Effects of interorbital hopping on orbital fluctuations and metal-insulator transitions: Extended linearized dynamical mean-field theory

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We study the effects of interorbital hopping on orbital fluctuations and Mott-Hubbard metal-insulator transition (MIT) in the two-orbital Hubbard model within the extended linearized dynamical mean-field theory. By mapping the model onto an effective model with different bandwidths through the canonical transformation, we find that at half-filling, the increases of the interorbital Coulomb interaction $U'$ and the Hund’s coupling $J$ drive the MIT, and the critical $J_c$ for MIT increases with the lift of the inter-orbital hopping integral $t_{ab}$. Meanwhile at quarter filling and in the strong correlation regime, the system without $t_{ab}$ exhibits MIT with the decreasing of $J$, and favors the orbital liquid ground state. However, the system transits from metal to insulator with the increasing of $t_{ab}$, accompanied with the rising of the orbital order parameter. These results show the important role of the interorbital hopping in the orbital fluctuation and orbital ordering.

I. INTRODUCTION

In recent years, significant interest has been attracted to the problem of orbital ordering and its effect on Mott-Hubbard metal-insulator transition (MIT) of some transition-metal oxides.\textsuperscript{3} As a result of the addition of orbital degree of freedom, some strongly correlated 3d transition-metal oxides exhibit very rich and complicated phase diagrams.\textsuperscript{2,3,4,5} In these strongly correlated systems with charge, spin and orbital degrees of freedom, various orbital, magnetic and charge orders coexist or compete with each other. Since many different quantum phases are almost degenerate, a little change in orbital configuration usually leads to quantum phase transition. This has been a hot topic in recent years since the long-range orbital ordered ground state is found in colossal magnetoresistive parent material $LaMnO_3$ and the typical MIT system $V_2O_5$. The quantum fluctuations are important in these compounds, and it comes to be the key issue to realize what role the orbital degree of freedom plays in driving the quantum phase transitions. The conventional self-consistent mean-field approach underestimates the effect of the orbital quantum fluctuations, the dynamical mean-field theory (DMFT)\textsuperscript{5} is an useful tool to unveil the role of the quantum fluctuations on the Mott-Hubbard MIT in these strongly correlated systems.

The DMFT, which is based on a mapping of lattice models onto effective quantum impurity models subject to a self-consistency condition, has been very successful in describing many aspects of strongly correlated electron systems.\textsuperscript{3} Many well-established numerical methods have been applied to solve the effective quantum impurity model, such as the quantum Monte Carlo,\textsuperscript{9,10,11} the exact diagonalization,\textsuperscript{12,13,14} and the renormalization-group method.\textsuperscript{15,16,17} Although these methods are successful in studying the MIT in single-band Hubbard model, computational limits are met in applying the DMFT methods to more complicated multi-band models. Recently Bulla and Potthoff\textsuperscript{18} proposed the linearized DMFT (LDMFT) to solve the effective impurity Anderson model with one impurity site and one bath site only, and this ansatz shows minimum computational effort in dealing with the MIT of Hubbard model. However, the LDMFT is bound to the critical point in parameter space. Then Potthoff\textsuperscript{19} extended this method (ELDMFT), which is able to access the entire parameter space. The ELDMFT reduces to the LDMFT at half-filling and at $U = U_c$. The ELDMFT simplifies the procedure of DMFT by linearizing the self-consistent equations in the low and high energy regions, and can be easily applied to study some more complicated models which are hard to be treated by the full DMFT. The results obtained for the Hubbard model are in good agreement with the other numerical techniques.\textsuperscript{15}

The minimal model to describe the Mott-Hubbard MIT including the orbital degree of freedom is the two-orbital degenerate Hubbard model. This model has been investigated with DMFT by several groups\textsuperscript{20,21,22,23,24,25}. Rozenberg\textsuperscript{20} found that the successive MIT occurs when the electron occupation number varies from $n=0$ to 4; Koga \textit{et al.}\textsuperscript{22} showed that two MITs may occur for the two subbands at different Coulomb interaction; and Puschke \textit{et al.}\textsuperscript{25} recently demonstrated that the Hund’s coupling plays an important role on the MIT. Whereas most of these studies neglected the charge transfer between the two different orbitals, the inter-orbital charge fluctuation was prohibited and the effect of orbital fluctuation was greatly underestimated. This paper is to understand the orbital physics in multi-band Hubbard model at finite temperatures, especially for the influences of the interorbital hopping and Coulomb interaction on the orbital fluctuation, orbital ordering and the MIT in...
the systems with various electron fillings.

