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Orbital-selective Mott phase in multiorbital models for iron pnictides and chalcogenides

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There is increasing recognition that the multiorbital nature of the $3d$ electrons is important to the proper description of the electronic states in the normal state of the iron-based superconductors. Earlier studies of the pertinent multiorbital Hubbard models identified an orbital-selective Mott phase, which anchors the orbital-selective behavior seen in the overall phase diagram. An important characteristics of the models is that the orbitals are kinetically coupled – *i.e.* hybridized – to each other, which makes the orbital-selective Mott phase especially nontrivial. A $U(1)$ slave-spin method was used to analyze the model with nonzero orbital-level splittings. Here we develop a Landau free-energy functional to shed further light on this issue. We put the microscopic analysis from the $U(1)$ slave-spin approach in this perspective, and show that the intersite spin correlations are crucial to the renormalization of the bare hybridization amplitude towards zero and the concomitant realization of the orbital-selective Mott transition. Based on this insight, we discuss additional ways to study the orbital-selective Mott physics from a dynamical competition between the interorbital hybridization and collective spin correlations. Our results demonstrate the robustness of the orbital-selective Mott phase in the multiorbital models appropriate for the iron-based superconductors.

I. INTRODUCTION

In many strongly correlated systems, superconductivity is closely connected to a strongly-correlated bad-metal normal state and a nearby antiferromagnetic order. As such, there has been considerable effort devoted to the understanding of the electron correlation effects and the associated magnetism. In the case of the iron-based superconductors (FeSCs) [1–6], recent developments have further highlighted the importance of electron correlations. For instance, angle-resolved photoemission spectroscopy (ARPES) has found an orbital-selective Mott phase (OSMP) in the iron chalcogenides [7–10]. The OSMP phase arises in multiorbital Hubbard models of the FeSCs, which contain both Hubbard interactions and Hund's coupling[11,12]. Evidence for the OSMP has also come from a variety of other measurements[13–16]. A complementary approach to the electron correlations of the FeSCs describes the localization-delocalization phenomena in the form of an orbital differentiation and a coherence-incoherence crossover[17,18], though OSMP is not explicitly invoked. In addition, recent experiments have identified a Mott insulating system in the copper-doped iron pnictides[19], which accompanies the earlier observations of Mott insulating states in the iron chalcogenides[20–22]. These observations considerably expand on the bad-metal behavior known, since early on in the field, through other properties of the iron pnictides[23–25]. For example, the room-temperature electrical resistivity is large (reaching the Mott-Ioffe-Regel limit, as defined by the normalized mean free path $k_F\ell$ being of order unity), in contrast to good metals such as Cr (for which $k_F\ell$ at room temperature is much larger than 1). Moreover, the Drude optical weight is much reduced[23].

The parent systems of FeSCs have the iron valence $+2$, with $n = 6$ electrons occupying the $3d$ orbitals. Correspondingly, multiple $3d$-electron orbitals are important[24–30]. In order to address the bad-metal physics, an important question is how the itinerancy of the electronic states is reduced with increasing Coulomb interactions. The appropriate multiorbital Hubbard models include the intra- and interorbital Hubbard interactions (U and U') and the Hund's coupling ($J_{\rm H}$).

The OSMP phase appears in the paramagnetic solution to the multiorbital Hubbard models[11]. In this phase, the non-degenerate $3d$ xy orbital loses its coherent spectral weight at the Fermi energy, while this weight remains nonzero for the other orbitals (including the degenerate $3d$ xz/yz orbitals). These features have been clearly identified in the ARPES measurements[7–10].

From a theoretical perspective, it is important to stress that, the orbitals are kinetically coupled – *i.e.* hybridized – to each other in these models. In particular, the bare kinetic hybridization between the $3d$ xy orbital and the other $3d$ orbitals is nonzero. In the OSMP phase, this hybridization is renormalized to zero and the $3d$ xy orbital is no longer mixed with the other orbitals in the low-energy electronic excitations.

More generally, orbital selectivity has been discussed in the correlation effects; see, for example, Refs. 17, 31–35. It can be defined in terms of the mass enhancement (m^*/m_b, the ratio of the effective mass observed experimentally to that of the non-interacting band dispersion) being different for the electronic states with predominantly different orbital contents. In practice, m^*/m_b for electronic states with predominantly $3d$ xy orbital character is much larger (reaching $10-20$ in the iron selenides) than that for the electronic states with predominantly $3d$ xz/yz (typically $3-4$) and other orbital characters[4,10].

Strictly speaking, the orbital selectivity is in itself not precisely defined, because the hybridization mixes the different orbitals in the electronic band states. However, it becomes sharply defined as a precursor to the OSMP[11]. In other words, the OSMP anchors the notion of orbital selectivity in general. Note that the picture of the orbitally-differentiated coherence-incoherence crossover has also yielded the $3d$ xy orbital to be localized at sufficiently high temperatures, while itinerant at zero temperature [36,37]. Hence the generalization of the no-

tion of OSMP is relevant in this case as well. These highlight the conceptual importance of the OSMP in characterizing the orbital selectivity in general.

A. Orbital vs. band basis

OSMP for the multiorbital Hubbard model has been discussed in several contexts. Most of these studies start from multiple inequivalent bands, and define the Hubbard and Hund's interactions in the band states [38–43]. By definition, the band basis diagonalizes the noninteracting part of the Hamiltonian. In other words, kinetically, they are decoupled from each other. In the presence of interactions, the weight of the coherent electrons near the Fermi surface will be renormalized below 1 in a band-dependent way. An OSMP corresponds to the regime where the renormalized coherent spectral weights for some of the bands vanish while those for the others remain nonzero.

For the FeSCs, multiorbital Hubbard models are defined in the orbital basis [12,24–35]. The definition of the non-degenerate orbitals is unambiguous. For the degenerate $3d$ xz/yz orbitals, there can be alternative definitions, but the degeneracy ensures that the different definitions are equivalent to each other.

In the orbital basis, the kinetic part of the Hamiltonian is not diagonal. Therefore, in the Hamiltonian, the orbitals are kinetically coupled – *i.e.* hybridized – to each other. In the OSMP solution of Ref. 11, the destruction of the quasiparticle spectral weight, Z_{xy}, is accompanied by the suppression of the renormalized interorbital kinetic hybridization between the $3d$ xy orbital and the other ones.

The purpose of this paper is to clarify how the above happens. We do so by formulating a Landau free-energy functional, which also demonstrates the robustness of the OSMP. Viewed from this perspective, we show the crucial role that the intersite spin correlations play in generating the OSMP (*cf.* Fig. 1) within the the microscopic $U(1)$ slave-spin approach[11,32].

