Orbitally-selective Breakdown of the Fermi Liquid and Simultaneous Enhancement of Metallic and Insulating States in Correlated Multi-band Systems with Spin-orbit Coupling

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(Dated: July 2, 2021)

We show that spin-orbit coupling (SOC) plays Janus-faced roles on the orbitally-selective Mott transitions in a three-orbital Hubbard model with crystal field splitting at a specific filling of 2/3, which is a minimal Hamiltonian for ruthenates. While the SOC favors metallic state due to enhancement of orbital hybridization at smaller on-site Coulomb repulsions, it stabilizes the Mott insulating state ascribed to lifting of orbital degeneracies and enhancement of band polarizations at larger electronic interaction. Moreover, an orbitally-selective non-Fermi liquid (OSnFL), where breakdown and retention of the Fermi liquid coexist in different orbitals, emerges between the orbitally-selective Mott phase and the Fermi-liquid state. This novel state can be used to account for the exotic metallic behavior observed in 4d materials, such as Ca1.8Sr0.2RuO4, Ba2RuO4 under strain and Sr2RuO4 under uniaxial pressure. We propose that orbitally-selective Kondo breakdown may account for the OSnFL.

I. INTRODUCTION

Multi-orbital correlated electronic systems have been extensively investigated for decades since the discoveries of iron-based superconductors [1, 2], and 4d, 5d materials like ruthenates and iridates [3–5], etc. Interplay of the following factors like the kinetic energy, crystal field splitting, spin-orbit coupling (SOC), Hund’s rule coupling and the Hubbard interaction dominates various exotic properties of these systems. For example, sizable SOC and Coulomb repulsion in 4d and 5d materials [5] lead to unconventional superconductivity [6, 7], SOC-assisted Mott transition [8–13], quantum spin liquid [14], spin-orbit exciton condensation [15, 16], and exotic magnetic order [15, 17–19]. Among all the phenomena mentioned above, SOC-assisted Mott transition is of particular interest, where the SOC lifts orbital degeneracy, resulting in an effective half-filled system. Then, the Mott transition occurs at intermediate Coulomb interaction, as observed in Sr2IrO4 [8].

Meanwhile, the Hund’s rule coupling served as a band decoupler [20], together with the crystal field splitting which lowers the orbital degeneracy, open a promising way to generate orbital selectivity which is believed to widely exist in ruthenates [21–28] and iron-based superconductors [21, 29–33]. The corresponding metallic state, so-called Hund’s metal, with electronic correlations dominated by Hund’s coupling, rather than the Hubbard interaction, are of current intensive interest since it may be responsible for exotic metallic behavior [21] and unconventional superconductivity [29]. And under certain circumstances [34–38], the orbitally-selective Mott (OSM) transition [39] takes place, where partial bands become Mott-insulating and the others remain metallic.

However, comprehensive understanding of quantum phase transitions in real materials with multiple active orbitals is still missing [22, 27, 39–41] since the SOC and the crystal field splitting are always separately taken into account [42–46] when the electronic correlations are theoretically treated within some reliable approximations like the dynamical mean field theory (DMFT) [47]. Such an unrealistic modelling may result in misleading of the effect of SOC on the Hund’s metals, the orbital selectivity, and the Mott insulators.

In this article, we have studied a three-orbital Hubbard model to investigate the influence of SOC on the orbital-differentiated correlations induced by both the

FIG. 1. (color online) The schematic phase diagram for the three-orbital Hubbard model in the plane of λ and U. FL, OSM, OSnFL, and Mott denote the Fermi liquid, orbital-selective Mott phase, orbitally-selective non-Fermi liquid, and Mott insulator, respectively.

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lifted degeneracies due to the crystal field splitting and the orbital decoupling ascribed to the Hund’s coupling at zero temperature. The main results are schematically summarized in Fig. 1. In the absence of SOC, two phases are identified within the interacting range we studied, including the Fermi-liquid state and the OSM state. The SOC is found to effectively suppress the electronic correlations at small Coulomb interactions, respectively. The Hund’s rule term observed in Ca$_1$Sr$_{0.2}$RuO$_4$ by recent angle-resolved photoemission spectroscopy (ARPES) experiments [27] and early transport measurements [49]. Contrastingly, the SOC enhances electronic correlations at large Coulomb repulsions and results in reduced critical values of phase transitions from the OSM state to the Mott insulator.

II. MODEL AND METHOD

To obtain above phase diagram, the three-orbital Hubbard model on the bethe lattice is considered, which is defined as

$$H = t \sum_{\langle ij \rangle \alpha \sigma} C_{i \alpha \sigma}^\dagger C_{j \alpha \sigma} + \sum_{i \alpha \sigma} (\Delta_{\alpha} - \mu) n_{i \alpha \sigma}$$

$$+ U \sum_{i \sigma} n_{i \alpha \sigma} n_{i \alpha \bar{\sigma}} + (U' - J_z) \sum_{i \alpha \beta \bar{\beta}} n_{i \alpha \sigma} n_{i \beta \bar{\sigma}}$$

$$+ U' \sum_{i \alpha \beta \bar{\beta}} n_{i \alpha \sigma} n_{i \beta \bar{\sigma}} - J_f \sum_{i \alpha \beta} \left[ S_{i \alpha}^+ S_{i \beta}^- + S_{i \alpha}^- S_{i \beta}^+ \right]$$

$$+ J_p \sum_{i \alpha \beta \neq \beta} C_{i \alpha \sigma}^\dagger C_{i \alpha \pi} C_{i \beta \bar{\pi}} C_{i \beta \bar{\sigma}} + H_{SOC},$$

