Evolution between two orbital-selective Mott phases driven by interorbital hopping

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The effect of interorbital hopping on the orbital selective Mottness in a two-band correlation system is investigated by using the dynamical mean-field theory with the Lanczos method as impurity solver. We construct the phase diagram of the two-orbital Hubbard model with interorbital hopping ($t_{12}$), where the orbital selective Mott phases (OSMP) show different evolution trends. We find that the negative interorbital hopping ($t_{12} < 0$) can enhance the OSMP regime upon tuning the effective bandwidth ratio. On the contrary, for the cases with positive interorbital hopping ($t_{12} > 0$), the OSMP region becomes narrow with the increase of orbital hybridization until it disappears. It is also shown that a new OSMP emerges for a large enough positive interorbital hopping, owing to the role exchange of wide and narrow effective orbitals caused by the large $t_{12}$. Our results are also applicable to the hole-overdoped Ba$_2$CuO$_{2-\delta}$ superconductor, which is an orbital-selective Mott compound at half-filling.

I. INTRODUCTION

The orbital selective Mottness is helpful for exploring the nature of strong correlation systems due to its discovery in some transition metal compounds, such as Ca$_{2-x}$Sr$_x$RuO$_4$, transition metal dichalcogenides, and Fe-based superconductors. When the carries on a subset of orbitals get localized while the others remain itinerate, the orbital-selective Mott transition (OSMT) happens. The simplest theoretical realization of the OSMT occurs in the two-orbital Hubbard model. The dynamical mean-field theory (DMFT) is a powerful framework to study the correlation-driven phase transitions in the one-band Hubbard model, and its extension to the two-orbital Hubbard model is also effective.

Several theoretical approaches have been used to build the impurity solver of the DMFT procedure, such as quantum Monte Carlo simulations (QMC), renormalization-group theory, and slave-variable representations, etc. For the multi-orbital extensions combined with the DMFT algorithm, each solver has its limitations. The QMC method faces the sign problem in the doped fermion system, renormalization-group theory cannot solve the one-band model well but it is hard to be expanded to multi-band system, and slave-variable representations cannot treat the interaction effect accurately. For the multi-orbital correlation system, the DMFT with the Lanczos method as impurity solver can accurately treat the multi-orbital correlations including the intraorbital interaction $U$, interorbital correlation $U'$, and Hund’s rule coupling $J_H$. But the off-diagonal Green’s function induced by the interorbital hopping will add complexity of self-consistency and need a lot of computing resources.

The interorbital hoppings induce strong orbital hybridization, which is crucial in many multi-band correlated transition-metal compounds. However, it is a tremendous challenge to solve the extend multi-band Hubbard model which also has the off-diagonal Hamiltonian induced by the interorbital hopping. We introduce the canonical transformation to diagonalize the tight-binding part of the extended two-orbital Hubbard Hamiltonian, and the effective orbitals obtained can reflect the effect of orbital hybridization in the multi-orbital correlation system. To comprehensively study the cooperative effects of multi-orbital interactions, we also develop the Lanczos method as the DMFT impurity solver. Comparing with the previous modified DMFT procedure, our present work can treat the Coulomb interactions and Hund’s rule coupling strictly, especially the critical points of the phase transitions can be determined accurately. We use the DMFT with Lanczos solver to study the electron correlation effect of two-orbital Hubbard model with sign convertible interorbital hopping, and we find two OSMP regions in the phase diagram. We also apply our results to analyze the recently discovered two-orbital superconductor Ba$_2$CuO$_{4-\delta}$. We find the orbital-select Mott transition in the half-filled Ba$_2$CuO$_{4-\delta}$.