The remainder of the paper is organized as follows. In Sec. II, we define the model and summarize the $U(1)$ slave-spin approach. Sec. III is devoted to the formulation of the Landau free-energy functional in terms of the orbital-dependent quasiparticle weight and how the OSMP appears as a distinct phase permitted by the Landau functional. We then address, in Sec. IV, the OSMP as derived by the microscopic $U(1)$ slave-spin approach from the perspective of the Landau free-energy functional. Landau analysis has been useful in clarifying the Mott transition in the dynamical mean-field theory (DMFT) context[44]. Sec. V discusses the implications of the insight gained in the present work for further studies on the OSMP, and Sec. VI summarizes the paper. Finally, in Appendices A through C, we present further details on the saddle-point equations of the $U(1)$ slave-spin approach.

II. MULTIORBITAL HUBBARD MODEL AND THE $U(1)$ SLAVE-SPIN APPROACH

We now define the model and, to facilitate the analysis in the next section, summarize the microscopic approach[32] based on a $U(1)$ slave-spin representation.

A. Multiorbital Hubbard model

The multiorbital Hubbard model for the FeSCs takes the following form,

$$H = H_0 + H_{\rm int}. \tag{1}$$

H_0 contains the tight-binding parameters among the multiple orbitals,

$$H_0 = \frac{1}{2}\sum_{ij\alpha\beta\sigma} t_{ij}^{\alpha\beta} d_{i\alpha\sigma}^\dagger d_{j\beta\sigma} + \sum_{i\alpha\sigma}(\Delta_\alpha - \mu) d_{i\alpha\sigma}^\dagger d_{i\alpha\sigma}, \tag{2}$$

where $d_{i\alpha\sigma}^\dagger$ creates an electron in orbital α ($= 1, ..., 5$) with spin σ at site i, Δ_α refers to the energy level associated with the crystal field splitting (which is diagonal in the orbital basis), and μ is the chemical potential. In general, $t_{ij}^{\alpha\beta} \neq 0$ for $\alpha \neq \beta$, corresponding to a nonzero kinetic hybridization between the different orbitals. For latter references, we note that the onsite energy for the $3d$ xy orbital is different from any of the other four $3d$ orbitals: for any orbital $\beta \neq xy$, the level splitting $\Delta_{xy,\beta} \equiv \Delta_{xy} - \Delta_\beta \neq 0$. The onsite interaction $H_{\rm int}$ reads

$$\begin{aligned} H_{\rm int} = \frac{U}{2}\sum_{i,\alpha,\sigma} n_{i\alpha\sigma} n_{i\alpha\bar{\sigma}} \\ + \sum_{i,\alpha<\beta,\sigma} \{U' n_{i\alpha\sigma} n_{i\beta\bar{\sigma}} + (U' - J_{\rm H}) n_{i\alpha\sigma} n_{i\beta\sigma} \\ - J_{\rm H}(d_{i\alpha\sigma}^\dagger d_{i\alpha\bar{\sigma}} d_{i\beta\bar{\sigma}}^\dagger d_{i\beta\sigma} + d_{i\alpha\sigma}^\dagger d_{i\alpha\bar{\sigma}}^\dagger d_{i\beta\sigma} d_{i\beta\bar{\sigma}})\Big\} \end{aligned} \tag{3}$$

where $n_{i\alpha\sigma} = d_{i\alpha\sigma}^\dagger d_{i\alpha\sigma}$. Here, U, U', and $J_{\rm H}$ respectively denote the intraorbital repulsion, the interorbital repulsion, and the Hund's rule exchange coupling. In the following, we will take $U' = U - 2J_{\rm H}$.[45]

B. $U(1)$ slave-spin theory

The metal-insulator transition in the model has been studied by using a $U(1)$ slave-spin theory, which was introduced in Ref. 32. Here we summarize the approach to set the stage for our consideration of the OSMP in the next two sections. For further details, we refer to Ref. 32 as well as Appendices A and B. In addition, we refer to Appendix C for a comparison with the Z_2 slave-spin theory of Ref. 46 (see also Refs. 47 and 48).

In the $U(1)$ slave-spin formulation, the XY component of a quantum $S = 1/2$ spin operator ($S_{i\alpha\sigma}^+$) is used to represent the charge degree of freedom of the electron at each site i, for each

orbital α and each spin flavor σ. Correspondingly, a fermionic "spinon" operator ($f^\dagger_{i\alpha\sigma}$) is used to carry the spin degree of freedom. The electron creation operator is then represented as follows,

$$d^\dagger_{i\alpha\sigma} = S^+_{i\alpha\sigma} f^\dagger_{i\alpha\sigma}. \tag{4}$$

This is implemented by a constraint,

$$S^z_{i\alpha\sigma} = f^\dagger_{i\alpha\sigma} f_{i\alpha\sigma} - \frac{1}{2}, \tag{5}$$

which restricts the Hilbert space to the physical one.

This representation contains a $U(1)$ gauge redundancy corresponding to $f^\dagger_{i\alpha\sigma} \to f^\dagger_{i\alpha\sigma} e^{-i\theta_{i\alpha\sigma}}$ and $S^+_{i\alpha\sigma} \to S^+_{i\alpha\sigma} e^{i\theta_{i\alpha\sigma}}$. Therefore, the slave spins carry the $U(1)$ charge, similarly as in the slave-rotor approach [49].

To ensure that the saddle point captures the correct quasiparticle spectral weight in the non-interacting limit (being equal to 1), we define a dressed operator in the Schwinger boson representation of the slave spins (in a way similar to the standard slave-boson theory[50]):

$$\hat{z}^\dagger_{i\alpha\sigma} = P^+_{i\alpha\sigma} a^\dagger_{i\alpha\sigma} b_{i\alpha\sigma} P^-_{i\alpha\sigma}, \tag{6}$$

where $P^\pm_{i\alpha\sigma} = 1/\sqrt{1/2 + \delta \pm (a^\dagger_{i\alpha\sigma} a_{i\alpha\sigma} - b^\dagger_{i\alpha\sigma} b_{i\alpha\sigma})/2}$, and δ is an infinitesimal positive number to regulate $P^\pm_{i\alpha\sigma}$.