In what follows, we study the two-orbital Hubbard model to explore the role of orbital degrees of freedom and the interorbital hopping, Hund’s coupling and the interorbital Coulomb correlation on MIT both in the half and quarter filling cases, respectively. We find the Hund’s coupling plays different roles in the half- and quarter-filling systems; the interorbital Coulomb interaction further splits the two Hubbard bands and drives the system from metal to insulator at half filling; the orbital fluctuation in the presence of interorbital (off-diagonal) orbital hopping is so strong that the metallic phase is stable at quarter filling; also the interorbital hopping may establish the orbital order and drives the system to the insulating phase. The paper is organized as follows: in Sec.II, we transform the two-orbital Hubbard model with interorbital hopping into an effective model with different bandwidth by the canonical transformation, which is easily mapped into an impurity model in the framework of the DMFT. Then we describe the extended linearized DMFT approach in Sec.III. Our numerical results for the systems with half and quarter filling at finite temperatures are presented in Sec.IV. And Sec.V is devoted for the discussion and summary.

II. THE TWO-ORBITAL HUBBARD MODEL

The two-orbital Hubbard model consists of the kinetic energy and the Coulomb potential parts,

\[ H = H_t + H_U \] (1)

with

\[ H_t = -\sum_{\langle ij \rangle \sigma \sigma'} t_{ij} C_{il\sigma}^+ C_{jl\sigma'} \]

\[ H_U = U \sum_{il} n_{il\uparrow} n_{il\downarrow} + \frac{J}{2} \sum_{i,l \neq i',\sigma,\sigma'} C_{il\sigma}^+ C_{il\sigma'}^+ C_{il'\sigma'} C_{il'\sigma} \]

\[ + \sum_{l \neq l', \sigma, \sigma'} (\frac{U'}{2} n_{il\sigma} n_{il'\sigma'} + \frac{J}{2} C_{il\sigma}^+ C_{il'\sigma'}^+ C_{il\sigma'} C_{il'\sigma}) \] (2)

Here \( l (l') = a \) or \( b \), and \( t_{aa} \) (\( t_{bb} \)) and \( t_{ab} \) denote the nearest-neighbor intraorbital and interorbital hopping integrals, respectively; \( U \) describes the on-site intraorbital repulsion between electrons and \( U' \) the on-site interorbital interaction; and \( J \) denotes the Hund’s coupling. There are two terms with \( J \) in Eq. (2). The first one corresponds to the spin exchange of the two intraorbital electrons, and the second one to the orbital exchange between two different orbital electrons. Such a full Hamiltonian keeps the rotation invariance of the Hamiltonian (1) in the spin and orbital spaces. Usually the spin exchange parameter is slightly different from the orbital one, while for clarity we assume the two parameters are the same. For an isolated ion we have the rotation invariant relation \( U - U' = 2J \); in some crystals, however, the direct Coulomb interactions \( U \) and \( U' \) are modified by the screening effect, and the parameter \( U' \) and \( J \) should be considered as independent parameters. Here we consider these two cases, respectively; and for clarity, we concentrate on the orbital fluctuation, and fix the spin configuration as the paramagnetic phase, that is, we look for dynamic mean-field solutions that do not break the spin rotational symmetry in this paper.

For such multi-orbital systems with off-diagonal orbital hopping, it is hard to map the Hamiltonian (1) onto the single impurity effective model. We introduce two fermions \( \alpha \) and \( \beta \) via a canonical transformation, and the kinetic terms become of orbital diagonal in this quasiparticle representation. The canonical transformation is expressed as:

\[ C_{\alpha \sigma} = u \alpha_{\sigma} + v \beta_{\sigma} \]

\[ C_{\beta \sigma} = -v \alpha_{\sigma} + u \beta_{\sigma}, \] (3)

with

\[ u^2 = \frac{1}{2} [1 + \sqrt{1 - \frac{t_{ab}^2}{t_{aa}^2 + (t_{aa} - t_{bb})^2}}], \]

\[ v^2 = \frac{1}{2} [1 - \sqrt{1 - \frac{t_{ab}^2}{t_{ab}^2 + (t_{aa} - t_{bb})^2}}]. \] (4)

Here \( \alpha \) and \( \beta \) are the new fermion operators, respectively. In this situation the twofold degenerate orbital degree of freedom is converted into two different kinds of fermions, and the orbital correlation is transformed into the particle-particle correlation. By Eq.(3), the kinetic energy \( H_t \) in Eq.(1) is expressed as,

\[ H_t = -t_{\alpha} \sum_{<ij>,\sigma} (\alpha_{i\sigma}^+ \alpha_{j\sigma} - \beta_{i\sigma}^+ \beta_{j\sigma}) \]

\[ -\mu \sum_{i,\sigma} (\alpha_{i\sigma}^+ \alpha_{i\sigma} + \beta_{i\sigma}^+ \beta_{i\sigma}), \] (5)

