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Analytical slave-spin mean-field approach to orbital selective Mott insulators

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We use the slave-spin mean-field approach to study particle-hole symmetric one- and two-band Hubbard models in the presence of Hund's coupling interaction. By analytical analysis of the Hamiltonian, we show that the locking of the two orbitals vs orbital selective Mott transition can be formulated within a Landau-Ginzburg framework. By applying the slave-spin mean field to impurity problems, we are able to make a correspondence between impurity and lattice. We also consider the stability of the orbital selective Mott phase to the hybridization between the orbitals and study the limitations of the slave-spin method for treating interorbital tunnelings in the case of multiorbital Bethe lattices with particle-hole symmetry.

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I. INTRODUCTION

Iron-based superconductors are the subject of intensive study in the pursuit of high-temperature superconductivity [1–7]. These systems are interacting via Coulomb repulsion and Hund's rule coupling and they require the consideration of multiple bands with crystal field and interorbital tunneling [8,9]. Early DMFT studies pointed out the importance of the correlations [10] and Hund's rule coupling [11], and reported a noticeable tendency towards orbital differentiation, with the d_{xy} orbital more localized than the rest [12]. They also demonstrated orbital-spin separation [13–15]. Note that the orbital differentiations have been recently observed in experiments [16].

Another perspective on the electron correlations in these materials is that the combination of Hubbard interaction and Hunds coupling place them in proximity to a Mott insulator [17] and, correspondingly, the role of the orbital physics is provided by the orbital selective Mott picture [18,19]. Reference [18] demonstrated an orbital selective Mott phase in the multiorbital Hubbard models for such materials, in the presence of the interorbital kinetic tunneling. In such a phase, the wave function renormalization for some of the orbitals vanishes. Such a phase has been observed in angle-resolved photoemission spectroscopy (ARPES) experiments [20,21]. Although desirable, these effects have not been understood analytically in the past, partly due to the fact that an analytical study is difficult for realistic models. However, there are simpler models, capable of capturing part of the relevant physics, which are amenable to such analytical understanding, and this is what we study in this paper.

The mean-field approaches to study these problems rely on various parton constructions or slave-particle techniques. The latter include slave-bosons [22,23], the Kotliar-Ruckenstein four-boson method [24] and its rotationally invariant version [25], slave-rotor [26], Z_2 slave-spin [27–30] and its $U(1)$ version [18,31], slave spin-1 method [32], and the Z_2 mod-2 slave-spin method [33–35]. For a comparison of some of these methods see Appendix A. While these methods are all equivalent in the sense that they are exact representations of the partition function if the degrees of freedom are taken into account exactly, different approximation schemes required for analytical tractability lead to different final results and therefore they have to be tested against an unbiased method like the dynamical mean-field theory (DMFT) [36–44] in large dimensions or density matrix renormalization group (DMRG) [45] in one dimension.

We use the Z_2 slave-spin [27–30] in the following to study the orbital selectivity with and without Hund's coupling. We briefly go through the method for the sake of completeness and setting the notations. By studying the free energy analytically we show that close to the Mott transition the Hamiltonian can be described by a two-level system and develop a Landau-Ginzburg theory for the orbital selectivity. A Landau-like picture has been useful in understanding the Mott transition in infinite dimensions. Using a Landau-Ginzburg approach, we show how the interaction in the slave-spin sector tends to lock the two bands together in the absence of Hund's coupling and that the Hund's coupling promotes orbital selectivity. We also apply the method to an impurity problem (finite-U Anderson impurity) and its use as an impurity shows that the slave-spin mean-field result can be understood as the DMFT solution with a slave-spin impurity solver. This puts the method in perspective by showing that the mean-field result is a subset of DMFT. Additionally, we study the effect on the orbital selective Mott phase produced by interorbital kinetic tunneling and point out some of the limitations of the slave-spin for treating such interorbital tunneling in particle-hole symmetric Bethe lattices. Finally, we study the instability of the orbital selective Mott phase by including hybridization between the two orbitals.