Here $a_{i\alpha\sigma}$ and $b_{i\alpha\sigma}$ are Schwinger bosons representing the slave-spin operators: $S^+_{i\alpha\sigma} = a^\dagger_{i\alpha\sigma} b_{i\alpha\sigma}$, $S^-_{i\alpha\sigma} = b^\dagger_{i\alpha\sigma} a_{i\alpha\sigma}$, and $S^z_{i\alpha\sigma} = (a^\dagger_{i\alpha\sigma} a_{i\alpha\sigma} - b^\dagger_{i\alpha\sigma} b_{i\alpha\sigma})/2$. They satisfy an additional constraint,

$$a^\dagger_{i\alpha\sigma} a_{i\alpha\sigma} + b^\dagger_{i\alpha\sigma} b_{i\alpha\sigma} = 1. \tag{7}$$

In other words, they are hard-core bosons. In this representation, the constraint in Eq. (5) becomes

$$a^\dagger_{i\alpha\sigma} a_{i\alpha\sigma} - b^\dagger_{i\alpha\sigma} b_{i\alpha\sigma} = 2 f^\dagger_{i\alpha\sigma} f_{i\alpha\sigma} - 1. \tag{8}$$

At the same time, Eq. (4) becomes

$$d^\dagger_{i\alpha\sigma} = \hat{z}^\dagger_{i\alpha\sigma} f^\dagger_{i\alpha\sigma}. \tag{9}$$

The Hamiltonian, Eq. (1), can then be effectively rewritten as

$$H = \frac{1}{2} \sum_{ij\alpha\beta\sigma} t^{\alpha\beta}_{ij} \hat{z}^\dagger_{i\alpha\sigma} \hat{z}_{j\beta\sigma} f^\dagger_{i\alpha\sigma} f_{j\beta\sigma} + \sum_{i\alpha\sigma} (\Delta_\alpha - \mu) f^\dagger_{i\alpha\sigma} f_{i\alpha\sigma} - \lambda_{i\alpha\sigma} [f^\dagger_{i\alpha\sigma} f_{i\alpha\sigma} - \frac{1}{2}(\hat{n}^a_{i\alpha\sigma} - \hat{n}^b_{i\alpha\sigma})] + H^S_{\rm int}. \tag{10}$$

Here, $\lambda_{i\alpha\sigma}$ is a Lagrange multiplier to enforce the constraint in Eq. (8). In addition, $H^S_{\rm int}$ is the interaction Hamiltonian, Eq. (3), rewritten in the slave-spin representation $H_{\rm int} \to H_{\rm int}(\mathbf{S})$,[32] and subsequently with the slave-spin operators substituted by the Schwinger bosons. The quasiparticle spectral weight

$$Z_{i\alpha\sigma} = |z_{i\alpha\sigma}|^2 \equiv |\langle \hat{z}_{i\alpha\sigma} \rangle|^2. \tag{11}$$

A metallic phase corresponds to $Z_{i\alpha\sigma} > 0$, and a Mott insulator corresponds to $Z_{i\alpha\sigma} = 0$ in all orbitals with a gapless spinon spectrum.

After decomposing the boson and spinon operators and treating the constraint on average, we obtain two saddle-point Hamiltonians for the spinons and the Schwinger bosons, respectively:

$$H^{\rm mf}_f = \sum_{k\alpha\beta} \left[\epsilon^{\alpha\beta}_k \langle \tilde{z}^\dagger_\alpha \rangle \langle \tilde{z}_\beta \rangle + \delta_{\alpha\beta} (\Delta_\alpha - \lambda_\alpha + \tilde{\mu}_\alpha - \mu) \right] f^\dagger_{k\alpha} f_{k\beta}, \tag{12}$$

$$H^{\rm mf}_S = \sum_{\alpha\beta} \left[Q^f_{\alpha\beta} \left(\langle \tilde{z}^\dagger_\alpha \rangle \tilde{z}_\beta + \langle \tilde{z}_\beta \rangle \tilde{z}^\dagger_\alpha \right) + \delta_{\alpha\beta} \frac{\lambda_\alpha}{2} (\hat{n}^a_\alpha - \hat{n}^b_\alpha) \right] + H^S_{\rm int}, \tag{13}$$

where $\delta_{\alpha\beta}$ is Kronecker's delta function, $\epsilon^{\alpha\beta}_k = \frac{1}{N} \sum_{ij\sigma} t^{\alpha\beta}_{ij} e^{ik(r_i - r_j)}$, and

$$Q^f_{\alpha\beta} = \sum_{k\sigma} \epsilon^{\alpha\beta}_k \langle f^\dagger_{k\alpha\sigma} f_{k\beta\sigma} \rangle / 2, \tag{14}$$

$$\tilde{z}^\dagger_\alpha = \langle P^+_\alpha \rangle a^\dagger_\alpha b_\alpha \langle P^-_\alpha \rangle. \tag{15}$$

In addition, $\tilde{\mu}_\alpha$ is an effective onsite potential defined as

$$\tilde{\mu}_\alpha = 2 \bar{\epsilon}_\alpha \eta_\alpha \tag{16}$$

where

$$\bar{\epsilon}_\alpha = \sum_\beta \left(Q^f_{\alpha\beta} \langle \tilde{z}^\dagger_\alpha \rangle \langle \tilde{z}_\beta \rangle + \text{c.c.} \right) \tag{17}$$

and

$$\eta_\alpha = (2 n^f_\alpha - 1)/[4 n^f_\alpha (1 - n^f_\alpha)], \tag{18}$$

with $n^f_\alpha = \frac{1}{N} \sum_k \langle f^\dagger_{k\alpha} f_{k\alpha} \rangle$.

Eqs. (12) and (13) represent the main formulation of the $U(1)$ slave-spin approach at the saddle-point level. Note that the slave-spin part is single-site in nature. By contrast, the pseudofermion part must contain intersite couplings, which will play an important role in the analysis (see next section). We study the metal-to-insulator transitions in the paramagnetic phase preserving the translational symmetry. These allow us to drop the spin and/or site indices of the Schwinger bosons (slave spins) and the Lagrange multiplier λ_α in the above saddle-point equations. We refer to Appendices A and B for a detailed derivation of these saddle-point Hamiltonians. The parameters z_α and λ_α are solved self-consistently. The parameter $\tilde{\mu}_\alpha$ introduced above is crucially important to ensuring that the noninteracting limit is properly captured (with $Z_\alpha = |\langle \tilde{z}_\alpha \rangle|^2 = |z_\alpha|^2 = 1$ and correct electron dispersion) regardless of whether the system is at or away from half filling (see Appendix C for more details). By contrast, in the Z_2 slave-spin formulation, the parameter $\tilde{\mu}_\alpha$ is absent in the saddle-point equations, and the proper non-interacting limit cannot be easily recovered for the generic case of multiple non-degenerate orbitals away from half filling; see Appendix C for further discussions on this point as well.

III. LANDAU FREE-ENERGY FUNCTIONAL AND THE ORIGIN OF THE ORBITAL-SELECTIVE MOTT TRANSITION

In a multiorbital system, an OSMP may exist besides the metallic and the Mott insulating phases. In an OSMP, some of the orbitals are Mott localized and the others are still metallic; the quasiparticle spectral weight Z vanishes for the former orbitals and remains nonzero for the latter ones. In this section, we clarify how an OSMP can arise in the slave-spin approach and develop a Landau theory to describe the orbital-selective Mott transition (OSMT).