with \( t_{\alpha} = t_{aa} u^2 + t_{bb} v^2 - t_{ab} u v \) and \( t_{\beta} = t_{aa} v^2 + t_{bb} u^2 + t_{ab} u v \). In addition, we transform the potential energy \( H_U \) via the canonical transformation Eq.(3), and obtain an effective two-orbital Hamiltonian with different bandwidths so long as \( t_{ab} \neq 0 \). Through the canonical transformation the two-orbital fermions with interorbital hopping are transferred into two new fermions without interorbital hopping, which can be treated more easily in the DMFT scheme as to the single Hubbard model. On the other hand, the on-site Coulomb energy and the Hund’s coupling in \( H_U \) inevitably become very complicated, which is not hard to treat in the DMFT framework in the present fermion representation.
III. THE EXTENDED LINEARIZED DMFT

In the DMFT, the above effective lattice model can be mapped into an impurity model with two orbitals,

\[
H_{\text{imp}} = \sum_{l,\sigma} \epsilon_{l\gamma\sigma} a_{l\gamma\sigma}^+ a_{l\gamma\sigma} - \mu \sum_{\sigma} \{ \alpha_{0\sigma} a_{0\sigma} + \beta_{0\sigma} b_{0\sigma} \} + \sum_{l,\sigma} [V_{l\sigma} (a_{l\alpha\sigma}^+ a_{l\gamma\sigma} + h.c) + V_{l\sigma}^\beta (a_{l\beta\sigma}^+ b_{l\gamma\sigma} + h.c)] + H_0^\alpha (\alpha, \beta),
\]

where \( \alpha_{0\sigma} \) (or \( \beta_{0\sigma} \)) annihilates a fermion with spin \( \sigma \) at the impurity site \( i = 0 \). The impurity couple with the bath which is described by operators \( (a_{l\gamma\sigma}^+, a_{l\gamma\sigma}) \) with energy \( \epsilon_{l\gamma\sigma} \) via hybridization \( V_{l\sigma} \) \( (\gamma = \alpha \text{ or } \beta) \). For this model, the free \( (U = U' = J = 0) \) impurity Green's function \( G_0^\alpha (\gamma, \gamma') = \langle \gamma_0 | a_{l\gamma\sigma}^+ a_{l\gamma'\sigma} | 0 \rangle \) \( (\gamma_0 \sigma', \gamma'_0 \sigma) = \alpha_0 \text{ or } \beta_{0\sigma} \) is a \( 2 \times 2 \) matrix, and it can be obtained via,

\[
(G_0^\alpha (\omega))^{-1} = \begin{pmatrix} \omega + \sum_{l,\sigma} \frac{V_{l\sigma}^2}{\omega - \epsilon_{l\sigma}} & 0 \\ 0 & \omega + \sum_{l,\sigma} \frac{|V_{l\sigma}|^2}{\omega - \epsilon_{l\sigma}} \end{pmatrix}.
\]

The Green's function \( G_\sigma (\omega) \) of the impurity model in Eq. (6) is obtained by the exact diagonalization method\(^8\), and thus the self-energy matrix is directly extracted by Dyson equation,

\[
\Sigma_\sigma (\omega) = (G_0^\alpha (\omega))^{-1} - G_\sigma (\omega)^{-1}.
\]

Therefore, the on-site Green's function reads,

\[
G_\sigma (\omega) = \int_{-\infty}^{\infty} \frac{\rho_0 (\epsilon)}{\omega + \mu - \epsilon - \Sigma_\sigma (\omega)} \, d\epsilon.
\]

Eq. (10) is the first self-consistent equation for the ELDMFT. To satisfy the DMFT self-consistent equation (Eq. (9)) in the low frequencies and match the features of the central quasiparticle peak, Potthoff introduced the second self-consistent equation\(^9\),

\[
V^2 = Z M_2^{(0)}.
\]

with \( M_2^{(0)} = \int d c e^2 \rho_0 (\epsilon) \). For a metal, \( Z \) denotes the quasi-particle weight, which represents the single particle excitation near the Fermi surface of the metal. As \( Z \) approaches zero, the single particle excitation vanishes, indicating the occurrence of MIT. The results for the single-band Hubbard model are in good agreement with other numerical techniques\(^9\).

To study the two-orbital Hubbard model, we introduce four bath parameters \( (\epsilon_{\alpha}, \epsilon_{\beta}, V^\alpha, \text{ and } V^\beta) \) to describe the paramagnetic phase of the bath, and thus four self-consistent conditions are introduced to fix them accordingly,

\[
\begin{align*}
\rho_{\gamma_{\text{imp}}} (\epsilon) &= n_{\gamma}, \\
V_{\gamma}^2 &= Z M_2^{(0)}_{\gamma} \quad (\gamma = \alpha, \beta),
\end{align*}
\]

with \( M_2^{(0)}_{\gamma} = \int d c e^2 \rho_0 (\epsilon)_{\gamma} \). These equations renormalize the high- and low-frequency regimes of the original self-consistency conditions in an integral, qualitative form, and are thus well motivated.