This paper is organized as follows. In Sec. II we introduce the canonical transformation used for the two-orbital Hubbard model including interorbital hopping. In Sec. III we explain the numerical method adopted to solve the transformed effective model: the DMFT approach with Lanczos solver. In Sec. IV we present the results of the orbital-selective Mott transitions in the two-orbital Hubbard model, and discuss the cooperate effect of electron correlation and interorbital hopping in the multi-band correlation system. In Sec. V we apply the method to the two-orbital superconductor Ba$_2$CuO$_{3.5}$ and introduce our finding. The principal conclusions of this paper are summarized in Sec. VI.
II. CANONICAL TRANSFORMATION

The two-orbital Hamiltonian consists of two parts: tight-binding Hamiltonian $H_t$ and interaction Hamiltonian $H_I$, where the tight-binding Hamiltonian $H_t$ reads

$$H_t = -\sum_{(ij)\sigma} t_{ij\sigma} d_{ij\sigma}^\dagger d_{ij\sigma} - \sum_{(ij)\sigma} t_{ij\sigma'} d_{ij\sigma}^\dagger d_{ij\sigma'},$$

$$-\mu \sum_{i\sigma} d_{i\sigma}^\dagger d_{i\sigma},$$

and interaction Hamiltonian $H_I$ is given by

$$H_I = \frac{U}{2} \sum_{i\sigma} n_{i\sigma} n_{i\sigma'} + \sum_{i,l\sigma} (U' - \delta_{\sigma\sigma'} J_H) n_{i\sigma} n_{il\sigma'},$$

$$+ \frac{J_H}{2} \sum_{i,l,\sigma} d_{il\sigma}^\dagger d_{il\sigma'} d_{i\sigma} d_{i\sigma'},$$

$$+ \frac{J_H}{2} \sum_{i,l,\sigma} d_{il\sigma}^\dagger d_{il'\sigma'} d_{i\sigma} d_{i\sigma'},$$

where $d_{ij\sigma}^\dagger$ ($d_{i\sigma}$) is an electron creation (annihilation) operator for orbital $i$ at site $j$ with spin $\sigma$, and $(ij)$ represent nearest neighbor (NN) sites. $t_l$ denotes the NN intraorbital hopping and $t_{ij}$ denotes the NN interorbital hopping. $U$ ($U'$) corresponds to the intraorbital (interorbital) interaction, and $J_H$ is the Hund’s rule coupling.

We introduce two effective decoupled orbitals $\alpha$ and $\beta$ by a canonical transformation, that decoupling the interorbital hopping

$$d_{i1\sigma} = u_{\alpha i\sigma} + v_{\beta i\sigma},$$

$$d_{i2\sigma} = -v_{\alpha i\sigma} + u_{\beta i\sigma},$$

with

$$u = \frac{1}{\sqrt{2}} \left( 1 + \frac{(t_{11} - t_{22})^2}{(t_{12})^2 + (t_{11} - t_{22})^2} \right)^{1/2},$$

$$v = \frac{1}{\sqrt{2}} \left( 1 - \frac{(t_{11} - t_{22})^2}{(t_{12})^2 + (t_{11} - t_{22})^2} \right)^{1/2},$$

where $\alpha_{i\sigma}$ and $\beta_{i\sigma}$ are fermion annihilation operators for the two newly introduced $\alpha$ and $\beta$ orbitals. The values of parameters $u$ and $v$ determined by Eq. (3) will make the interorbital hopping between the $\alpha$ and $\beta$ orbitals vanish.

The canonical transformation, the original two-orbital Hamiltonians shown in Eq. (1) and Eq. (2) are converted into an effective two-orbital Hamiltonian $H_{t,\text{eff}}$, which consists of the tight-binding part $H_{t,\text{eff}}^I$ and the interaction part $H_{I,\text{eff}}^I$ for the two effective orbitals as:

$$H_{t,\text{eff}}^I = -\sum_{(ij)\sigma} \left( t_{i\alpha j\sigma} \alpha_{i\sigma}^\dagger \alpha_{j\sigma} + t_{i\beta j\sigma} \beta_{i\sigma}^\dagger \beta_{j\sigma} \right),$$

$$-\mu \sum_{i\sigma} \left( \alpha_{i\sigma}^\dagger \alpha_{i\sigma} + \beta_{i\sigma}^\dagger \beta_{i\sigma} \right),$$

and

$$H_{I,\text{eff}}^I = \frac{U}{2} \sum_{i\sigma} (n_{i\alpha\sigma} n_{i\beta\sigma} + n_{i\beta\sigma} n_{i\beta\sigma}^\dagger)$$

$$+ \sum_{i\sigma\sigma'} \left( U' - \delta_{\sigma\sigma'} J_H \right) n_{i\alpha\sigma} n_{i\beta\sigma'},$$

$$+ \frac{J_H}{2} \sum_{i,\sigma} \left( \alpha_{i\sigma}^\dagger \alpha_{i\sigma}^\dagger \beta_{i\sigma} \beta_{i\sigma} + \beta_{i\sigma} \beta_{i\sigma} ^\dagger \alpha_{i\sigma} \alpha_{i\sigma}^\dagger \right).$$