We start from the two saddle-point Hamiltonians, Eqs. (12) and (13). Consider first Eq. (12), where the kinetic hybridization between two different orbitals $\alpha \neq \beta$ is $W_k^{\alpha\beta} f_{k\alpha}^\dagger f_{k\beta}$, with $W_k^{\alpha\beta} = \epsilon_k^{\alpha\beta} \langle \tilde{z}_\alpha^\dagger \rangle \langle \tilde{z}_\beta \rangle \propto \langle \tilde{z}_\alpha^\dagger \rangle \langle \tilde{z}_\beta \rangle$. Recall that $\langle f_{k\alpha}^\dagger f_{k\beta} \rangle$ is determined by an averaging of $f_{k\alpha}^\dagger f_{k\beta}$ with respect to $H_f^{\rm mf}$, and it is nonzero in response to an effective "field" $W_k^{\alpha\beta}$ applied to the kinetic hybridization operator $f_{k\alpha}^\dagger f_{k\beta}$ in $H_f^{\rm mf}$. For the case we consider, with a nonzero orbital level difference, $\Delta_{\alpha,\beta} \equiv \Delta_\alpha - \Delta_\beta \neq 0$, the susceptibility describing the linear response of $\langle f_{k\alpha}^\dagger f_{k\beta} \rangle$ to $W_k^{\alpha\beta}$ will be finite, leading to $\langle f_{k\alpha}^\dagger f_{k\beta} \rangle \propto W_k^{\alpha\beta} \propto \langle \tilde{z}_\alpha \rangle \langle \tilde{z}_\beta^\dagger \rangle$; this is illustrated in Fig. 1, top panel. As a result, the kinetic hybridization of the spinons is

$$\langle H_f^{\rm mf} \rangle_{\alpha\beta} = \sum_k \epsilon_k^{\alpha\beta} \langle \tilde{z}_\alpha^\dagger \rangle \langle \tilde{z}_\beta \rangle \langle f_{k\alpha}^\dagger f_{k\beta} \rangle \propto |\langle \tilde{z}_\alpha \rangle|^2 |\langle \tilde{z}_\beta \rangle|^2. \tag{19}$$

Consider next Eq. (13), which shows that the slave-spin operator $\tilde{z}_\alpha$ for orbital α experiences an effective field of $h_\alpha = \sum_\beta Q_{\alpha\beta}^f \langle \tilde{z}_\beta \rangle$, where $Q_{\alpha\beta}^f$ is defined in Eq. (14). Similar reasoning as in the previous paragraph gives rise to

$$Q_{\alpha\beta}^f \propto \langle \tilde{z}_\alpha \rangle \langle \tilde{z}_\beta^\dagger \rangle, \tag{20}$$

for $\alpha \neq \beta$ and $\Delta_{\alpha,\beta} \neq 0$. In other words, $h_\alpha \propto \langle \tilde{z}_\alpha \rangle |\langle \tilde{z}_\beta \rangle|^2$, as illustrated in Fig. 1. Taking the expectation value of $\tilde{z}_\alpha^\dagger$ with respect to $H_S^{\rm mf}$ then yields the following component of the free energy from $H_S^{\rm mf}$:

$$\langle H_S^{\rm mf} \rangle_{\alpha\beta} \to |\langle \tilde{z}_\alpha \rangle|^2 |\langle \tilde{z}_\beta \rangle|^2. \tag{21}$$

From Eqs. (19) and (21), we see that for both the spinons and the slave spins, the interorbital correlations appear as a biquadratic coupling $|z_\alpha|^2 |z_\beta|^2$. This biquadratic interaction is a natural result of a self-consistent solution of the two saddle-point equations, Eqs. (12) and (13) (Fig. 1). It is crucial to the stabilization of an OSMP. As z_α approaches zero, so does $Q_{\alpha\beta}^f$; correspondingly, the effective field acting on the slave spin, h_α, also goes to zero in spite of a nonzero z_β, making the OSMP an internally consistent solution.

To see how the OSMP arises more explicitly, we can construct a Landau free-energy functional in terms of the quasiparticle weights, z_α. For simplicity of notation, we take the $3d$ xy and another $3d$ orbital as orbitals 1 and 2, but our analysis straightforwardly applies to the case of more than two

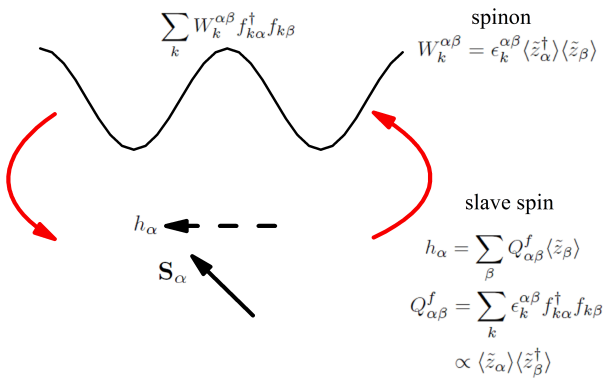

FIG. 1. (Color online) Illustrating the effect of the interorbital kinetic hybridization in the $U(1)$ slave-spin theory. The black curve shows the effective spinon dispersion, which is generated by $W_k^{\alpha\beta} f_{\alpha\sigma}^\dagger f_{\beta\sigma}$. (The physical spin index σ is suppressed in the figure legends.) Meanwhile, the slave-spin $\mathbf{S}_\alpha$ experiences a local field, $h_\alpha = \sum_\beta Q_{\alpha\beta}^f \langle \tilde{z}_\beta \rangle$, where $Q_{\alpha\beta}^f \propto \langle \tilde{z}_\alpha \rangle \langle \tilde{z}_\beta^\dagger \rangle$. The red arrows indicate the self-consistency between $W_k^{\alpha\beta}$ and h_α, which results in a biquadratic interorbital coupling as shown in Eqs. (19) and (21).

orbitals. The free-energy density reads

$$f = \sum_{\alpha=1,2} \left(r_\alpha |z_\alpha|^2 + u_\alpha |z_\alpha|^4 \right) + v |z_1|^2 |z_2|^2, \tag{22}$$

in which the biquadratic coupling v term comes from the kinetic hybridization as discussed above. The quadratic terms $r_\alpha |z_\alpha|^2$ arise from the kinetic energy of the saddle-point Hamiltonian in Eq. (13) [as well as in Eq. (12)]. For example, since $\sum_k \langle f_{k\alpha}^\dagger f_{k\alpha} \rangle$ is the spinon density in orbital α, which is of order $O(1)$ even when z_α approaches zero; thus, $Q_{\alpha\alpha}^f \sim O(1)$, and gives rise to the quadratic terms $(r_\alpha |z_\alpha|^2)$ in the Landau free-energy density. Taking the derivatives with respect to $|z_\alpha|$, we obtain

$$\frac{\partial f}{\partial |z_1|} = |z_1| (2r_1 + 4u_1 |z_1|^2 + 2v |z_2|^2) = 0, \tag{23}$$

$$\frac{\partial f}{\partial |z_2|} = |z_2| (2r_2 + 4u_2 |z_2|^2 + 2v |z_1|^2) = 0. \tag{24}$$

There could then be three solutions:

1. $r_1 + 2u_1 |z_1|^2 + v |z_2|^2 = r_2 + 2u_2 |z_2|^2 + v |z_1|^2 = 0$, which yields $|z_1| \neq 0$, $|z_2| \neq 0$, corresponding to a metallic phase;

2. $|z_1| = |z_2| = 0$, corresponding to a Mott insulator;

3. $|z_1| = 0$, $|z_2| = \sqrt{-\frac{r_2}{2u_2}}$ (or $|z_2| = 0$, $|z_1| = \sqrt{-\frac{r_1}{2u_1}}$), corresponding to an OSMP.