IV. THEORETICAL RESULTS

In studying the orbital fluctuations and MIT of the two-orbital Hubbard model at finite temperature by the ELDMFT method, we choose the original diagonal hopping as the unit, \( t_{\text{lat}} = t_{bb} = 1 \), and mainly consider two different conditions: one is the spin symmetric case with \( 2J = U = U' \), and the other one is the case with the parameters \( J \) and \( U' \) being independent. Without special note being made, the temperature in this paper is \( k_B T = 1/\beta = 1/16 \). We restrict the present study to the paramagnetic phase, the other possible magnetic ordered phases shall be encountered latter on. In the following studies, we focus on the systems with half filling (\( n = 2 \)) and quarter filling (\( n = 1 \)), respectively.
of the single-band Hubbard model by the full DMFT the system is a good metal. This result resembles to that quasiparticle band near the Fermi energy, indicating that quasiparticle spectra exhibit three distinct features: the For the systems with finite interaction in the half-filling systems. Theoretical parameters are $U=4$, $J=0$ and $t_{ab}=0$.

A. Half filling cases

The two-orbital Hubbard model reduces to two independent single-band Hubbard models at $t_{ab}=U'=J=0$. For the symmetric case with half filling $n=2$, the MIT is observed at the critical Coulomb interaction $U_c \approx 6.0$, which is consistent with the Potthoff’s result. We now consider the systems with $t_{ab}=J=0$ and $U=4$, and study the effect of the interorbital Coulomb interaction on the MIT and orbital fluctuations.

The DOS for the systems with $U'=0.0$, 2.0, 4.0, 4.7 and 5.0 are shown in Fig. 1. At $U'=0$ we find that the quasiparticle spectra exhibit three distinct features: the broad upper and lower Hubbard bands and the dominant quasiparticle band near the Fermi energy, indicating that the system is a good metal. This result resembles to that of the single-band Hubbard model by the full DMFT. For the systems with finite $U'$, the spectral characters in the regime of $U'<U'_c$ is quite different from that in $U'>U'_c$, here $U'_c$ denotes the MIT critical point. In the regime of $U'<U'_c$, our results clearly demonstrate that the interorbital correlations remove the orbital degeneracy of the Hubbard bands and further split the upper and lower Hubbard bands into four Hubbard subbands. Approaching the critical point $U'_c$, the DOS near the Fermi surface decreases very quickly with the increase of $U'$, as shown in Fig. 1. Large $U'$ suppresses the quasiparticle excitation near $E_F$, and as a result it leads to the MIT at the critical point of $U'_c=4.75$. What we obtained is in agreement with the previous results by Rozenberg and Koga et al., confirming the validity and the reliability of the present ELDMFT method.

To learn the effects of the orbital fluctuations more better, we also study the influence of thermal fluctuation on MIT at low temperature $\beta=32$ and high temperature $\beta=8$ by keeping the other parameters fixed. Considerable influence of the thermal fluctuations are found, and the corresponding upper critical points of MIT are $U'_c=5.0$ for $\beta=32$ and $U'_c=4.45$ for $\beta=8$, respectively. We do not consider a lower critical point of MIT with $U'>U$, presumptively unphysical. Obviously, the interorbital interaction drives the MIT at high temperature more easier than at low temperature, since the combination of the quantum and the thermal fluctuations drives the paramagnetic metal transition to the paramagnetic insulator more easily.

Next we study the influence of interorbital hopping on the orbital fluctuations and the MIT in the system with half filling. The dependences of the quasiparticle weights on the interorbital interaction in the cases with $t_{ab}=0.5$ and $t_{ab}=1.0$ are shown in Fig. 4. In Fig. 2 the two dashed lines with open and filled circles represent the quasiparticle weight $Z$ of the effective orbitals $\alpha$ and $\beta$ as $t_{ab}=0.5$ respectively, while the two solid lines with open and filled triangles are the corresponding results for $t_{ab}=1.0$. For the convenience of comparison, the result of the degenerate bands as $t_{ab}=0$ (dotted line) is also shown. Firstly, we find that the difference between the two effective bands $\alpha$ and $\beta$ is significant as the interorbital interaction drives the MIT at high temperature more easier than at low temperature, since the combination of the quantum and the thermal fluctuations drives the paramagnetic metal transition to the paramagnetic insulator more easily.

FIG. 1: Evolution of the DOS with the interorbital Coulomb interaction in the half-filling systems. Theoretical parameters are $U=4$, $J=0$ and $t_{ab}=0$.