where $t$ denotes the nearest-neighbor hopping, $\Delta_{\alpha}$ represents crystal field splitting for $t_{2g}$ basis with orbital indices $\alpha = \{yz, xz, xy\}$, and $\mu$ is the chemical potential. $U$ and $U'$ are the onsite intraorbital and interorbital Coulomb repulsions, respectively. The Hund’s rule couplings consist of the Ising-type coupling $J_z$, the spin-flip term $J_f$ and pair-hopping term $J_p$. The relationship $U = U' + 2J_z$ is employed to assure the electronic interaction rotationally invariant. $C_{i \alpha \sigma}^\dagger (C_{i \alpha \sigma})$ creates (annihilates) an electron with spin $\sigma$ in orbital $\alpha$ of lattice site $i$. $S$ and $n$ represent the spin and particle number operators, respectively. The relativistic SOC reads

$$H_{SOC} = \lambda \sum_{i \alpha \beta \pi \sigma_1} \sum_{\pi \sigma_2} \langle \alpha | L_{\pi \sigma_1} | \beta \rangle \langle \sigma_1 | S_{\pi \sigma_2} | \sigma_2 \rangle C_{i \alpha \sigma_1}^\dagger C_{i \beta \sigma_2},$$

where $\lambda$ is the strength of SOC, $L$ is the local orbital angular momentum operator. The matrix representations of $L = 2$ in the $t_{2g}$ basis are the same as the ones for $L = 1$ in cubic basis except for a sign in accordance with the T-P correspondence [5, 50].

We employed the DMFT in combination with exact diagonalization (ED) [47] as impurity solver to solve the model (1) on the bethe lattice with infinite coordinates at a filling of $n = 2/3$, namely 4 electrons in 3 orbitals, and at zero temperature. The noninteracting density of states is $\rho_0(\omega) = \frac{2}{\pi D^2} \sqrt{D^2 - \omega^2}$ and the half bandwidth $D$ is used as the energy unit. The effective inverse temperature was set to $\beta D = 200$ which serves as a low-frequency cutoff. On the bethe lattice, the DMFT self-consistent conditions simply read $\hat{\Delta}(\omega) = \frac{D^2}{4} \hat{G}(\omega)$, where $\Delta(\omega)$ is a matrix for hybrid functions, $\hat{G}(\omega)$ for local lattice Green’s functions. Totally 6 baths were used to fit the hybrid function $\Delta(\omega)$. In our calculations, the orbital degeneracy is lifted by crystal field splitting (i.e., $|\Delta_{yz} = \Delta_{xz} \neq \Delta_{xy}|$, leading to a nondegenerate $d_{xz}$ orbital and doubly degenerate $d_{yz/xx}$ orbitals. We fix electronic populations to be (1.5, 1.5, 1.0) in accordance with that of Ca$_1$Sr$_{0.2}$RuO$_4$ [27] in the absence of SOC, which can be realized by tuning the orbitally-dependent potential $\Delta_\alpha$ [36]. The calculations were performed in the paramagnetic state with isotropic Hund’s coupling where $J_z = J_f = J_p$. The broadening factor $\eta = 0.02D$ is used to calculate real-frequency dynamical quantities including the Green’s functions, self-energies, and dynamical susceptibilities for spin, orbital, and total angular momentums.

III. RESULTS

FIG. 2. (color online) (a) The quasiparticle residue $Z$ of $t_{2g}$ orbitals as a function of $U$ at $\lambda = 0.0$ and $\lambda = 0.14$; (b) a blowup for $Z$ of $d_{xy}$ orbital near the critical point $U_{cxy}(\lambda = 0.0)$ of about 2.3; those for $d_{yz/xx}$ orbitals are shown in the inset.

In order to explore the influence of SOC on the electronic correlations in multi-band systems, we have calculated the quasiparticle residue $Z_\alpha = (1 - \frac{\partial \text{Re} \Sigma_\alpha(\omega)}{\partial \omega}|_{\omega = 0})^{-1}$, as shown in Fig. 2 (a), where Re$\Sigma_\alpha(\omega)$ is the real part of self-energies of $t_{2g}$ orbitals. In the absence of SOC, $Z_{xy}$ is rapidly suppressed as $U$ increases and vanishes at a critical value of $U_{cxy}(\lambda = 0.0) \approx 2.3$, indicating a Mott-Hubbard gap opens in $d_{xy}$ band. In contrast, although $Z_{yz/xx}$ is drastically reduced at the beginning, it remains finite in a wide region of $U$ with $U_{cxy}(\lambda = 0.0)$ much larger than $U_{cxy}(\lambda = 0.0)$, which
suggests an occurrence of the OSM phase where electrons in \( d_{xy} \) band become Mott-localised and those in \( d_{yz/zx} \) bands remain itinerant. This is in excellent agreement with previous results [36].