IV. THE ORBITAL-SELECTIVE MOTT TRANSITION IN A FIVE-ORBITAL MODEL FOR IRON CHALCOGENIDES AS AN ILLUSTRATION OF THE LANDAU THEORY

In the previous section we have constructed a Landau theory, and shown that an OSMP is an allowed solution to the free-energy functional. Strictly speaking, the Landau theory works only when z_α is sufficiently small for each orbital. In the more realistic situation, such as in the five-orbital model for iron chalcogenides, $z_{xz/yz}$ may still be sizable across the OSMT for the localization of the $3d$ xy orbital. Therefore, it is instructive to show that the general consideration obtained in the previous section is valid in the five-orbital model.

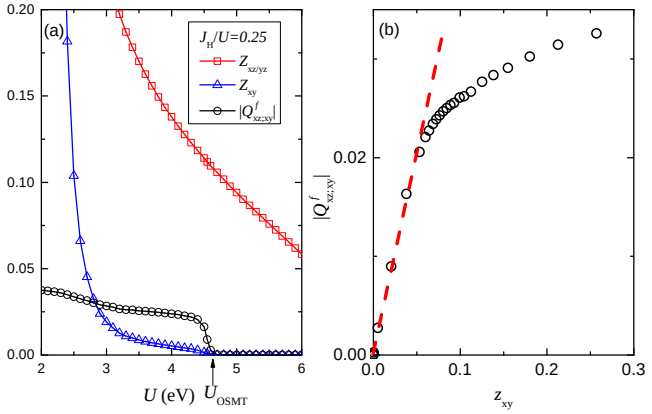

FIG. 2. (Color online) (a): The evolution of the quasiparticle spectral weights Z_{xy}, $Z_{xz/yz}$, and the renormalization factor for the interorbital hybridization $|Q^f_{xz/yz,xy}|$ as a function of U in a five-orbital model for $K_xFe_{2-y}Se_2$ (without ordered iron vacancies), with $J_H/U = 0.25$ and electron filling $n = 6$. An OSMT occurs at $U = U_{OSMT}$. (b): $|Q^f_{xz/yz,xy}|$ vs. z_{xy}. The linear dependence expected from the Landau analysis is shown by a linear fit (dashed line). The model parameters are the same as in (a).

For this reason, we revisit the OSMT in the five-orbital model for $K_xFe_{2-y}Se_2$ system.[11] For an illustrative purpose, we consider the case without iron-vacancy order and with the electron filling $n = 6$. For definiteness, we fix the ratio of the Hund's rule coupling to the intraorbital Hubbard interaction to $J_H/U = 0.25$. We have calculated the evolution of the quasiparticle spectral weights $Z_\alpha = |z_\alpha|^2$ with increasing U for the $3d$ xz/yz and xy orbitals. The results are summarized in Fig. 2(a). An OSMT takes place, at which Z_{xy} vanishes, where Z_{xz} (as well as $Z_{yz} = Z_{xz}$, $Z_{x^2-y^2}$ and $Z_{3z^2-r^2}$) remain nonzero.

On approach of the OSMT, we can investigate how the renormalization factor for the interorbital hybridization, $Q^f_{xz,xy}$ (and $Q^f_{yz,xy}$, which is equal to $Q^f_{xz,xy}$ as dictated by the C_4 symmetry) behaves. We see that for U smaller than 4 eV, where the system is sufficiently away from the OSMT, $Q^f_{xz,xy}$ decreases relatively slowly. By contrast, as U gets closer to U_{OSMT}, where the system enters the linear-response regime, $Q^f_{xz,xy}$ rapidly decreases. This behavior implies that suppressing the interorbital hybridization is key to the OSMT. Indeed, it follows from the general analysis in the previous section that $Q^f_{xz/yz,xy}$ would vanish as the OSMT is reached. The relationship $Q^f_{xz,xy} \propto z_{xz}z_{xy}$ would be expected if both z_{xy} and z_{xz} were small. In our case, since z_{xz} is still sizable across the OSMT, the relationship $Q^f_{xz,xy} \propto z_{xz}$ would acquire sizable corrections; such corrections will not affect the existence or critical behavior of the OSMT. On the other hand, near the transition, $Q^f_{xz,xy}$ is expected to be linearly proportional to z_{xy}. This proportionality is indeed satisfied, as shown in Fig. 2(b).

V. DISCUSSIONS

We have analyzed the OSMT in multiorbital models pertinent to the FeSCs. From a Landau free-energy functional, the OSMP can be realized because the effective coupling between the quasiparticle weights of the different orbitals is biquadratic (instead of bilinear). In our analysis, we have emphasized the role of a nonzero orbital level splitting between the $3d$ xy orbital and the other $3d$ orbitals (particularly the xz/yz orbitals).

We have clarified how the crucial feature of the Landau analysis, namely the absence of the bilinear coupling between the quasiparticle weights of the different orbitals, arises within the $U(1)$ slave-spin approach. Crucial to this feature is the coupling of the pseudofermions at different sites. At the saddle point level, the slave spins are treated through a local description, with its condensate capturing the quasiparticle weight. By contrast, the effective Hamiltonian of the pseudofermions, which is at least bilinear, must contain intersite coupling. Because the slave spins have a $U(1)$ symmetry, we can construct the saddle-point equations in the gauge with the slave spins alone describing the charge degrees freedom. Correspondingly, the physical spin degrees of freedom are entirely captured by the pseudofermions. Thus, the intersite pseudofermion coupling reflects the intersite coupling of the physical spin degrees of freedom. In this way, the analysis here highlights the importance of the intersite spin correlations in renormalizing the interorbital kinetic hybridization to zero, as the OSMP is realized.