FIG. 2: Quasiparticle weights $Z$ (dotted line), $Z_{\alpha}$ (filled symbols) and $Z_{\beta}$ (open symbols) as the function of $U'$ at half filling with different interorbital hopping $t_{ab}$. The other parameters are: $U=4$ and $J=0$. 

$\omega - \mu$

$\text{Im}G(\omega+i\epsilon)/\pi$

-8 -6 -4 -2 0 2 4 6 8

$\omega - \mu$

$\text{Im}G(\omega+i\epsilon)/\pi$

-8 -6 -4 -2 0 2 4 6 8

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$\omega - \mu$

$\text{Im}G(\omega+i\epsilon)/\pi$

-8 -6 -4 -2 0 2 4 6 8

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$\text{Im}G(\omega+i\epsilon)/\pi$

-8 -6 -4 -2 0 2 4 6 8

$\omega - \mu$

$\text{Im}G(\omega+i\epsilon)/\pi$

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-8 -6 -4 -2 0 2 4 6 8

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-8 -6 -4 -2 0 2 4 6 8

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$\text{Im}G(\omega+i\epsilon)/\pi$

-8 -6 -4 -2 0 2 4 6 8

$\omega - \mu$

$\text{Im}G(\omega+i\epsilon)/\pi$

-8 -6 -4 -2 0 2 4 6 8

$\omega - \mu$

$\text{Im}G(\omega+i\epsilon)/\pi$

-8 -6 -4 -2 0 2 4 6 8

$\omega - \mu$

$\text{Im}G(\omega+i\epsilon)/\pi$

-8 -6 -4 -2 0 2 4 6 8

$\omega - \mu$

$\text{Im}G(\omega+i\epsilon)/\pi$

-8 -6 -4 -2 0 2 4 6 8

$\omega - \mu$

$\text{Im}G(\omega+i\epsilon)/\pi$

-8 -6 -4 -2 0 2 4 6 8

$\omega - \mu$

$\text{Im}G(\omega+i\epsilon)/\pi$

-8 -6 -4 -2 0 2 4 6 8

$\omega - \mu$

$\text{Im}G(\omega+i\epsilon)/\pi$

-8 -6 -4 -2 0 2 4 6 8

$\omega - \mu$

$\text{Im}G(\omega+i\epsilon)/\pi$

-8 -6 -4 -2 0 2 4 6 8

$\omega - \mu$

$\text{Im}G(\omega+i\epsilon)/\pi$
of the \(\alpha\)-band to the metallic properties at \(t_{ab} = 1.0\) is small, the properties of the system is mainly controlled by the \(\beta\)-band, implying that the orbital excitation and orbital fluctuation are large and dominant in the metallic phase. Secondly, the MIT critical point of the system is \(U'_c = 4.5\) for \(t_{ab} = 1.0\), obviously smaller than \(U'_c = 4.7\) for \(t_{ab} = 0.5\). The interorbital hopping broadens the bandwidth of \(\beta\)-band and narrows that of \(\alpha\)-band, and more electrons transfer to the \(\beta\)-band with the increase of \(t_{ab}\). As we have obtained above, the interorbital interaction suppresses the quasiparticle excitation near Fermi surface in the cases without off-diagonal hopping. Similarly, the interorbital hopping also depresses the quasiparticle weight of the \(\alpha\)-band by narrowing its bandwidth. As a result, the MIT is more easier to happen when \(t_{ab}\) becomes large in the paramagnetic half-filling system.

Apart from the effects of interorbital hopping and Coulomb correlation on MIT, our calculations also show that the Hund’s coupling \(J\) plays a very important role in MIT. We find that for \(t_{ab}=0\), the behaviors of \(Z\) for the \(J \neq 0\) case are quite different from the \(J = 0\) case. There are two MIT critical points with \(J_c = 0.55\) and \(J'_c = 0.25\) (unphysical) for the spin rotation symmetry case \(2J = U - U'\), and the metallic phase can exist only in a narrow region \(J_c < J < J_c\), which is in agreement with Pruschke and Bulla’s result. The large Hund’s coupling \(J\) suppresses spin flip excitation, and as \(J\) increases the exchange splitting pushes the \(\alpha\)-bands higher with respect to the \(\beta\)-bands, resulting in the system to transition to the insulating phase. Therefore the role of the Hund’s coupling is similar to the on-site Coulomb Interaction \(U\), driving the MIT by preventing the electrons from double occupation. Meanwhile, instead of excluding the double occupation, the interorbital Coulomb correlation drives the MIT by removing the orbital degeneracy of the two Hubbard bands.