When the SOC is taken into account, e.g. \( \lambda = 0.14 \), the quasiparticle residues behave distinctly at small and large Coulomb repulsions in comparison to those at \( \lambda = 0.0 \). At large \( U \), the SOC enhances the electronic correlations in \( d_{yz/zx} \) bands as indicated by suppression of \( Z_{yz/zx} \), leading to a smaller critical value of Mott transition \( U_{yz/zx}(\lambda = 0.14) \) than that of \( \lambda = 0.0 \) case. Since the Mott-insulating state with a vanishing \( Z_{xy} \) preserves in \( d_{xy} \) band, it suggests that the SOC cooperates with the Coulomb interaction and stabilizes the Mott-insulating ground state. Conversely, at small \( U \), the SOC suppresses the electronic correlations in all bands as inferred by larger values of \( Z \) in comparison to those of \( \lambda = 0 \) case as shown in Fig. 2 (b) which is a blowup of Fig. 2 (a) at small \( U \) region. This gives rise to an intersection of \( Z_{yz/zx} \) between \( \lambda = 0.14 \) and \( \lambda = 0.0 \) cases at \( U \approx 2.5 \) as seen in the inset of Fig. 2 (b). Furthermore, the quasiparticle residue \( Z_{xy} \) of \( \lambda = 0.14 \) case remains nonzero for a wide range of \( U > U_{xy}(\lambda = 0) \), suggesting that a transition from Mott insulator to metal may take place in \( d_{xy} \) band when SOC is turned on. This indicates that the SOC competes with the on-site Coulomb repulsion and favors a metallic ground state at small \( U \). Obviously, the SOC shows opposite effects on the Mott transitions in multi-band systems.

![Diagram](image.png)

**FIG. 3.** (Color online) (a-b) Density of states projected onto the \( t_{2g} \) orbitals and (c-d) the imaginary part of self-energy on the Matsubara axis at \( U = 2.58 \) and \( U = 8.78 \) for \( \lambda = 0.0 \) and \( \lambda = 0.14 \).

We further demonstrate the pronounced effects of the SOC in the vicinity of phase transitions in Fig. 3 where the calculated density of states projected onto the \( t_{2g} \) basis and corresponding imaginary part of the Matsubara self-energy \( \text{Im} \Sigma_{0}(i\omega_{n}) \) are exhibited. In the absence of the SOC, at both \( U = 2.58 \) and \( U = 8.78 \), the density of states at the Fermi level vanishes in \( d_{xy} \) orbital and \( \text{Im} \Sigma_{0}(i\omega_{n}) \) diverges in proximity to zero frequency, which is a typical character of Mott insulator. Meanwhile, the \( d_{yz/zx} \) orbitals behave as Fermi liquids since the density of states is finite at \( \omega = 0 \) and \( \text{Im} \Sigma_{0}(i\omega_{n}) \) approaches zero at low frequency. It suggests that the system is in the OSM phase. When \( \lambda \) increases to 0.14, the SOC exhibits distinct effects at small and large \( U \), respectively. At \( U = 8.78 \), while the SOC barely influences the nature of \( d_{xy} \) orbital, the complete suppression of density of states of \( d_{yz/zx} \) orbitals at the Fermi level and the divergence of \( \text{Im} \Sigma_{yz/zx}(i\omega_{n}) \) as \( \omega_{n} \) goes to zero, suggests an appearance of the SOC-assisted Mott phase. On the other hand, at \( U = 2.58 \), the SOC drastically affects the properties of \( d_{xy} \) orbital but hardly influences that of \( d_{yz/zx} \) orbitals. The appearance of central peak of density of states for \( d_{xy} \) orbital at the Fermi level and \( \text{Im} \Sigma_{xy}(i\omega_{n}) \) extrapolating to zero as \( \omega_{n} \to 0 \) suggests a SOC-induced Fermi liquid behavior.

The occurrence of SOC-assisted Mott phase at large \( U \) can be easily understood within \(|J, \pm m\rangle\) basis where the local Hamiltonian (2) can be diagonalized. Here \( J \) denotes the total angular momentum and \( \pm m \) represents its projection in \( z \) direction. It is found that the SOC enhances band polarizations and leads to a full occupation of the \( |3/2, \pm 3/2\rangle \) bands at \( \lambda_{c} \) of about 0.1. Then, the rest two electrons reside in \( |3/2, \pm 1\rangle \) and \( |1/2, \pm 1\rangle \) bands, resulting in an effective half-filled system, rather than originally 4 electrons per 3 orbitals. Therefore, the SOC favors Mott transition at large \( U \) since the effective filling is changed.

On the contrary, in the small \( U \) region, an OSM phase requires decoupling between Mott-insulating \( d_{xy} \) orbital and metallic \( d_{yz/zx} \) orbitals, which is originally fulfilled by Hund’s rule interaction in the absence of SOC. However, the SOC introduces coupling between the \( d_{xy} \) and \( d_{yz/zx} \) orbitals, leading to the enhancements of both orbital fluctuations and the kinetic energies of all orbitals. Therefore, the SOC tends to destroy the Mott phase of \( d_{xy} \) orbital and favors metallic state due to the increase of bandwidth and decrease of band decoupling at small \( U \).

Besides the opposite effect of SOC on electronic correlations, it is also interesting to find an intermediate phase, called orbitally-selective non-Fermi liquid (OSNFL) where breakdown of the Fermi liquid happens only in \( d_{xy} \) orbitals, emerging between the Fermi-liquid state and the OSM phase in the small \( U \) and intermediate \( \lambda \) region, as presented in Fig. 1. This exotic metallic state can be clearly identified by the imaginary part of the Matsubara self-energy \( \text{Im} \Sigma_{0}(i\omega_{n}) \) as shown in Fig. 4 (a). For example, at \( U = 2.58 \), while \( \text{Im} \Sigma_{yz/zx}(i\omega_{n}) \) always goes to zero as \( \omega_{n} \to 0 \), indicating the Fermi liquids in \( d_{yz/zx} \) bands, (see the inset of Fig. 4 (a)), \( \text{Im} \Sigma_{xy}(i\omega_{n}) \) extrapolates to a finite value as \( \omega_{n} \to 0 \) around \( \lambda \approx 0.12 \), which is in sharp contrast to the divergent behavior for \( \lambda \leq 0.08 \) and the tendency to approach zero for \( \lambda \geq 0.14 \). The finite scattering rate suggests a finite lifetime of quasi-
particles and a breakdown of the Fermi liquid at zero temperature.