This insight suggests complementary means of studying the OSMP. In terms of physical variables, another setting in which interorbital hybridization has been shown to be dynamically suppressed is in the heavy fermion systems[51–53]. There, the RKKY spin-exchange interactions compete against the Kondo hybridization between the f and conduction electrons, and the resulting destruction of the Kondo hybridization can be viewed as an OSMT of f electrons. One of the means that captures this interplay between the hybridization and collective spin correlations is the extended dynamical mean field theory (EDMFT)[54]. In the EDMFT approach, such intersite spin correlations are treated in terms of physical spins (instead of the auxiliary fermions).

For the multiorbital Hubbard Hamiltonian, Eq. (1), the effect of intersite spin correlations can be taken into account by adding an explicit exchange interaction, J_{ij}, between the

spins at the different sites. The total Hamiltonian is then the multiorbital analogue of the one-band Hubbard-Heisenberg model[55]. (Alternatively, such a term can be considered as being effectively generated at an intermediate energy scale, by integrating out the incoherent part of the slave-spin fluctuation spectrum.) Within the EDMFT, the effects of such intersite correlations are studied dynamically through a bosonic bath, whose spectrum is determined self-consistently. This coupling of the bosonic bath to the local spin degrees of freedom competes with the hybridization term. When the competition is strong enough, it can drive the hybridization to zero, thereby realizing an OSMP. For the Anderson lattice model relevant to heavy fermion systems, this method has already shown that an OSMP arises, even when an on-site hybridization is present. This line of study holds a clear promise to bring about further new insights into the orbital-selective Mott physics in multiorbital models pertinent to the iron-based superconductors.

We close this section by noting that the orbital-selective Mott physics is also of interest in a variety of other contexts, such as VO_2[56] and multiorbital systems at low dimensions[57–59].

VI. CONCLUSION

In this paper, we have revisited on the orbital-selective Mott phase identified in previous studies in the multiorbital Hubbard models for iron pnictides and iron chalcogenides. This type of models contains kinetic hybridization between the $3d$ electron orbitals. We have constructed a Landau free-energy functional in terms of the quasiparticle renormalization factor, z_α. We have shown that a kinetic hybridization between the different orbitals introduces biquadratic couplings between the quasiparticle renormalization z factors of the different orbitals. The absence of bilinear couplings is a property that is generic to multiorbital models with nonzero orbital level splittings. It makes the orbital-selective Mott phase possible.

Within the microscopic $U(1)$ slave-spin approach, the absence of the bilinear coupling among the z's can be traced to the intersite spin correlations. This amounts to a linear relationship between the renormalized interorbital kinetic hybridization and the quasiparticle weight for the $3d$ xy orbital (when the latter is sufficiently small). Such a linear relationship is shown to be satisfied in the previously identified solution near the orbital-selective Mott transition.

More generally, our analysis here illustrates that intersite spin correlations are important in renormalizing the interorbital kinetic hybridization to zero, thereby generating the OSMP. This insight suggests additional means of studying the orbital-selective Mott physics in the multiorbital models. In particular, an extended dynamical mean field theory allows the study of the dynamical competition between the interorbital hybridization and collective spin correlations. This method has been used to demonstrate an OSMP in the case of Anderson lattice model, which contains an on-site hybridization. It would be a promising way to gain further insights into the dynamical suppression of the hybridization effect for the orbital-selective Mott phase in multiorbital models pertinent to the iron-based superconductors. Given the growing recognition that the orbital selectivity plays an important role in the iron pnictides and iron chalcogenides, such studies are clearly worth the efforts.

In short, through a Landau analysis, we have demonstrated the robustness of the orbital-selective Mott phase in multiorbital models pertinent to the iron-based superconductors. We have also suggested means for further theoretical studies of the orbital-selective Mott physics, which may be relevant to bad metals in a variety of correlated electron systems.

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After completing this manuscript, we became aware of another work [60] which studied a particle-hole-symmetric multiorbital Hubbard model with an inter-orbital kinetic and/or onsite hybridization and without an orbital-level splitting. The two works reached consistent conclusions where there is overlap.

Appendix A: Derivation of the saddle-point equations

To facilitate the detailed derivations and analyses presented in the next two appendices, we summarize here the derivation[32] of the equations Eqs. (12) and (13) from Eq. (10). By decomposing the slave (Schwinger) boson – or, equivalently, the slave spin – and the pseudofermion operators in Eq. (10), we obtain

$$H_f^{\rm mf} = \frac{1}{2}\sum_{ij\alpha\beta\sigma} t_{ij}^{\alpha\beta}\langle \hat{z}_{i\alpha\sigma}^\dagger \hat{z}_{j\beta\sigma}\rangle f_{i\alpha\sigma}^\dagger f_{j\beta\sigma} + \sum_{i\alpha\sigma}(\Delta_\alpha - \lambda_{i\alpha\sigma} - \mu) f_{i\alpha\sigma}^\dagger f_{i\alpha\sigma}, \qquad \text{(A1)}$$

$$H_S^{\rm mf} = \frac{1}{2}\sum_{ij\alpha\beta\sigma} t_{ij}^{\alpha\beta}\langle f_{i\alpha\sigma}^\dagger f_{j\beta\sigma}\rangle z_{i\alpha\sigma}^\dagger z_{j\beta\sigma} + \sum_{i\alpha\sigma}\frac{\lambda_{i\alpha\sigma}}{2}(\hat{n}_{i\alpha\sigma}^a - \hat{n}_{i\alpha\sigma}^b) + H_{\rm int}^S, \qquad \text{(A2)}$$

where $\langle\cdots\rangle$ denotes the averaging taken with respect to these Hamiltonians, and $\hat{n}^a_{i\alpha\sigma} = a^\dagger_{i\alpha\sigma}a_{i\alpha\sigma}$. Here, $H_S^{\rm mf}$ has an internal $U(1)$ symmetry of the bosons. For the single-orbital case, it is a Bose-Hubbard model for two species of hard-core bosons (or, equivalently, a model for interacting XY spins), and it possesses a phase transition from a bosonic Mott insulator to a superfluid. More generally, we start from the side with a Bose condensation in the composite boson field $z_{i\alpha\sigma}$. The leading term is captured by a single-site decomposition in Eq. (A1) and Eq. (A2), with $\hat{z}^\dagger_{i\alpha\sigma}\hat{z}_{j\beta\sigma} \approx \langle\hat{z}^\dagger_{i\alpha\sigma}\rangle\hat{z}_{j\beta\sigma} + \hat{z}^\dagger_{i\alpha\sigma}\langle\hat{z}_{j\beta\sigma}\rangle - \langle\hat{z}^\dagger_{i\alpha\sigma}\rangle\langle\hat{z}_{j\beta\sigma}\rangle$. We focus on the paramagnetic phase with the translational symmetry preserved, in which the spin and site indices can be dropped without causing ambiguity. The boson Hamiltonian then reads

$$H_S^{\rm mf} \approx \sum_{\alpha\beta} Q^f_{\alpha\beta}\left(\langle\hat{z}^\dagger_\alpha\rangle\hat{z}_\beta + \langle\hat{z}_\beta\rangle\hat{z}^\dagger_\alpha\right) + \sum_\alpha \frac{\lambda_\alpha}{2}(\hat{n}^a_\alpha - \hat{n}^b_\alpha) + H^S_{\rm int}. \tag{A3}$$