Further more we study the interplay between the interorbital hopping and the Hund’s coupling in driving the MIT. We show the dependence of the quasiparticle weight on the Hund’s coupling in the system with \(2J = U - U'\) and \(t_{ab} = 1.0\) in Fig. 3(b). For the convenience of comparison, the result of the degenerate bands as \(t_{ab} = 0\) (dotted line) is also shown. When \(J\) is small, the system is metallic, and the quasiparticle weight of the effective \(\beta\)-band is considerably larger than that of \(t_{ab} = 0\). Since the hopping channels of the former is more than the latter, the charge transfer between two different orbitals leads to more considerable orbital quantum fluctuation than that in \(t_{ab} = 0\). That means the presence of \(t_{ab}\) broads the conduction bandwidth and increases the DOS of the \(\beta\)-band, and thus enhances the quasiparticle weight \(Z_\beta\), as shown in Fig. 2. When \(J\) becomes large, a lot of spin flip excitation is suppressed, the system undergoes a MIT, corresponding defines a critical value \(J_c\). The MIT critical point \(J_c\) as a function of the interorbital hopping is shown in Fig. 3(b). Obviously the increase of the interorbital hopping enhance the orbital fluctuations, and contributes more excitations near the Fermi surface. As a result, more large \(J_c\) are needed to drive the MIT, and thus the MIT critical value \(J_c\) increases with the lift of the interorbital hopping.

B. Quarter filling cases

The two-orbital Hubbard model with quarter filling is appropriate to describe some important strongly correlated materials with twofold degenerate orbital degree of freedom, such as the hole-type compound \(KCuF_3\) and electron-type compound \(LaNiO_3\). To our knowledge, the strongly correlated systems with quarter filling have not been given enough attention by the conventional DMFT yet. In this subsection we study the two-orbital Hubbard model with quarter filling, we take large intraorbital interactions \((U = 8\) and 12), and assume the relationship \(U = U' + 2J\).

First we consider the case with \(t_{ab} = 0\). The evolution of the DOS with the Hund’s coupling \(J\) \((J = 0.0, 0.5, 1.0\) and 2.0) for \(U=8\) and 12 are shown in Fig. 4. The Hund’s coupling strongly modifies the orbital subbands. At \(J=0\), the presence of the interorbital and intraorbital Coulomb interactions \(U'\) and \(U\) removes nearly a half of the quasiparticle weight in the lower Hubbard band to the upper Hubbard band, and the lowest subband is thus almost filled up and the residue quasiparticle weight near the Fermi surface is very small. Therefore the system with \(J = 0\) at quarter filling is a bad metal or an insulator. In the system with \(U=8\), the DOS at the Fermi level increases gradually as \(J\) increases; as \(J > 0.5\) the system transits from bad metallic or insulating phase to metallic phase. Meanwhile, the increasing of Hund’s coupling can further split the energy bands into many subbands as shown in Fig. 4. It can be seen clearly that in the quarter-filling case, the influence of the Hund’s coupling \(J\) on
MIT is different to the half-filling case: in the former the increase of the Hund’s coupling indicates the reduction in the interorbital repulsion $U’$ and the enhancement of the ferromagnetic fluctuation, therefore the metallic phase is in favor; however in the latter, the increase of $J$ leads the system to transit from metal to insulator since the spin flip excitation is suppressed and the quasiparticle weight near Fermi surface greatly declines. On the other hand, for larger intraorbital Coulomb interaction $U = 12$, the system is always an insulator with the increasing of $J$ up to 2. As $J$ approaches to 2, the edge of the upper Hubbard bands is gradually shifted to the Fermi energy, indicating the MIT will occur at $J_e \approx 2$.

From Fig.4 one can see the striking difference of the quasiparticle weights between the systems with $U = 8$ and with $U=12$. At $U = 8$, the quasiparticle weight $Z$ monotonously increases with the lift of $J$, implying that the system is a good metal in the absence of the interorbital hopping. However, for the system with $U = 12$, the quasiparticle weight $Z$ is very small, and the total weight is 0.031 as the Hund’s coupling $J$ increases to 2. The double occupancy $D$, as one expects, decreases with the increasing of the intraorbital repulsion. At $U = 8$, the maximum magnitude of the double occupancy is about $D_m = 0.0012$. While at $U = 12$ the double occupancy $D_m$, about 0.0001, is negligible. Such strong single occupation and large Coulomb interaction in the System with quarter filling suggests that the system with $U=12$ is in the antiferromagnetic insulating phase, while the system with $U=8$ is a paramagnetic or ferromagnetic metal. We will discuss the cases with spin symmetry broken in a future paper.

In the two-orbital Hubbard model at quarter filling, it is very interesting how the interorbital hopping affects the MIT. Here we mainly study the MIT in the systems with $U=8$ and $J=1.0$. The evolution of the DOS of the $\alpha$- and $\beta$-bands with the interorbital hopping is shown in Fig.4. At small $t_{ab}$ both $\alpha$- and $\beta$-bands cross the Fermi surface, indicating that the system is metallic. Significantly different from the half-filling cases, the further increase of the interorbital hopping greatly reduces the quasiparticle states near the Fermi surface for both the $\alpha$- and $\beta$-bands. One finds that in the $\alpha$-band most states move to the high energy regime above the Fermi level, while in the $\beta$-band, most states move to the low energy regime below the Fermi level, thus the asymmetry of the DOS is smaller than the half-filling cases.