A. Z_2 slave-spin method

We consider the Hamiltonian $H = H_0 + H_{\rm int}$, where

$$H_0 = \sum_{\langle ij\rangle\alpha\beta} t_{ij}^{\alpha\beta} d_{i\alpha}^\dagger d_{j\beta}. \quad (1)$$

We must demand $t_{ij}^{\alpha\beta} = [t_{ji}^{\beta\alpha}]^*$ for this Hamiltonian to be Hermitian. Unless mentioned explicitly, α is a superindex that contains both spin and orbital degrees of freedom. We replace the d fermions with the parton construction [27]

$$d_{i\alpha}^\dagger = \hat{z}_{i\alpha} f_{i\alpha}^\dagger, \quad \hat{z}_{i\alpha} = \tau_{i\alpha}^x. \quad (2)$$

$\tau_{i\alpha}^\mu$, $\mu = x,y,z$ are SU(2) Pauli matrices acting on a slave-spin subspace per site/spin/flavor, that is introduced to capture the occupancy of the levels. Slave-spin states $|\Uparrow_{i\alpha}\rangle$ and $|\Downarrow_{i\alpha}\rangle$

correspond to occupied/unoccupied states of orbital/spin α at site i, respectively. Away from half-filling, [28] has shown that $\tau^x_{i\alpha}$ has to be replaced with $\tau^+_{i\alpha}/2 + c_\alpha \tau^-_{i\alpha}/2$ where c is a gauge degree of freedom and is determined to give the correct noninteracting result. Here, for simplicity we assume *p-h* (particle-hole) symmetry and thus maintain the form of Eq. (2). Note that this parton construction has a Z_2 gauge degree of freedom $\tau^{x,y} \to -\tau^{x,y}$ and $f \to -f$, thus the name Z_2 slave-spin. The representation (2) increases the size of the Hilbert space. Therefore, the constraint

$$2 f^\dagger_{i\alpha} f_{i\alpha} = \tau^z_{i\alpha} + 1 \tag{3}$$

is imposed to remove the redundancy and restrict the evolution to the physical subspace. Using Eqs. (2) and (3) it can be shown that the standard anticommutation relations of d electrons are preserved.

Plugging Eq. (2) in H_0, and imposing the constraint (on average) via a Lagrange multiplier, we have

$$H_0 = \sum_{\langle ij\rangle\alpha\beta} t^{\alpha\beta}_{ij} f^\dagger_{i\alpha} f_{j\beta} \hat{z}^\dagger_{i\alpha} \hat{z}_{j\beta} - \lambda_{i\alpha}\big[f^\dagger_{i\alpha} f_{i\alpha} - \big(\tau^z_{i\alpha} + 1\big)/2\big].$$

On a mean-field level, the transverse Ising model of slave-spins can be decoupled from fermions. The decoupling is harmless in large dimensions [46] as the leading operator introduced by integrating over the fermions becomes irrelevant at the critical point of the transverse Ising model. Therefore, writing $H_0 \approx H_f + H_{0S}$, we have

$$\begin{aligned} H_{0S} &= \sum_{\langle ij\rangle\alpha\beta} \mathcal{J}^{\alpha\beta}_{ij}\big[\hat{z}^\dagger_{i\alpha}\hat{z}_{j\beta} - Q^{\alpha\beta}_{ij}\big] + \sum_{\alpha} \lambda_{i\alpha}\tau^z_{i\alpha}/2, \\ H_f &= \sum_{\langle ij\rangle\alpha\beta} \tilde{t}^{\alpha\beta}_{ij} f^\dagger_{i\alpha} f_{j\beta} - \lambda_{i\alpha}(f^\dagger_{i\alpha} f_{i\alpha} - 1/2), \end{aligned} \tag{4}$$

where $\tilde{t}^{\alpha\beta}_{ij} = t^{\alpha\beta}_{ij} Q^{\alpha\beta}_{ij}$ with $Q^{\alpha\beta}_{ij} = \langle \hat{z}^\dagger_{i\alpha}\hat{z}_{j\beta}\rangle$ the renormalized tunneling and $\mathcal{J}^{\alpha\beta}_{ij} = t^{\alpha\beta}_{ij}\langle f^\dagger_{i\alpha} f_{j\beta}\rangle$ an Ising coupling between slave-spins. The advantage of the parton construction (2) is that the interaction $H_{\rm int}\{\tau\}$ can be often written only in terms of the slave-spin variables, so that $H = H_f + H_S$ and $H_S = H_{0S} + H_{\rm int}$.