The hopping parameters in the effective model are expressed as

$$t_{\alpha} = t_1 u^2 + t_2 v^2 - t_{12} uv,$$

$$t_{\beta} = t_1 v^2 + t_2 u^2 + t_{12} uv,$$

according to Eq. (3). The effective interaction $H_{I,\text{eff}}^I$ in Eq. (6) has a formulation similar to the original interaction terms when the spin rotation symmetry is kept with $U = U' + 2J_H$.

III. DYNAMICAL MEAN-FIELD THEORY

The canonical transformation decouples the hybridization of the two orbitals, so that the effective model is comparably easier to be solved by DMFT. In the framework of DMFT, we map the lattice Hamiltonian onto an impurity model with fewer degrees of freedom,

$$H_{\text{imp}} = \sum_{m\sigma} \left( c_{\gamma m\sigma}^\dagger c_{\gamma m\sigma} c_{\gamma m\sigma} + c_{\gamma m\sigma}^\dagger c_{\gamma m\sigma} c_{\gamma m\sigma}^\dagger \right)$$

$$+ \sum_{m\sigma} \left( V_{\gamma m\sigma} \alpha_{m\sigma} + \alpha_{m\sigma}^\dagger \right),$$

$$+ \sum_{m\sigma} \left( V_{\gamma m\sigma} \beta_{m\sigma} + \beta_{m\sigma}^\dagger \right),$$

$$-\mu \sum_{m\sigma} \alpha_{m\sigma}^\dagger \alpha_{m\sigma} - \mu \sum_{m\sigma} \beta_{m\sigma}^\dagger \beta_{m\sigma},$$

$$+ H_{t,\text{eff}}^I (\alpha, \beta),$$

where $c_{\gamma m\sigma}$ ($c_{\gamma m\sigma}^\dagger$) denotes the creation (annihilation) operator for the ‘environmental bath’ lattice of orbital $\gamma$ ($\gamma = \alpha, \beta$), $c_{\gamma m\sigma}$ denotes the energy of the $m$-th ‘environmental bath’ of orbital $\gamma$, and $V_{\gamma m\sigma}$ represents the coupling between the orbital $\gamma$ of the ‘impurity site’ and its ‘environmental bath’. We take the bath size $n_b = 3$ in our work. It has been proved that the critical points of OSMT calculated by DMFT with Lanczos solver in two-orbital Hubbard model29 are almost the same when $n_b \geq 3$.

By using the canonical transformation, the two orbitals are nonhybridized. Thus, the Green’s function and self-energy are all diagonal with respect to the orbital, so that
we can calculate the Green’s function and the parameters $V_{\gamma\sigma}$ and $\epsilon_{m\sigma}^\gamma$ independently. The Weiss function of the impurity model can be obtained through the parameters of the impurity Hamiltonian by

$$G^{-1}_{\gamma\sigma}(i\omega_n) = i\omega_n + \mu - \varepsilon_\gamma - \sum_m \frac{(V_{m\sigma}^\gamma)^2}{i\omega_n - \varepsilon_{m\sigma}^\gamma}. \quad (9)$$

Employing the Lanczos solver, we can obtain the Green’s function $G^{(\gamma)}_{\text{imp}}$ and $G^{(\gamma)}_{\text{non}}$, which is expressed as

$$G^{(\gamma)}_{\text{imp}}(i\omega_n) = G^{(+)}_{\gamma}(i\omega_n) + G^{(-)}_{\gamma}(i\omega_n), \quad (10)$$