The self-energy $\Sigma_{xy}(\omega)$ on the real frequency axis again reveals the SOC-induced non-Fermi-liquid behavior in $d_{xy}$ band. Fig. 4 (c) and (d) shows the real part of self-energy $\text{Re}\Sigma_{xy}(\omega)$ and imaginary part of self-energy $\text{Im}\Sigma_{xy}(\omega)$ at $U = 2.58$ for $\lambda = 0.0$, $\lambda = 0.12$ and $\lambda = 0.14$. When $\lambda = 0.12$, the positive slope of $\text{Re}\Sigma_{xy}(\omega)$ at the Fermi level and the finite $\text{Im}\Sigma_{xy}(\omega)$ suggests the breakdown of quasiparticle picture. The development of additional low-energy poles of $\omega + \mu - \varepsilon - \text{Re}\Sigma_{xy}(\omega) = 0$ close to the Fermi level and the finite scattering rate at $\omega = 0$ lead to the appearance of a pseudogap in $d_{xy}$ band, as depicted in Fig. 4 (b), reminiscent of that observed in Hubbard model within cluster DMFT [51]. This is strikingly different from those for $\lambda = 0.0$ and 0.14. For the former, the divergent $\text{Im}\Sigma_{xy}(\omega)$ at $\omega = 0$ and the steep positive slope of $\text{Re}\Sigma_{xy}(\omega)$ suggest a Mott-insulating state. In contrast, for the latter, the $\text{Im}\Sigma_{xy}(\omega)$ can be fitted by $\omega^2$ and the $\text{Re}\Sigma_{xy}(\omega)$ is linearly $\omega$-dependent, indicating a typical Fermi-liquid behavior at zero temperature. Fig. 4 (b) shows the density of states for $d_{xy}$ band in the Mott, pseudogap, and the Fermi-liquid states at $\lambda = 0.00$, 0.12 and 0.14, respectively.

Now we discuss the underlying physics for the OSnFL state. Since the nature of correlated metals is controlled by the low-energy excitations in the absence of SOC for multi-band systems [52, 53], we performed similar calculations for the dynamical susceptibilities $\chi^i(\omega)$ of total, orbital, and spin angular momentums with $i = J$, $L$, and $S$, respectively, at $U = 2.58$ and $\lambda = 0.12$, as shown in Fig. 5 (a). The dynamical spin susceptibilities are defined as

$$\chi^{SS}(\omega = \omega + i\eta) = -\text{Im} \int_{-\infty}^{\infty} dt e^{\omega t} \chi^{SS}(t).$$

We only display the imaginary parts since the real parts can be reproduced by the Kramers-Kronig relations. The dynamical susceptibilities $\chi^{LL}(\omega)$ and $\chi^{JJ}(\omega)$ for the corresponding orbital and total angular momentums can be obtained similarly. The calculation details regarding dynamical correlations are given in Appendix B. From Fig. 5 (a), it is found that the low-energy excitations mainly come from spin fluctuations, while the high-energy parts are ascribed to the excitations of orbital momentum $L$. Thus we focus on analyses of dynamical spin susceptibilities $\chi^{SS}(\omega)$ at $U = 2.58$ for $\lambda = 0.0$, 0.12, and 0.14. At $\lambda = 0.0$, the system is in the OSM phase. The low-energy spin fluctuations consist of two parts, one is attributed to the Kondo screening of spins in $d_{yz/yz}$ bands by itinerant electrons, and the other is ascribed to the existence of spin triplets formed by 4 electrons in $t_{2g}$ orbitals [52, 53]. At $\lambda = 0.14$, the system becomes a Fermi liquid. The intensity of low-energy spin excitations is drastically enhanced. Since the low-energy spin excitations of $d_{yz/yz}$ bands remains almost unchanged for different $\lambda$ as seen in the inset of Fig. 5 (b), the abrupt increase should be ascribed to additional Kondo resonances between spins in $d_{xy}$ band and itinerant electrons. At $\lambda = 0.12$, while electrons in $d_{xy}$ band become itinerant, the corresponding low-energy spin excitations are similar to those for $\lambda = 0.0$, indicating that the spins in $d_{xy}$ band do not take part in the Kondo screening. The lack of Kondo screening in $d_{xy}$ band leads to the emergence of non-Fermi liquid. Hence we conclude that the OSnFL state is a result of orbitally-selective Kondo breakdown.
IV. DISCUSSION

The calculated results show the Janus-faced influence of SOC on the Mott transitions in the presence of crystal field splitting at a filling of \( n = 2/3 \). Owing to the orbital degeneracy lifted by crystal field splitting, the Mott transitions in different orbitals take place separately as \( U \) increases. The opposite effect of SOC on the electronic correlations leads to the increase of \( U_{xy} \) and decrease of \( U_{yz/z^2} \), which is in sharp contrast to previous theoretical results in the absence of crystal field splitting, where a common Mott transition occurs and the critical value of \( U_c \) can only be increased or decreased by the SOC for given integer fillings [44–46]. Furthermore, the competition between SOC and Coulomb repulsion results in the OSnFL state, characterized by the coexistence of the Fermi liquid and non-Fermi liquid in different orbitals, which is fundamentally distinct from the case of \( \lambda = 0.0 \), where the metallic ground state is always a Fermi liquid, as displayed in Fig. 1. The coexisting region is of particular importance as it provides a unique platform to study the breakdown of the Fermi-liquid picture and the nature of non-Fermi-liquid state. The appearance of OSnFL state requires remarkable orbital-differentiated correlations and sizable orbital hybridizations, reminiscent of the non-Fermi-liquid state. The appearance of OSnFL state is originated from the orbitally-selective Kondo breakdown and can be applied to understand the exotic metals in 4d materials.