Particle-hole symmetry. *p-h* symmetry on the original Hamiltonian is defined as (n is a site index)

$$d_{n\alpha} \to (-1)^n d^\dagger_{n\alpha}, \quad d^\dagger_{n\alpha} \to (-1)^n d_{n\alpha}. \tag{5}$$

On a bipartite lattice, the nearest neighbor tunneling term preserves *p-h* symmetry, even in the presence of interorbital tunneling. So, if the system is at half-filling the Hamiltonian is invariant under *p-h* symmetry. We have to decide what *p-h* symmetry does to our slave-spin fields. We choose

$$f_{n\alpha} \to (-1)^n f^\dagger_{n\alpha}, \quad \tau^x_{n\alpha} \to \tau^x_{n\alpha}, \quad \tau^z_{n\alpha} \to -\tau^z_{n\alpha}. \tag{6}$$

So, we see that if the original Hamiltonian had *p-h* symmetry, we necessarily have $\lambda_{i\alpha} = 0$.

B. Single-site approximation

The Hamiltonian H_S is a multiflavor transverse Ising model which is nontrivial in general. Following [27–34] we do a further single-site mean field for the Ising model, exact in the limit of large dimensions:

$$\hat{z}^\dagger_{i\alpha}\hat{z}_{j\beta} \approx \langle \hat{z}^\dagger_{i\alpha}\rangle \hat{z}^\dagger_{j\beta} + \hat{z}^\dagger_{i\alpha}\langle \hat{z}_{j\beta}\rangle - \langle \hat{z}^\dagger_{i\alpha}\rangle\langle \hat{z}_{j\beta}\rangle. \tag{7}$$

The last term together with the second term of Eq. (8) contributes a $-2\sum_{\langle ij\rangle\alpha\beta}\mathcal{J}^{\alpha\beta}_{ij} Q^{\alpha\beta}_{ij}$. We define $z_{i\alpha} = \langle \hat{z}_{i\alpha}\rangle$ and $Z_{i\alpha} = |z_{i\alpha}|^2$ as the wave function renormalization of orbital α at site i. The slave-spin Hamiltonian becomes (using the symmetry of $\mathcal{J}^{\alpha\beta}_{ij}$)

$$H_{0S} = \sum_{i\alpha}(h^*_{i\alpha}\hat{z}_{i\alpha} + \text{H.c.}), \quad h_{i\alpha} = \sum_{j\beta}\mathcal{J}^{\alpha\beta}_{ij} z_{j\beta}. \tag{8}$$

In translationally invariant cases $h_{i\alpha}$ and $z_{i\alpha}$ become independent of the site index and $\mathcal{J}^{\alpha\beta}_{ij}$ depends on the distance between sites i and j. Therefore, we can simply write $h_\alpha = \sum_\beta \mathcal{J}_{\alpha\beta} z_\beta$ where

$$\mathcal{J}_{\alpha\beta} \equiv \sum_{(i-j)} \mathcal{J}^{\alpha\beta}_{(i-j)} = \sum_j t^{\alpha\beta}_{ij}\langle f^\dagger_{i\alpha} f_{j\beta}\rangle.$$

In the absence of interorbital tunneling, $\mathcal{J}$ is a diagonal matrix, corresponding to individual orbitals, where for each orbital $\mathcal{J}_\alpha = \int_{-D_\alpha}^{D_\alpha} d\epsilon \rho_\alpha(\epsilon) f(\epsilon)\epsilon$ is the average kinetic energy and depends only on bare parameters, unaffected by the renormalization factor z. For semicircular band (Bethe lattice), $\mathcal{J} = -0.2122D$, while for a 1D tight-binding model, $\mathcal{J}_{\rm 1D} = -0.318D$ with $D = 2t$. Since the operator $\hat{z}_\alpha = \tau^x_\alpha$ is Hermitian, we can write the slave-spin Hamiltonian (for each site) as [47]

$$H_S = \sum_\alpha a_\alpha \tau^x_\alpha + H_{\rm int}, \tag{9}$$

where $a_\alpha = 2\sum_\beta \mathcal{J}_{\alpha\beta} z_\beta$ (at half-filling). The only nontrivial part of computation is the diagonalization of H_S. This is a 4^M dimensional matrix where M is the number of orbitals. The free energy (per site) is

$$\begin{aligned} F &= -\frac{1}{\beta}\sum_{nk}\text{Tr}\log[-\mathbb{G}^{-1}_f(k,i\omega_n)] - 2\sum_n \mathcal{J}_{\alpha\beta} z^*_\alpha z_\beta \\ &\quad - \frac{1}{\beta}\log\{\text{Tr}[e^{-\beta H_S}]\}. \end{aligned} \tag{10}$$