where

$$G^{(+)}_{\gamma}(i\omega_n) = \frac{\langle \phi_0 | \gamma^+ | \phi_0 \rangle}{i\omega_n - a_0^{(+)} - \frac{a_1^{(+)} a_2^{(+)} \cdot \cdot \cdot}{i\omega_n + a_0^{(-)} + \frac{a_1^{(-)} a_2^{(-)} \cdot \cdot \cdot}{i\omega_n + a_0^{(-)} + \frac{a_1^{(-)} a_2^{(-)} \cdot \cdot \cdot}}}} \quad (11)$$

and

$$G^{(-)}_{\gamma}(i\omega_n) = \frac{\langle \phi_0 | \gamma^- | \phi_0 \rangle}{i\omega_n + a_0^{(-)} - \frac{a_1^{(-)} a_2^{(-)} \cdot \cdot \cdot}{i\omega_n + a_0^{(-)} + \frac{a_1^{(-)} a_2^{(-)} \cdot \cdot \cdot}{i\omega_n + a_0^{(-)} + \frac{a_1^{(-)} a_2^{(-)} \cdot \cdot \cdot}}}}. \quad (12)$$

The DMFT simulate lattice model with impurity model through the self-consistent equation of impurity Weiss function and the noninteracting Green’s function of lattice model. Considering the semicircular DOS of the Bethe lattice, the on-site component of the Green’s function of each orbital $[G^{(\gamma)}_{\text{imp}}(i\omega_n) = \sum_k G^{(\gamma)}_{\sigma}(i\omega_n, k)]$ satisfies a simple self-consistent relation,

$$\left\{ g^{(\gamma)}_0(i\omega_n) \right\}^{-1} = i\omega_n + \mu - t_G^{2} G^{(\gamma)}_{\text{imp}}(i\omega_n) \quad (13)$$

where $g_0$ is the noninteracting Green’s function of lattice model. Adjusting the parameters $V_{m\sigma}^\gamma$ and $\epsilon_{m\sigma}^\gamma$ to make the impurity Weiss function $G_0$ equal with lattice model $g_0$, the process of DMFT is completed.

We calculate the orbital-resolved spectral density of the effective orbital $\gamma$ by

$$A_\gamma(\omega) = -\frac{1}{\pi} \text{Im} G^{(\gamma)}_{\sigma}(\omega + i\eta), \quad (14)$$

where $\eta$ is an energy broadening factor. The orbital-dependent quasiparticle weight is determined by the self-energy

$$Z_\gamma = (1 - \frac{\partial}{\partial \omega} \text{Re} \Sigma_\gamma(\omega + i\eta)|_{\omega=\theta})^{-1}. \quad (15)$$

IV. RESULTS AND DISCUSSIONS

We study the effects of interaction and interorbital hopping on phase transition in the extended two-orbital Hubbard model. The chemical potential $\mu$ is kept as $\mu = U/2 + U' - J_H/2$ to satisfy the particle-hole symmetry. We compare in Fig. 1 the quasiparticle weights for different interaction $U$ and interorbital hopping $t_{12}$. While $t_{12} = 0$, the quasiparticle weight $Z$ denotes that the critical interaction of metal-insulator transition (MIT) $U_{c\alpha} = 3.7$ for the wide effective orbital $\alpha$, and the critical interaction for the narrow effective orbital $\beta$ is $U_{c\beta} = 2.3$, indicating that the OSMP occurs when interaction $2.3 \leq U \leq 3.7$. The OSMP region of effective model narrows to $2.6 \leq U < 3.2$ when $t_{12} = 0.4$ as shown in Fig. 1, where the critical point of MIT for orbital $\alpha$ shifts to the weak interaction region and the narrow orbital critical interaction becomes strong. The positive interorbital hopping ($t_{12} > 0$) suppresses the region of OSMP by decreasing the difference of two effective orbital hopping integrals, i.e. $t_\beta/t_\alpha = 0.67$ according to Eq. (17), which is opposite to previous results for the negative interorbital hopping that enhances the OSMP.