V. CONCLUSION

In conclusion, we have investigated the three-orbital Hubbard model with both SOC and crystal field splitting using the DMFT combined with ED at 2/3 filling. The OSM transitions take place as the orbital degeneracy is lifted by crystal field splitting in the absence of SOC. It is found that the SOC plays Janus-faced roles on the OSM transitions. While it suppresses the OSM transition at smaller \( U \), it favors the OSM transition at larger \( U \). The competition between the SOC and electronic correlations leads to the emergence of an OSnFL state, where the Fermi liquid coexists with non-Fermi liquid. The OSnFL state is originated from the orbitally-selective Kondo breakdown and can be applied to understand the exotic metals in 4d materials.

ACKNOWLEDGMENTS

This work is financially supported by the National Natural Science Foundation of China (Grant No. 11774258, 12004283) and Postgraduate Education Reform Project of Tongji University (Grant No. GH1905), Z. Y. Song acknowledges the financial support by China Postdoctoral Science Foundation (Grant No. 2019M651563).

Appendix A: Dynamical Mean Field Theory for Multi-orbital Hubbard Models

The DMFT [47] was employed to investigated the multi-orbital Hubbard model (1) on the bethe lattice with infinite coordination number, on which the DMFT has already been proved to be exact and the model (1) can be exactly mapped onto an Anderson impurity model with self-consistent conditions \( \Delta(\omega) = \frac{U^2}{4} \tilde{G}(\omega) \), where \( \tilde{G}(\omega) \) is the matrix of local lattice Green’s functions, \( \Delta(\omega) \) denotes the matrix of hybridization functions for the Anderson impurity model, and \( D \) represents the half bandwidth. Note that the hat symbol is used to denote a matrix. When the spin-orbit coupling is considered, it is convenient to do the calculations in the \( |J, \tau,m⟩ \) basis, where \( J = \{ \frac{1}{2}, \frac{3}{2} \} \), \( m = \{ \frac{1}{2}, \frac{3}{2} \} \), \( m \leq J \) and \( \tau = ± \) specifying a pair of Kramers doublet \( m \), which are the eigenvectors of the Hamiltonian (2). In this representation, the Anderson impurity model reads

\[
H_{\text{imp}} = \sum_{\kappa \tau m} \epsilon_{\kappa m} C^\dagger_{\kappa \tau m} C_{\kappa \tau m} + \sum_p \tilde{E}_p d^\dagger_p d_p + \sum_{pq} \tilde{M}_{pq} d^\dagger_p d_q \\
+ \sum_{k \tau m} V_{k \tau m} \left( C^\dagger_{k \tau m} d_{\tau m} + d^\dagger_{\tau m} C_{k \tau m} \right) \\
+ \frac{1}{4} \sum_{pqrst} \tilde{U}_{rst} d^\dagger_p d^\dagger_q d_s d_t, \tag{A1}
\]

where \( \epsilon_{\kappa m} \) denotes the dispersion relationship of bath electrons, \( p, q, s, t \) are the orbital indices of \( |J, \tau,m⟩ \),
It is found that the Weiss field $\hat{g}(i\omega_n) = (\hat{\Sigma}(i\omega_n) + G^{-1}(i\omega_n))^{-1}$ with $\hat{\Sigma}(\omega)$ the matrix of self-energy can be well reproduced by the noninteracting impurity Green’s function $\hat{g}_{\text{imp}}(i\omega_n)$ defined by (A3) in the OSM ((a)-(c)), the OSnFL ((d)-(f)), and the Fermi-liquid (FL) ((g)-(i)) phases, suggesting that the finite size effects are negligible and the results presented in the paper are convincing. The procedures of the DMFT calculations in combination with ED as the impurity solver are described below.

Starting from an initial set of bath parameters $\{\epsilon_{km}, V_{k;j\tau m}\}$, we construct the Anderson model (A1). The hybridization function of the corresponding impurity model (A1) is written as

$$\hat{\Delta}_{j,\tau m; j',\tau m}(i\omega_n) = \sum_k \frac{V_{k;j\tau m} V_{k;j'\tau m}}{i\omega_n - \epsilon_{km}},$$

where $\omega_n = \frac{(2n-1)\pi}{\beta}$ is the Matsubara frequency with a fictitious temperature $\beta D = 200$, which serves as a low frequency cutoff. The noninteracting impurity Green’s
function of the Anderson model (A1) is
\[ \hat{g}_{\text{imp}}(i\omega_n) = i\omega_n + \mu - \hat{E} - \hat{M} - \Delta^{-1}(i\omega_n). \] (A3)

After the impurity Green’s function \( \hat{G}_{\text{imp}}(i\omega_n) \) is obtained by solving model (A1) with ED, the self-energy \( \hat{\Sigma}(i\omega_n) \) can be calculated based on the Dyson’s equation
\[ \hat{\Sigma}(i\omega_n) = \hat{g}_{\text{imp}}^{-1}(i\omega_n) - \hat{G}_{\text{imp}}^{-1}(i\omega_n). \] (A4)

Finally, the local Green’s function of the three-orbital Hubbard model (1) in the \( |J, \tau m\rangle \) basis is calculated as
\[ \hat{G}(i\omega_n) = \int_{-\infty}^{+\infty} \frac{\rho(\epsilon)d\epsilon}{i\omega_n + \mu - \hat{E} - \hat{M} - \hat{\Sigma}(i\omega_n) - \epsilon}, \] (A5)
where \( \rho(\omega) = \frac{2}{D^{2D}} \sqrt{D^2 - \omega^2} \) is the density of states for three Kramers doublets, which is the same as the counterpart for the \( t_{2g} \) orbitals. Considering the self-consistent conditions \( \Delta(\omega_n) = \frac{1}{D^2} \hat{G}(i\omega_n) \), we can iteratively calculate the local Green’s function \( \hat{G}(i\omega_n) \) through equations (A1) — (A5).