Here $\beta = 1/T$ is the inverse temperature and the second part comes from two constants introduced in Eqs. (4) and (7). At zero temperature, the first term is just $\mathcal{J}_{\alpha\beta} z^*_\alpha z_\beta$ and the last term is E_S which depends on z via a. Hence,

$$F = -\sum_{\alpha\beta}\mathcal{J}_{\alpha\beta} z^*_\alpha z_\beta + E_S(\{a\}). \tag{11}$$

II. ONE-BAND MODEL

In the one-band case the interaction is $H_{\rm int} = U\sum_i \tilde{n}_{i\uparrow}\tilde{n}_{i\downarrow}$, where $\tilde{n}_{i\sigma} \equiv n_{i\sigma} - 1/2$. Representing the latter with $\tau^z_{i\sigma}/2$ and using translational symmetry we obtain $H_{\rm int} \to (U/4)\tau^z_\uparrow\tau^z_\downarrow$. Since we are in the paramagnetic phase ($a_\uparrow = a_\downarrow$), only the sum of the two spins $2\vec{T} = \vec{\tau}_\uparrow + \vec{\tau}_\downarrow$ enter (the singlet decouples) and the Hamiltonian can be written as $H_S = 2aT^x + \frac{U}{2}(T^z)^2 - U/4$, creating a connection to the spin-1 representation of [32]. Furthermore, we can form even and odd linear combinations of the empty and filled states and at

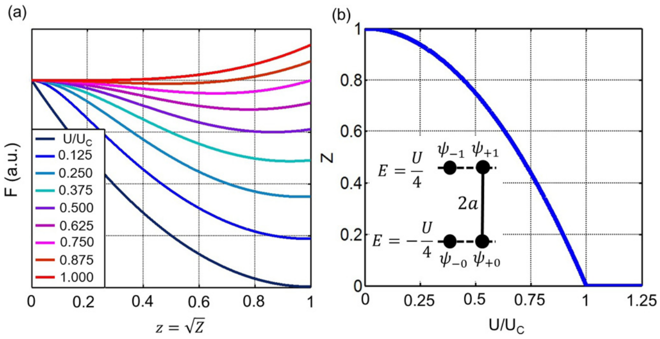

FIG. 1. (a) Free energy (at $T = 0$) as a function of z showing a second-order phase transition as U/U_C is varied. (b) Wave function renormalization $Z = |z|^2$ as a function of U has the Brinkman-Rice form. Inset: Diagrammatic representation of the slave-spin Hamiltonian. Each dot denotes an atomic state. Two states decouple and H_S is equivalent to that of Z_2 mod-2 slave-spin.

the half-filling only the even linear superpositions enters the the Hamiltonian. Thus, choosing atomic states of H_S as

$$|\psi_{\pm 0}\rangle = \frac{|\Uparrow\rangle \pm |\Downarrow\rangle}{\sqrt{2}}, \quad |\psi_{\pm 1}\rangle = \frac{|\Uparrow\Downarrow\rangle \pm |O\rangle}{\sqrt{2}}, \tag{12}$$

with $E_{\pm 0} = -U/4$ and $E_{\pm 1} = U/4$, the Hamiltonian can be written as $H_S = 2a\tau^x + (U/4)\tau^z$, where $\vec{\tau}$ are Pauli matrices acting between $|\psi_{+0}\rangle$ and $|\psi_{+1}\rangle$, i.e., it reduces to the Z_2 mod-2 slave-spin method [33,34]. In writing the states in Eq. (12) we have used a short-hand notation (also used in the next section) $|\Uparrow_\uparrow\Downarrow_\downarrow\rangle \to |\Uparrow\rangle$ and $|\Downarrow_\uparrow\Uparrow_\downarrow\rangle \to |\Downarrow\rangle$, $|\Uparrow_\uparrow\Uparrow_\downarrow\rangle \to |\Uparrow\Downarrow\rangle$ and so on. The inset of Fig. 1(b) shows a diagrammatic representation of the slave-spin Hamiltonian and two states decouple. The ground state of H_S is that of a two-level system

$$E_S = -\frac{U}{4}\sqrt{1 + (4\alpha/U)^2}, \tag{13}$$

with the level-repulsion $\alpha = 2a$ and the zero-temperature (free) energy is given by (factor of 2_s due to spin)