In the presence of the strong Coulomb correlation, the system with symmetric orbitals tends to break the orbital symmetry to lower the ground state energy and form long-range orbital order. The orbital order parameter, $<\mathbf{T}>$, is usually defined as the average of the pseudospin operator $\mathbf{T} = \sum_{ab} C_{ia}^{\dagger} \sigma_{ab} C_{ib}$, with $\sigma$ being the Pauli matrix, representing the orbital polarization of the electrons occupation in the two orbitals. In the quarter-
filling system with $U=12$, we calculate the three components of $T$, $T^x$, $T^y$, and $T^z$, and the results are shown in Fig. 6 From the preceding study, we have found that in the absence of the interorbital hopping the system with large interorbital interaction is in a para-orbital phase. Switching on the off-diagonal or interorbital hopping, we find that the symmetry of the orbital space is broken, and the $x$-component of orbital order parameter $T^x$ is finite, while the $z$-component $T^z$ is always zero. This result is also confirmed by the self-consistent mean-field method for the effective spin-orbital superexchange interaction in the limit of large $t_{ab}^{27}$. In addition, large interorbital hopping results in strong orbital fluctuations, and large Hund’s coupling favors the ferro-orbital occupation, the competition of these factors favors the orbital polarization in the $x$-direction, leads to the orbital order parameter $T$ lying in the $x$-direction, and $T^x$ increases with the increasing of the interorbital hopping integrals and the Hund’s coupling $J$, as seen in Fig. 6.

In the absence of the interorbital hopping $t_{ab}$, the interorbital Coulomb interaction $U'$ and the Hund’s coupling $J$ adjust the relative positions of the four subbands; though the electrons occupying one orbital configuration is favorable in energy, no electron can transfer between these orbitals, and the orbital occupations of the electrons in the two orbitals are the same, giving rising to orbital disordered phase. In the presence of $t_{ab}$, the electrons can transfer between orbitals and occupy the most favorable orbital configuration in energy, and therefore the orbital ordering can establish, as we find in the present results. It is worthy of noting that we only consider a possible ferro-orbital phase, while more complicated orderings are out of reach from the present single-impurity DMFT study. Further study will be addressed in the future paper.

V. CONCLUSIONS

From the proceeding study it is clear that the interorbital hopping plays an important role in the MIT of the two-orbital degenerate Hubbard models. The presence of the interorbital hopping not only enhances the orbital fluctuations and quasi-particle excitation near Fermi surface, but also leads to some unusual results. At half filling, since more and more electrons transfer from one orbital to the another, the critical value of the interorbital Coulomb interaction $U''$ for MIT decreases with the increase of the interorbital hopping; while the critical value of the Hund’s coupling $J_c$ for MIT lifts with the increase of $t_{ab}$. In the systems with $2J = U - U'$, metallic phase can exist in a very narrow region with the variation of $J$, since both intra- and interorbital Coulomb interactions, $U$ and $U'$, split the Hubbard subbands and drive the MIT. At quarter filling, the increase of $J$ may lead to insulator-metal transition, and this role in MIT is completely contrary to that in the half-filling case; and the increase of the interorbital hopping may also drive the MIT due to strong orbital fluctuation, and leads to weak ferro-orbital ordering in the system with large onsite Coulomb interaction.

Meanwhile, the interorbital Coulomb correlation also drives the MIT by expanding the separation of two orbital Hubbard subbands both in half- and quarter-filling systems. In the present paper we mainly concentrate our study on the paramagnetic and para/ferro-orbital phase, little attention is paid to complicated spin and orbital orderings. At present, it is not possible to compare the theoretical results with the experimental results in candidate compounds KCuF$_3$ and LaNiO$_3$, since more complicated spin and orbital orders are involved in these two realistic compounds, thus more than two impurities must be considered in the study, beyond the single-impurity DMFT theory.

Recently it receives great interest whether the wide and the narrow Hubbard subbands exhibit MIT separately, i.e. the orbital-selective Mott transition (OSMT) in two-orbital Hubbard model. Obviously our results do not show that there exist such Mott transition in the presence of interorbital hopping $t_{ab} \neq 0$. While in the absence of $t_{ab}$, it is not difficult to expect the existence of OSMT since the charge transfer between orbitals is forbidden, and the role of the $a$-band is to exert an effective potential on the $b$-band and to change the chemical potential of the subband, therefore the MIT of the $a$-band and the $b$-band occur separately. On the contrary for $t_{ab} \neq 0$ there exists charge transfer between the two orbitals, and the MIT will occur at the same critical points for both bands. While for the system involving two subbands of different bandwidths and omitting the interorbital hopping, we find in the new quasi-particle representation in Fig. 3a, the OSMT seems happen as the Hund’s coupling is large enough. Further studies are deserved to investigate the OSMT in the whole parameters space to determine the phase diagram of the two-band Hubbard model.
model with nondegenerate subbands.