In our calculations, the parameters \( \{\epsilon_{km}, V_{k,l\tau m}\} \) to build the model (A1) are obtained by using the conjugate gradient method to minimizing the cost function
\[ \chi = \frac{1}{N_{\text{max}}} \sum_{n=1}^{N_{\text{max}}} \frac{1}{\omega_n^2} \sum_{pq} |(\hat{g}(i\omega_n) - \hat{g}_{\text{imp}}(i\omega_n))_{pq}|, \] (A6)
where \( N_{\text{max}} = 256 \) is the upper limit of the summation. Starting from a guessed Weiss field \( \hat{g}(i\omega_n) \), we can self-consistently obtain the converged results when the difference \( \Delta_g \) between the new Weiss field \( \hat{g}_{\text{new}}^{\text{new}}(i\omega_n) \) and the old Weiss field \( \hat{g}_{\text{old}}^{\text{old}}(i\omega_n) \) is less than \( 10^{-6} \). The difference \( \Delta_g \) is defined as
\[ \Delta_g = \max \{|\hat{g}_{pq}^{\text{new}}(i\omega_n) - \hat{g}_{pq}^{\text{old}}(i\omega_n)|\} \] (A7)

Although the present DMFT calculations were performed in the \( |J, \tau m\rangle \) basis, the dynamical quantities, like local lattice Green’s function \( \hat{G}_{t_{2g}}(i\omega_n) \) and self-energy \( \hat{\Sigma}_{t_{2g}}(i\omega_n) \), in the \( t_{2g} \) basis can be readily obtained via a unitary transformation
\[ \hat{G}_{t_{2g}}(i\omega_n) = \hat{A}\hat{G}(i\omega_n)\hat{A}^\dagger, \] (A8)
and
\[ \hat{\Sigma}_{t_{2g}}(i\omega_n) = \hat{A}\hat{\Sigma}(i\omega_n)\hat{A}^\dagger. \] (A9)

Since ED has direct access to the real-frequency dynamical correlations as described in Appendix B, we can calculate the local lattice Green’s function \( \hat{G}(i\omega + i\eta) \) after the self-energy is obtained via the Dyson equation
\[ \hat{\Sigma}(i\omega + i\eta) = \hat{g}_{\text{imp}}^{-1}(i\omega + i\eta) - \hat{G}_{\text{imp}}^{-1}(i\omega + i\eta), \]
where the impurity Green’s function \( \hat{G}_{\text{imp}}(i\omega + i\eta) \) is directly produced by ED. Similar to the Matsubara Green’s function \( \hat{G}_{t_{2g}}(i\omega_n) \), the local Green’s function \( \hat{G}_{t_{2g}}(i\omega + i\eta) \) and self-energy \( \hat{\Sigma}_{t_{2g}}(i\omega + i\eta) \) in the \( t_{2g} \) basis are calculated as
\[ \hat{G}_{t_{2g}}(i\omega + i\eta) = A\hat{G}(i\omega + i\eta)A^\dagger, \] (A10)
and
\[ \hat{\Sigma}_{t_{2g}}(i\omega + i\eta) = A\hat{\Sigma}(i\omega + i\eta)A^\dagger. \] (A11)

On the basis of \( \hat{G}_{t_{2g}}(i\omega + i\eta) \), the projected density of states, as shown in the main text, is defined as
\[ \rho_{\alpha\sigma}(\omega) = -\frac{1}{\pi} \text{Im} \left( \hat{G}_{t_{2g}}(i\omega + i\eta) \right)_{\alpha\sigma,\alpha\sigma}, \] (A12)
where \( \alpha \) is the orbital index for \( t_{2g} \) orbitals and \( \sigma \) denotes electron spin.

**Appendix B: Exact Diagonalization**

When ED is employed as impurity solver of the DMFT, it needs two steps to obtain the dynamical correlation functions. The first step is to calculate the ground-state energy \( E_g \) and corresponding eigenvector \( |\rangle \) of the Anderson impurity model (A1) by the Lanczos method. On the basis of the Lanczos method, the \( E_g \) and \( |\rangle \) can be obtained by iteratively constructing a Krylov space \( \{|\phi_n\rangle\} \) from an arbitrary initial configuration \( |\phi_1\rangle \) via
\[ |\phi_{n+1}\rangle = H_{\text{imp}}|\phi_n\rangle - a_n|\phi_n\rangle - b_n^2|\phi_{n-1}\rangle, \] (B1)
where \( n = 2, 3, 4, \ldots \), \( a_n = \langle \phi_n| H_{\text{imp}}|\phi_n\rangle, \) \( b_n^2 = \langle \phi_{n+1}| \phi_{n+1}\rangle. \) Note \( |\phi_n\rangle \) denotes a normalized vector, \( b_1 = 0, |\phi_0\rangle = 0, |\phi_2\rangle = H_{\text{imp}}|\phi_1\rangle - a_1|\phi_1\rangle \) and \( a_1 = \langle \phi_1| H_{\text{imp}}|\phi_1\rangle. \) The iteration (B1) continues until \( b_n \) is less than a threshold. In this basis, the Hamiltonian for the Anderson impurity model (A1) is a tridiagonal matrix and simply reads
\[ \begin{bmatrix}
a_1 & b_2 & 0 & 0 & \cdots \\
b_2 & a_2 & b_3 & 0 & \cdots \\
0 & b_3 & a_3 & b_4 & \cdots \\
0 & 0 & b_4 & a_4 & \cdots \\
\vdots & \vdots & \vdots & \vdots & \ddots 
\end{bmatrix}, \] (B2)

which can be diagonalized by the modern standard library subroutines.

