Takagi H 2007 Phys. Rev. Lett. 99 167402
[6] Tsunetsugu H 2002 J. Phys. Soc. Jpn 71 1844
[7] Yamashita Y and Ueda K 2003 Phys. Rev. B 67 195107
[8] Georges A, Kotliar G, Krauth W and Rozenberg M J 1996 Rev. Mod. Phys. 68 13
[9] Kotliar G and Kajueter H 1996 Phys. Rev. B 54 R14221
[10] Rozenberg M J 1997 Phys. Rev. B 55 R4855
[11] Momoi T and Kubo K 1998 Phys. Rev. B 58 R567
[12] Inaba K and Koga A 2007 J. Phys. Soc. Jpn 76 094712
[13] Held K and Vollhardt 1998 Eur. Phys. J. B 5 473
[14] Shimoyamada A, Ishizaka K, Tsuda S, Nakatsuji S, Maeno Y and Shin S 2009 Phys. Rev. Lett. 102 086401
[15] Neupane M et al., 2008 arXiv:0808.0346
[16] Bickers N E 1987 Rev. Mod. Phys. 59 845
[17] Kotliar G, Sergeev V, Paulson G and Biroli G 2001 Phys. Rev. Lett. 87 186401
[18] Stanescu T D, Civelli M, Hauke K and Kotliar G 2006 Ann. of Phys. 321 1682
[19] Kita T, Ohashi T and Suga S I arXiv:0812.4019, to appear in Phys. Rev. B.
[20] Miyashita S, Yamashita Y, Yonemitsu K, Koga A and Kawakami N 2009 J. Phys.: Conf. Ser. 150 042128
[21] Ohashi T, Kawakami N and Tsunetsugu H 2006 Phys. Rev. Lett. 97 066401
[22] Ohashi T, Momoi T, Tsunetsugu H and Kawakami N 2008 Phys. Rev. Lett. 100 076402