In Eq. (A3), we Taylor-expand $\hat{z}_\alpha$ and $\hat{z}^\dagger_\alpha$ in terms of $\hat{A} - \langle\hat{A}\rangle$ (where $\hat{A} = \hat{n}^a, \hat{n}^b, a^\dagger b$), and keep up to the linear terms in $\hat{A} - \langle\hat{A}\rangle$. This leads to

$$\hat{z}^\dagger_\alpha \approx \tilde{z}^\dagger_\alpha + \langle\tilde{z}^\dagger_\alpha\rangle\eta_\alpha[\hat{n}^a_\alpha - \hat{n}^b_\alpha - (2n^f_\alpha - 1)], \tag{A4}$$

where $\tilde{z}^\dagger_\alpha = \langle P^+_\alpha\rangle a^\dagger_\alpha b_\alpha\langle P^-_\alpha\rangle$. The details involved in the derivation of Eq. (A4) is given in Appendix B. Note that $n^f_\alpha = \langle\hat{n}^a_\alpha\rangle = 1-\langle\hat{n}^b_\alpha\rangle$ from the constraints. With this, we find that $\langle\hat{z}_\alpha\rangle = \langle\tilde{z}_\alpha\rangle$, which is defined as z_α (*cf.* Eq. (11)). Using Eq. (A4), the saddle-point Hamiltonian given in Eq. (A3) becomes

$$H_S^{\rm mf} \approx \sum_{\alpha\beta} Q^f_{\alpha\beta}\left(\langle\tilde{z}^\dagger_\alpha\rangle\tilde{z}_\beta + \langle\tilde{z}_\beta\rangle\tilde{z}^\dagger_\alpha\right) + \sum_\alpha\left(\frac{\lambda_\alpha}{2} + \bar{\epsilon}_\alpha\eta_\alpha\right)(\hat{n}^a_\alpha - \hat{n}^b_\alpha) + H^S_{\rm int}. \tag{A5}$$

Further using the constraint Eq. (5), we can redefine λ_α to move the term proportional to η_α to $H_f^{\rm mf}$ by introducing an effective onsite potential $\tilde{\mu}_\alpha$. We then arrive at the two saddle-point Hamiltonians, Eqs. (12) and (13). Recognizing the hard-core nature of the bosons (or, equivalently, recognizing that they can be transformed back to XY spins), we can exactly diagonalize the Hamiltonian in Eq. (13) even thought it contains quartic terms of the boson operators in $H^S_{\rm int}$.

Appendix B: Derivation of Eq. (A4)

Starting from the definition of the projectors $P^\pm_{i\alpha\sigma} = 1/\sqrt{1/2 + \delta \pm (\hat{n}^a_{i\alpha\sigma} - \hat{n}^b_{i\alpha\sigma})/2}$, we expand $\hat{n}^a_{i\alpha\sigma} - \hat{n}^b_{i\alpha\sigma}$ about its saddle-point value and obtain

$$P^+_\alpha = \frac{1}{\sqrt{\left[\frac{1}{2} + \frac{1}{2}(\langle\hat{n}^a_\alpha\rangle - \langle\hat{n}^b_\alpha\rangle) + \delta\right]\left[1 + \frac{\Delta\hat{n}}{1+\langle\hat{n}^a_\alpha\rangle - \langle\hat{n}^b_\alpha\rangle + 2\delta}\right]}} \approx \frac{1}{\sqrt{\frac{1}{2} + \frac{1}{2}(\langle\hat{n}^a_\alpha\rangle - \langle\hat{n}^b_\alpha\rangle) + \delta}}\left\{1 - \frac{\Delta\hat{n}}{2(1 + \langle\hat{n}^a_\alpha\rangle - \langle\hat{n}^b_\alpha\rangle + 2\delta)}\right\}, \tag{B1}$$

where $\Delta\hat{n} = (\hat{n}^a_\alpha - \hat{n}^b_\alpha) - (\langle\hat{n}^a_\alpha\rangle - \langle\hat{n}^b_\alpha\rangle)$. Here we have again dropped the site and spin indices for simplicity. By using the constraint in Eq. (5) we have $\langle\hat{n}^a_\alpha\rangle - \langle\hat{n}^b_\alpha\rangle = 2n^f_\alpha - 1$. This further simplifies Eq. (B1) to

$$P^+_\alpha \approx \frac{1}{\sqrt{n^f_\alpha + \delta}}\left(1 - \frac{\Delta\hat{n}}{4(n^f_\alpha + \delta)}\right). \tag{B2}$$

Similarly, we have

$$P^-_\alpha \approx \frac{1}{\sqrt{1 - n^f_\alpha + \delta}}\left(1 + \frac{\Delta\hat{n}}{4(1 - n^f_\alpha + \delta)}\right). \tag{B3}$$

Inserting these into the definition of $\hat{z}^\dagger_\alpha$ in Eq. (6), we obtain

$$\hat{z}^\dagger_\alpha \approx \langle P^+_\alpha\rangle\left(1 - \frac{\Delta\hat{n}}{4(n^f_\alpha + \delta)}\right)\left[\langle a^\dagger_\alpha b_\alpha\rangle + (a^\dagger_\alpha b_\alpha - \langle a^\dagger_\alpha b_\alpha\rangle)\right]\langle P^-_\alpha\rangle\left(1 + \frac{\Delta\hat{n}}{4(1 - n^f_\alpha + \delta)}\right) \approx \langle P^+_\alpha\rangle a^\dagger_\alpha b_\alpha\langle P^-_\alpha\rangle + \langle P^+_\alpha\rangle\langle a^\dagger_\alpha b_\alpha\rangle\langle P^-_\alpha\rangle\frac{(2n^f_\alpha - 1)\Delta\hat{n}}{4n^f_\alpha(1 - n^f_\alpha) + \delta} + O(\Delta\hat{n}^2), \tag{B4}$$

where we have defined $\langle P^+_\alpha\rangle = 1/\sqrt{n^f_\alpha + \delta}$ and $\langle P^-_\alpha\rangle = 1/\sqrt{1 - n^f_\alpha + \delta}$. Using the definition of $\tilde{z}^\dagger_\alpha$ given in Eq. (15) and that of η_α given in Eq. (18), we arrive at

$$\hat{z}^\dagger_\alpha \approx \tilde{z}^\dagger_\alpha + \langle\tilde{z}^\dagger_\alpha\rangle\eta_\alpha\Delta\hat{n}, \tag{B5}$$

which, then, yields Eq. (A4).