The second step is to calculate the dynamical correlation function based on the ground-state energy \( E_g \) and ground-state eigenvector \( |\rangle \) obtained in the first step. For the given operator \( O \), the real-time dynamical correlation function is defined as
\[ C_{\alpha\beta}(t) = -i\theta(t) \{ |O_\alpha(t), O_\beta\rangle \xi \} \] (B3)
where \( \theta(t) \) is a step function of time \( t, O_\alpha(t) = e^{iH_{\text{imp}}t} O_\alpha e^{-iH_{\text{imp}}t}, \) \( \xi \) denotes the commutator of two operators, \( \xi = 1 \) if \( O \) is a Fermi operator and \( \xi = -1 \) if \( O \) is a non-Fermi operator.
otherwise. After performing a Fourier transformation, the dynamical correlation function on the real frequency axis can be written as

\[ C_{\alpha\beta}(\omega + i\eta) = C_{\alpha\beta}^> (\omega + i\eta) + \xi C_{\alpha\beta}^< (\omega + i\eta), \]  

where \( \eta \) is a broadening factor and

\[ C_{\alpha\beta}^> (\omega + i\eta) = \langle |O_\alpha - H_{\text{imp}} + E_g + i\eta|O_\beta \rangle \frac{1}{\omega - H_{\text{imp}} - E_g + i\eta}, \]  

\[ C_{\alpha\beta}^< (\omega + i\eta) = \langle |O_\beta - H_{\text{imp}} - E_g + i\eta|O_\alpha \rangle \frac{1}{\omega + H_{\text{imp}} - E_g + i\eta}. \]

Similar to calculate the ground-state energy \( E_g \) and eigenvector \(|\rangle\rangle\), the method of the Krylov space can be applied to calculate both dynamical correlation functions above.

In order to calculate \( C_{\alpha\beta}^> (\omega + i\eta) \), we start the Lanczos iterations with the initial vector \(|\phi_1^\beta\rangle = O_{\beta}|\rangle\rangle\) to construct the new basis \(|\phi_n^\alpha\rangle\rangle\). By inserting the completeness \( \sum_n |\phi_n^\alpha\rangle\langle\phi_n^\alpha| = 1 \) into equation (B5), it yields

\[ C_{\alpha\beta}^> (\omega + i\eta) = \frac{1}{\sqrt{\langle |O_\alpha O_\alpha^\dagger |\rangle}} \sqrt{\langle |O_\beta O_\beta^\dagger |\rangle} \times \sum_n U_{n\alpha}^\beta V_n^\beta (\omega + i\eta) \]  

where

\[ V_n^\beta (\omega + i\eta) = \langle \phi_n^\beta | \frac{1}{\omega - H_{\text{imp}} + E_g + i\eta} |\phi_1^\beta\rangle, \]

and \( U_{n\alpha}^\beta = \langle \phi_n^\alpha | \phi_1^\beta\rangle \) with \( \langle \phi_1^\beta | = \langle |O_\alpha / \sqrt{\langle |O_\alpha O_\alpha^\dagger |\rangle} \). It is obvious that the main difficulties are to calculate \( V_n^\beta (\omega + i\eta) \) in the new basis. By taking advantage of the completeness of \( \sum_n |\phi_n^\beta\rangle\langle\phi_n^\beta| = 1 \) and the identity

\[ \langle \phi_m^\alpha | (\omega - H_{\text{imp}} + E_g) \frac{1}{\omega - H_{\text{imp}} + E_g} |\phi_1^\beta\rangle = \delta_{m,1}, \]

\[ V_n^\beta (\omega + i\eta) \) can be obtained through

\[ S_{mn}^\beta (\omega + i\eta) V_n^\beta (\omega + i\eta) = E_m, \]

where \( E_m = \delta_{m,1}\) and \( S_{mn}^\beta (\omega + i\eta) \) is a tridiagonal matrix

\[ S_{mn}^\beta (\omega + i\eta) = \begin{bmatrix} \omega - a_1 + E_g + i\eta & -b_2 & 0 & 0 & \cdots \\ -b_2 & \omega - a_2 + E_g + i\eta & -b_3 & 0 & \cdots \\ 0 & -b_3 & \omega - a_3 + E_g + i\eta & -b_4 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix}. \]

**Appendix C: Results with Eight Bath Sites Coupled to Three Kramers Doublets**

In order to further investigate the effect of bath discretization on the OSnFL phase, we have done the DMFT calculations with eight bath sites at zero temperature using ED as the impurity solver, where four bath sites couple to \( |\frac{1}{2}, \pm \frac{3}{2}\rangle \) and \( |\frac{3}{2}, \pm \frac{1}{2}\rangle \) Kramers doublets and the remaining four bath sites couple to \( |\frac{3}{2}, \pm \frac{3}{2}\rangle \) doublet. The calculated results at \( U = 2.51 \) are displayed in Fig. 7, which are similar to those obtained with six bath sites. The OSnFL state can be clearly identified by the imaginary part of self-energy \( \text{Im}\Sigma(\omega_n) \) on the Matsubara frequency axis. As shown in the inset of Fig. 7 (a), \( \text{Im}\Sigma_{yz/xx}(\omega_n) \) for \( d_{yz/xx} \) orbitals always extrapolates to zero when \( \omega_n \) goes to zero, suggesting the typical Fermi-liquid behavior in \( d_{yz/xx} \) orbitals. In contrast, at around \( \lambda \approx 0.12 \), \( \text{Im}\Sigma_{xy}(\omega_n) \) for \( d_{xy} \) orbital approaches a finite value at low frequencies, which is distinctly different from
indicate the breakdown of the Fermi liquid at zero temperature. Im \( \Sigma_{xy}(\omega) \) of self-energy \( \text{Re} \Sigma_{xy} \) indicate the SOC-induced non-Fermi-liquid nature of the Fermi-liquid breakdown in \( d_{xy} \) orbital due to the finite scattering rate at zero temperature.