$$F = 2_s|\mathcal{J}|z^2 + E_S(z). \tag{14}$$

The free energy is plotted in Fig. 1(a) and it shows a second-order phase transition as U is varied. Close to the the transition $\alpha \to 0$, we can approximate $E_S \approx -2\alpha^2/U + 8\alpha^4/U^3$. Writing the first term of the free energy as $+\alpha^2/8|\mathcal{J}|$, we can read off the critical interaction $U_C = 16|\mathcal{J}|$. Minimization of the free energy gives the Gutzwiller projection formula of Brinkman and Rice [48]

$$Z = \begin{cases} 1 - u^2, & u < 1, \\ 0, & u > 1, \end{cases} \tag{15}$$

with $u = U/U_C$ and is plotted in Fig. 1(b). At finite temperature this procedure gives a first-order transition terminating at a critical point [34].

Spectral function. The Green's functions of the d fermions $G_d(\tau) \equiv \langle -T d_\sigma(\tau) d_\sigma^\dagger(0)\rangle$ factorizes

$$G_{d,\sigma}(\tau) \approx \langle -T f_\sigma(\tau) f_\sigma^\dagger(0)\rangle \langle T_\tau \tau_\sigma^x(\tau)\tau_\sigma^x(0)\rangle \tag{16}$$

to the product of f-electron Green's function and the slave-spin susceptibility and thus the spectral function is obtained from a convolution with the slave-spin function $A_d(\omega) = A_f(\omega) * A_S(\omega)$, in which A_f is a semicircular density of states with the width Z and within single-site approximation A_S is

$$A_S(\omega) = Z\delta(\omega) + \frac{1 - Z}{2}[\delta(\omega + 2E_S) + \delta(\omega - 2E_S)]. \tag{17}$$

The spectral density has the correct sum rule (in contrast to the usual slave-bosons [22,23]) since the commutation relations of the slave-spins are preserved. However, the single-site approximation does not capture incoherent processes, and this reflects in sharp Hubbard peaks in the Mott phase ($Z = 0$) where $A_f = \delta(\omega)$. Also, the spatial independence of the self-energy implies that the inverse effective mass of "spinons" $m/\tilde{m} = Z[1 + (m/k_F)\partial_k\Sigma]$ is zero in the Mott phase. This is again an artifact of the single-site approximation. Both of these problems are remedied, e.g., by doing a cluster mean-field calculation [28,33] or including quantum fluctuations around the mean-field value within a spin-wave approximation to the slave-spins [33].

The fact that (beyond single-site approximation) spinons disperse in spite of $\langle\tau^x\rangle \to 0$ and they carry a $U(1)$ charge as seen by Eq. (2), implies that vanishing of $\langle\tau^x\rangle$ does not generally correspond to the Mott phase in finite dimensions. However, in large dimensions, this is correct [34] and that is what we refer to in the following.

III. TWO-BAND MODEL

In absence of interorbital tunnelings, the free energy is

$$F = a_1^2/2|\mathcal{J}_1| + a_2^2/2|\mathcal{J}_2| + E_S(a_1, a_2), \tag{18}$$

where E_S is the ground state of the slave-spin Hamiltonian. For two bands we have the interaction

$$\begin{aligned} H_{\text{int}} = &\, U(\tilde{n}_{1\uparrow}\tilde{n}_{1\downarrow} + \tilde{n}_{2\uparrow}\tilde{n}_{2\downarrow}) \\ &+ U'(\tilde{n}_{1\uparrow}\tilde{n}_{2\downarrow} + \tilde{n}_{1\downarrow}\tilde{n}_{2\uparrow}) \\ &+ (U' - J)(\tilde{n}_{1\uparrow}\tilde{n}_{2\uparrow} + \tilde{n}_{1\downarrow}\tilde{n}_{2\downarrow}) + H_{XP}, \end{aligned} \tag{19}$$

where $\tilde{n}_\alpha \equiv n_{f\alpha} - 1/2 = \tau_\alpha^z/2$. The spin-flip and pair-tunneling terms are

$$\begin{aligned} H_{XP} = &-J_X[d_{1\uparrow}^\dagger d_{1\downarrow} d_{2\downarrow}^\dagger d_{2\uparrow} + d_{1\downarrow}^\dagger d_{1\uparrow} d_{2\uparrow}^\dagger d_{2\downarrow}] \\ &+ J_P[d_{1\uparrow}^\dagger d_{1\downarrow}^\dagger d_{2\downarrow} d_{2\uparrow} + d_{2\uparrow}^\dagger d_{2\downarrow}^\dagger d_{1\downarrow} d_{1\uparrow}]. \end{aligned} \tag{20}$$