Appendix C: Recovery of the proper noninteracting limit in the $U(1)$ slave-spin approach

In this section we show how the saddle-point equations of the $U(1)$ slave-spin theory recovers the correct noninteracting ($U = J_{\rm H} = 0$) limit for a general multiorbital Hubbard model.

In the noninteracting limit, the quasiparticle spectral weight of the itinerant electrons is not renormalized by the electron correlations; therefore

$$Z_\alpha = 1 \tag{C1}$$

for each orbital. In addition, the spinon dispersion should be identical to the original tight-binding dispersion of the physical d electrons. Both features would be captured if Eq. (C1) is accompanied by

$$\lambda_\alpha = \tilde{\mu}_\alpha. \tag{C2}$$

Indeed, in this case Eq. (12) becomes

$$H_f^{\rm mf} = \sum_{k\alpha\beta} \left\{ \epsilon_k^{\alpha\beta} + \delta_{\alpha\beta}(\Delta_\alpha - \mu) \right\} f_{k\alpha}^\dagger f_{k\beta}. \tag{C3}$$

This generates exactly the same dispersion as for the original tight-binding model of the $3d$ electrons in Eq. (2).

We now show that Eqs. (C1) and (C2) indeed solve the saddle-point equations in the non-interacting case. Our strategy is to show that $\lambda_\alpha = \tilde{\mu}_\alpha$ leads to $Z_\alpha = 1$ in this case. With $\lambda_\alpha = \tilde{\mu}_\alpha$, the Hamiltonian $H_S^{\rm mf}$ at $U = J_{\rm H} = 0$ in Eq. (13) becomes

$$\begin{aligned} H_S^{\rm mf} &= \sum_{\alpha\beta} \left\{ Q_{\alpha\beta}^f \left(\langle \tilde{z}_\alpha^\dagger \rangle \tilde{z}_\beta + \langle \tilde{z}_\beta \rangle \tilde{z}_\alpha^\dagger \right) + \delta_{\alpha\beta} \frac{\tilde{\mu}_\alpha}{2} (\hat{n}_\alpha^a - \hat{n}_\alpha^b) \right\} \\ &= \sum_\alpha \left\{ h_\alpha \tilde{z}_\alpha^\dagger + h_\alpha^* \tilde{z}_\alpha + (h_\alpha \langle \tilde{z}_\alpha^\dagger \rangle \eta_\alpha + h_\alpha^* \langle \tilde{z}_\alpha \rangle \eta_\alpha)(\hat{n}_\alpha^a - \hat{n}_\alpha^b) \right\}, \\ &= \sum_\alpha (a_\alpha^\dagger, b_\alpha^\dagger) \mathcal{H}_{S\alpha}^{\rm mf} \begin{pmatrix} a_\alpha \\ b_\alpha \end{pmatrix}, \end{aligned} \tag{C4}$$

where $h_\alpha = \sum_\beta Q_{\alpha\beta}^f \langle \tilde{z}_\beta \rangle$, and $\mathcal{H}_{S\alpha}^{\rm mf}$ is a 2×2 matrix,

$$\mathcal{H}_{S\alpha}^{\rm mf} = \begin{pmatrix} \frac{(2n_\alpha^f - 1)(h_\alpha \langle \tilde{z}_\alpha^\dagger \rangle + \text{c.c.})}{4n_\alpha^f (1 - n_\alpha^f)} & \frac{h_\alpha}{\sqrt{n_\alpha^f (1 - n_\alpha^f)}} \\ \frac{h_\alpha^*}{\sqrt{n_\alpha^f (1 - n_\alpha^f)}} & \frac{-(2n_\alpha^f - 1)(h_\alpha \langle \tilde{z}_\alpha^\dagger \rangle + \text{c.c.})}{4n_\alpha^f (1 - n_\alpha^f)} \end{pmatrix}. \tag{C5}$$

Without losing generality, we take $\langle \tilde{z}_\alpha \rangle$ to be real, in which case h_α is also real. By diagonalizing $\mathcal{H}_{S\alpha}^{\rm mf}$, we obtain that, at $T = 0$,

$$|\langle \tilde{z}_\alpha \rangle| = \frac{1}{2\sqrt{(n_\alpha^f - 1/2)^2 |\langle \tilde{z}_\alpha \rangle|^2 + n_\alpha^f (1 - n_\alpha^f)}}. \tag{C6}$$

This equation has two solutions, either $|\langle \tilde{z}_\alpha \rangle| = 1$ or $|\langle \tilde{z}_\alpha \rangle| = -1/(2n_\alpha^f - 1)^2 < 0$. Because the second solution is unphysical, we have $|\langle \tilde{z}_\alpha \rangle| = 1$, corresponding to $Z_\alpha = 1$ for each orbital α.

Therefore, in the noninteracting case, $\lambda_\alpha = \tilde{\mu}_\alpha$, and the saddle-point equations of the $U(1)$ slave-spin theory recover the correct noninteracting limit of the multiorbital Hubbard model. In the case of degenerate orbitals at half-filling, this result is straightforward. On the other hand, for the generic case of non-degenerate orbitals, when the electron density of orbital α (which is proportional to $\langle \hat{n}_\alpha^a \rangle - \langle \hat{n}_\alpha^b \rangle$) is away from half-filling, λ_α is generally nonzero, and a nonzero $\tilde{\mu}_\alpha$ is crucial for the recovery of the proper noninteracting limit.

1. Comparison with the Z_2 slave-spin theory

We now make a comparison between the $U(1)$ and the Z_2 slave-spin theory. In the Z_2 formulation, the field $\tilde{\mu}_\alpha$ is absent. Therefore, for multiorbital models with non-degenerate orbitals away from half-filling, the saddle-point equations of the Z_2 formulation do not correctly capture the limit of zero interactions. It has been shown in Ref. 32 that by choosing a particular projector, the saddle-point Hamiltonian $H_S^{\rm mf}$ of the $U(1)$ theory – which does incorporate the parameters $\tilde{\mu}_\alpha$ – can be written in a form appropriate for the Z_2 slave-spin theory. This suggests a route to remedy the Z_2 formulation in the generic case of multiorbital models with non-degenerate orbitals away from half-filling, such that the $\tilde{\mu}_\alpha$ parameters be introduced; whether this can be done in a natural way remains unclear. Note that, even if this is achieved, the agreement between the saddle-point results of the $U(1)$ and Z_2 formulations only applies to the metallic phase where the slave spins are ordered. The Z_2 theory is insufficient to describe a Mott insulating state, due to the fact that the pseudofermions must carry not only the physical spin degrees of freedom but also the physical charge degrees of freedom[48].

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