In summary, utilizing the extended linearized DMFT, we find in the two-orbital Hubbard models with the interorbital hopping and half filling, the increase of Hund’s coupling drives the MIT; on the other hand, the quarter-filling two-orbital systems remain metallic due to large orbital fluctuations. The systems with only intraorbital hopping favors metallic and orbital liquid phase; as a contrast, there exists the long-range orbital ordering in the quarter-filling two-orbital systems with interorbital hopping and large U.

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1 M. Imada, A. Fujimori and Y. Tokura, Rev. Mod. Phys., 70, 1039 (1998).
2 Y. Tokura, A. Urushibara, Y. Moritomo, T. Arima, A. Asamitsu, G. Kido, and N. Furukawa, J. Phys. Soc. Jpn. 63, 3931 (1994).
3 S. A. Carter, T. F. Rosenbaum, P. Metcalf, J. M. Honig, and J. Spalek, Phys. Rev. B 48, R16841 (1993).
4 Y. Maeno, H. Hashimoto, K. Yoshida, S. Nishizaki, T. Fujita, J. G. Bednorz, and F. Lichtenberg, Nature (London) 372, 532 (1994).
5 S. Nakatsuji and Y. Maeno, Phys. Rev. Lett. 84, 2666 (2000).
6 S. Ishihara and S. Maekawa, Phys. Rev. Lett. 80, 3799 (1998).
7 L. Paolasini, C. Vettier, F. de Bergevin, F. Yakhou, D. Mannix, A. Stunault, W. Neubeck, M. Altarelli, M. Fabrizio, P. A. Metcalf, and J. M. Honig, Phys. Rev. Lett. 82, 4719 (1999).
8 A. Georges, G. Kotliar, W. Krauth and M. J. Rozenberg, Rev. Mod. Phys. 68, 13 (1996).
9 M. Jarrell, Phys. Rev. Lett. 69, 168 (1992).
10 M. J. Rozenberg, X. Y. Zhang, and G. Kotliar, Phys. Rev. Lett. 69, 1236 (1992).
11 A. Georges and W. Krauth, Phys. Rev. Lett. 69, 1240 (1992).
12 M. Caffarel and W. Krauth, Phys. Rev. Lett. 72, 1545 (1994).
13 M. J. Rozenberg, G. Moeller, and G. Kotliar, Mod. Phys. Lett. B 8, 535 (1994).
14 Q. Si, M. J. Rozenberg, G. Kotliar, and A. E. Ruckenstein, Phys. Rev. Lett. 72, 2761 (1994).
15 R. Bulla, A. C. Hewson, and Th. Pruschke, J. Phys: Condens. Matter 10, 8365 (1998).
16 R. Bulla, Phys. Rev. Lett. 83, 136 (1999).
17 R. Bulla, T. A. Costi, and D. Vollhardt, Phys. Rev. B 64, 045103 (2001).
18 R. Bulla and M. Potthoff, Eur. Phys. J. B 13, 257 (2000).
19 M. Potthoff, Phys. Rev. B 64, 165114 (2001).
20 M. J. Rozenberg, Phys. Rev. B 55, R4855 (1997).
21 Y. Ono, M. Potthoff, and R. Bulla, Phys. Rev. B 67, 035119 (2003).
22 A. Koga, Y. Imai, and N. Kawakami, Phys. Rev. B 66, 165107 (2002); A. Koga, N. Kawakami, T. M. Rice, and M. Sigrist, Phys. Rev. Lett. 92, 216402 (2004).
23 A. Liebsch, Phys. Rev. Lett. 91, 226401 (2004).
24 R. Sato, T. Ohashi, A. Koga, and N. Kawakami, J. Phys. Soc. Jpn. 73, 1864 (2004).
25 T. Pruschke and R. Bulla, cond-mat/0411186.
26 D. I. Khomskii and M. V. Mostovoy, J. Phys. A 36, 9197 (2003); M. V. Mostovoy and D. I. Khomskii, Phys. Rev. Lett. 92, 167201 (2004).
27 D.-M. Chen and Liang-Jian Zou, unpublished.
28 L. de’ Medici, A. Georges and S. Biermann, cond-mat/0503764; R. Arita and K. Held, cond-mat/0503764; A. Liebsch, cond-mat/0505393.