Fig. 2 shows the details of spectral density evolution with increasing interaction $U$ for $t_{12} = 0.4$ when $t_2/t_1 = 0.4$ and $J_H = 0.25U$. At the condition of $U = 2.0$, there exist resonance peaks around the Fermi level for both effective orbital $\alpha$ [Fig. 2 (a)] and orbital $\beta$ [Fig. 2 (b)]. The finite spectral weights indicate that both effective orbitals are metallic, so that the system is in metal phase. When interaction $U = 3.0$, the spectral weight at the Fermi level of orbital $\alpha$ is finite [Fig. 2 (c)], but a Mott gap opens around the Fermi level in orbital $\beta$ [Fig. 2 (d)]. This is the typical characteristic of OSMP. Increasing interaction to $U = 4.0$, Mott gaps can be found in the spectral density of both bands in Fig. 2 (e) and (f), and then the system transforms into insulating phase.

We construct phase diagrams in the plane of interaction $U$ and hopping integral $t_2/t_1$ with different interorbital hopping in Fig. 3. In a two-orbital system without
interorbital hopping, as shown in Fig. 3 (a), the OSMP can exist for any hopping integral ratio except \( t_2/t_1 = 1 \) because of the effect of Hund’s rule coupling, and the OSMP region narrows with increasing \( t_2/t_1 \), which is consistent with the previous research on OSMP. When we introduce the interorbital hopping, the hopping ratio of two effective orbitals will increase, as a result the normal OSMP region (orange region) shrinks as shown in Fig. 3 (b) and (c) with \( t_{12} = 0.2 \) and \( t_{12} = 0.4 \) respectively. It is worth noting that a new OSMP (yellow region) appears and its region expands with the increasing interorbital hopping. In the new OSMP, the effective orbital \( \alpha \) translates into insulator while orbital \( \beta \) keeps in metal phase.

In order to exhibit the change of OSMP region directly, we show the \( t_{12} \) dependence of \( \Delta U_c \) in Fig. 3 (d). When \( t_{2}/t_1 = 0.1 \), \( \Delta U_c \) (orange square symbol) decreases as \( t_{12} \) increases, which denotes the normal OSMP region gradually shrinks under the effect of \( t_{12} \). Conversely, the rising blue curve denotes the new OSMP region expands with increasing \( t_{12} \) when \( t_{2}/t_1 = 1.0 \). The effective hopping integral ratio \( t_\beta/t_\alpha \) increases with increasing \( t_{2}/t_1 \) under the effect of interorbital hopping \( t_{12} \). When \( t_{12} = 0.2 \) and \( t_{2}/t_1 = 0.8 \), the effective orbital hopping \( t_\alpha = t_\beta = 0.70 \) according to Eq. (7). If \( t_{2}/t_1 > 0.8 \), \( t_\beta \) is greater than \( t_\alpha \), thus the new OSMP region appears in Fig. 3 (b). Correspondingly, \( t_\alpha = t_\beta = 0.80 \) when \( t_{12} = 0.4 \) and \( t_{2}/t_1 = 0.6 \). It causes the movement of intersection and the change of OSMP region in Fig. 3 (c).

Electronic structures of solid materials are complicated and various. The phase difference between the plane wave of electron in different orbitals may make the interorbital hopping integral be negative. Thus we extend the interorbital hopping to \(-0.8 \leq t_{12} \leq 1.0\), and construct the phase diagram under the effect of interorbital hopping in Fig. 4. Two interleaved OSMP regions separate the metal phase and insulator phase. At the region of \( t_{12} > 0 \), normal OSMP region decreases accompanying with increasing \( t_{12} \) until \( t_{12} = 0.6 \). It transforms into a new OSMP while \( t_{12} > 0.6 \). The physical mechanism is consistent with the Fig. 3 (b) and (c). Fig. 4 also shows the OSMT while \( t_{12} < 0 \), the normal OSMP region expands with the increasing \( |t_{12}| \) indicating negative interorbital hopping integral \( t_{12} \) is beneficial to normal OSMP. The interorbital hopping will increase the difference of two effective orbital hopping integrals if \( t_{12} < 0 \) according to Eq. (7), thus the multi-orbital character will be enhanced under the effect of correlation. As a result, the normal OSMP region enlarges in the phase diagram.