The self-energy \( \Sigma_{xy}(\omega) \) on the real frequency axis further manifest the SOC-induced non-Fermi-liquid nature of \( d_{xy} \) orbital. Fig. 7 (c) and (d) shows the real part of self-energy \( \text{Re} \Sigma_{xy}(\omega) \) and the imaginary part of self-energy \( \text{Im} \Sigma_{xy}(\omega) \) of \( d_{xy} \) orbital at \( U = 2.51 \) for \( \lambda = 0.0 \), \( \lambda = 0.12 \) and \( \lambda = 0.16 \). For the case of \( \lambda = 0.12 \), the positive slop of \( \text{Re} \Sigma_{xy}(\omega) \) and finite value of \( \text{Im} \Sigma_{xy}(\omega) \) at the Fermi level indicate the breakdown of the Fermi liquid at zero temperature. In contrast, the sharp slop of \( \text{Re} \Sigma_{xy}(\omega) \) and divergent \( \text{Im} \Sigma_{xy}(\omega) \) at \( \omega = 0 \) suggest a Mott-insulating state for \( \lambda = 0.0 \) case, and the linearly \( \omega \)-dependent \( \text{Re} \Sigma_{xy}(\omega) \) and quadratically \( \omega^2 \)-dependent \( \text{Im} \Sigma_{xy}(\omega) \) in the vicinity of the Fermi level indicate a typical Fermi-liquid behavior for \( \lambda = 0.16 \) case. Fig. 7 (c) displays the density of states for \( d_{xy} \) orbital in the Mott, non-Fermi-liquid and Fermi-liquid states at \( \lambda = 0.0 \), 0.12 and 0.16, respectively.

In order to reveal the mechanism which is responsible for the appearance of the OSM state, we have calculated the dynamical susceptibilities \( \chi^{xy}(\omega) \), defined by Eq (3) and (4), for total spin momentum \( S \), total orbital angular momentum \( L \) and total angular momentum \( J \) at \( U = 2.51 \) and \( \lambda = 0.12 \), as displayed in Fig. 8 (a). This result is similar to that obtained with totally six bath sites. It is obvious that the low-energy excitations of the total angular momentum \( J \) are mainly contributed by the spin fluctuations and the high-energy ones are ascribed to the excitations of the total orbital angular momentum \( L \). Since the low-energy excitations were found to dominate the physical properties of the correlated multiorbital systems [52, 53], we now pay attention on the low-energy spin fluctuations. Fig. 8 (b) depicts the spin susceptibilities at \( U = 2.51 \) for \( \lambda = 0.0 \), 0.12 and 0.16 cases. As explained in the main text, at \( \lambda = 0.0 \), the system is in the OSM state. The appearance of low-energy spin excitations is due to the spins in \( d_{yz/zx} \) orbitals screened by their itinerant electrons and the formation of the local triplets with three \( t_{2g} \) orbitals filled by four electrons. At \( \lambda = 0.16 \), the abrupt jump in spin excitations is attributed to the presence of the additional Kondo resonances in \( d_{xy} \) orbital because the spin susceptibilities for \( d_{yz/zx} \) orbitals keep almost unchanged, as displayed in the inset of Fig. 8 (b). In contrast, at \( \lambda = 0.12 \), the spin susceptibilities are almost the same with those at \( \lambda = 0.0 \), indicating the spins in \( d_{xy} \) band do not participate in the Kondo screening. Obviously, the lack of the Kondo resonances in \( d_{xy} \) orbital leads to the non-Fermi liquid behavior.

In summary, the results calculated with eight bath sites are qualitatively consistent with those obtained with six bath sites, suggesting the finite-size effect is negligible.

**FIG. 7.** (color online) The influence of spin-orbit coupling on the imaginary part of Matsubara self-energy for \( d_{xy} \) band, those for \( d_{yz/zx} \) bands are shown in the inset. (a) Density of states for \( d_{xy} \) band in the Mott (\( \lambda = 0.0 \)), non-Fermi-liquid (\( \lambda = 0.12 \)) and the Fermi-liquid (\( \lambda = 0.16 \)) states. (b) Real and (d) imaginary part of self-energy of \( d_{xy} \) band on the real frequency axis. Here, the electron repulsion is fixed at \( U = 2.51 \).

**FIG. 8.** (color online) (a) Dynamical susceptibilities for spin (\( S \)), orbital (\( L \)) and total (\( J \)) angular momentums at \( U = 2.51 \) and \( \lambda = 0.12 \). (b) Dynamical spin susceptibilities at \( U = 2.51 \) for \( \lambda = 0.0 \), 0.12 and 0.16 cases, the inset shows corresponding orbitally-resolved dynamical spin susceptibilities, where solid lines denote \( d_{yz/zx} \) orbitals and dashed lines \( d_{xy} \) orbital.

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