V. APPLICATION

In this section, we apply the extended DMFT in recently discovered superconductor Ba2CuO4−\( \delta \), which can be described with two-orbital Hubbard model. Based on the DFT-calculated band structure of the compressed half-filled Ba2CuO3.5 compound, the electronic states near the Fermi level consist primarily of the Cu \( d_{x^2−y^2} \) and \( d_{3z^2−r^2} \) orbitals. The model parameters of the tight-binding Hamiltonian \( H_t \) in Eq. (1) take the following val-

![FIG. 2: (Color online) Evolution of the orbital-resolved spectral density \( A(\omega) \) with the increasing Coulomb interaction \( U \) when \( t_{12} = 0.4 \), \( t_2/t_1 = 0.4 \) and \( J_H = 0.25U \). Left panels show the results of effective orbital \( \alpha \) and right panels are for effective orbital \( \beta \). The energy boarding factor in our calculation takes \( \eta = 0.05 \).](image1.png)

![FIG. 3: (Color online) Phase diagrams of the effective two-orbital Hubbard model with different interorbital hopping: (a) \( t_{12} = 0.0 \), (b) \( t_{12} = 0.2 \) and (c) \( t_{12} = 0.4 \), when \( J_H = 0.25U \). The black circles (red triangles) denote the critical points of MIT for effective orbital \( \alpha \) (\( \beta \)). (d) The \( t_{12} \) dependence of the difference between the critical interactions of the two effective orbitals (\( \Delta U_c = |U_{c\alpha} - U_{c\beta}| \)) for \( t_2/t_1 = 0.1 \) (orange square symbol) and \( t_2/t_1 = 1.0 \) (blue diamond symbol).](image2.png)
The orbital-dependent quasiparticle weight $Z$ as a function of the interaction $U$ when $J_H = 0.25U$ is shown in Fig. 5 (a). According to quasiparticle weight $Z$, the two-orbital system is metallic when $U < 2.1$ eV, and it transforms into insulator while $U \geq 2.3$ eV. A narrow OSMP region exists within $2.1$ eV $\leq U < 2.3$ eV, in which the wide $\alpha$ band is metallic and the narrow $\beta$ band behaves insulating. Fig. 5 (b) (c) and (d) reveal the effects of interaction $U$ on the orbital-resolved spectrum $A(\omega)$ for both the effective $\alpha$ and $\beta$ bands in Ba$_2$CuO$_{3.5}$ with $J_H = 0.25U$. When the interaction is weak, such as $U = 1.0$ eV, the spectral weights at the Fermi level are finite for both bands, as shown in Fig. 5 (b), indicating a metallic phase for the two-orbital system. With increasing interaction $U$ to 2.5 eV, Mott gaps can be found in the DOS of both bands in Fig. 5 (d), thus the system is insulator at this condition. When $U = 2.2$ eV as shown in Fig. 5 (c), the wide $\alpha$ band is still metallic with the resonance peaks in its DOS at the Fermi level, but a Mott gap around the Fermi level exists in the narrow $\beta$ band, indicating the system is in the OSMP.$^{35-36,41}$

The phase diagram of Ba$_2$CuO$_{3.5}$ in the plane of interaction $U$ and Hund’s rule coupling $J_H$ for Ba$_2$CuO$_{3.5}$. The region of OSMP becomes narrower with the decreasing $J_H$ and increasing $U$, and OSMT vanishes around $J_H = 0.34$ eV and $U = 2.7$ eV.

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VI. CONCLUSIONS

To conclude, we study the effects of interaction and interorbital hopping on the OSMT in two-orbital Hubbard model by using DMFT with Lanczos solver, and we find that the interorbital hopping influences phase transition by changing the hopping integral ratio of effective orbitals: (1) if the interorbital hopping $t_{12} > 0$, the wide band becomes narrow but the narrow band is getting broaden with increasing $t_{12}$, and the OSMP is suppressed until $t_{\alpha} = t_{\beta}$. Conversely, a new OSMP appears when we increase $t_{12}$ continuously, where the effective orbital $\beta$ becomes metallic and orbital $\alpha$ behaves as insulator; (2) if $t_{12} < 0$, interorbital hopping enhances the OSMP by increasing the difference of the two effective orbitals. We apply the extended DMFT method to construct the phase diagram of the recently discovered two-orbital superconductor Ba$_2$CuO$_{3.5}$, and we demonstrate that the half-filled Ba$_2$CuO$_{3.5}$ should be an OSMP compound.

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