This term mixes the Hilbert space of the f electron with that of slave-spins. Following [27–29] we include this term approximately by $d_{\alpha\sigma}^\dagger \to \tau_{\alpha\sigma}^+$ and $d_{\alpha\sigma} \to \tau_{\alpha\sigma}^-$ substitution so that it acts only in the slave-spin sector. The justification is that such a term captures the physics of spin-flip and pair-hopping. Using the spherical symmetry $U' = U - J$ this can be written as

$$\begin{aligned} H_{\text{int}} = &\frac{U}{2}(\tilde{n}_{1\uparrow} + \tilde{n}_{1\downarrow} + \tilde{n}_{2\uparrow} + \tilde{n}_{2\downarrow})^2 - \frac{U}{2} + H_{XP} \\ &- J[\tilde{n}_{1\uparrow}\tilde{n}_{2\downarrow} + \tilde{n}_{1\downarrow}\tilde{n}_{2\uparrow} + 2\tilde{n}_{1\uparrow}\tilde{n}_{2\uparrow} + 2\tilde{n}_{1\downarrow}\tilde{n}_{2\downarrow}]. \end{aligned} \tag{21}$$

For $J_X = J$ and $J_P = 0$ it has a rotational symmetry [49]. Alternatively, $U' = U - 2J$ and $J_X = J_P = J$ has rotational symmetry. The choice does not affect the discussion qualitatively. We keep the former values in the following.

Atomic orbitals. We start by diagonalizing the atomic Hamiltonian in absence of the hybridizations. Close to

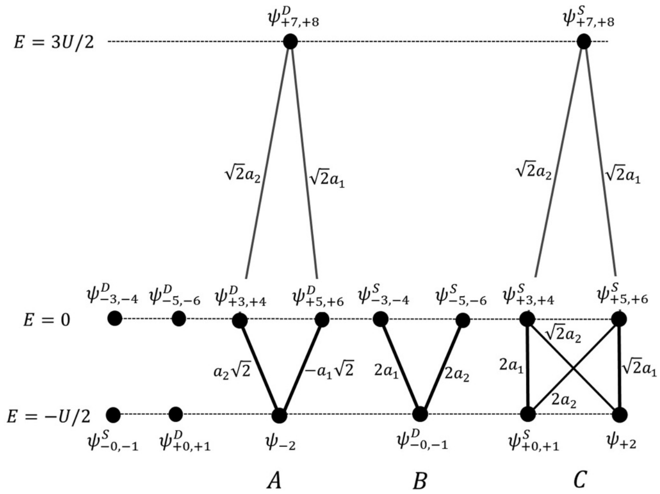

FIG. 2. Diagrammatic representation of the slave-spin Hamiltonian H_S in the two-band model with $J = 0$ and $\lambda_1 = \lambda_2 = 0$. Each dot represents an atomic state with a certain energy, denoted on the left, whereas the connecting lines represent off-diagonal elements of the Hamiltonian matrix, all assumed to be real. We have used the short-hand notation $\sqrt{2}\psi^{S/D}_{a,b} \equiv \psi_a \pm \psi_b$. Also note that $a_i = 2\mathcal{J}_i z_i$. The Hamiltonian factorizes into several sectors.

half-filling the doubly occupied states have the lowest energy and are given by

$$|\psi_{\pm 0}\rangle = \frac{|\Uparrow_1\Uparrow_2\rangle \pm |\Downarrow_1\Downarrow_2\rangle}{\sqrt{2}}, \quad E_{\pm 0} = -U - J/2,$$

$$|\psi_{\pm 1}\rangle = \frac{|\Uparrow_1\Downarrow_2\rangle \pm |\Downarrow_1\Uparrow_2\rangle}{\sqrt{2}}, \quad E_{\pm 1} = -U + J/2 \mp J_X,$$

$$|\psi_{\pm 2}\rangle = \frac{|\Uparrow\Downarrow_1, O_2\rangle \pm |O_1\Uparrow\Downarrow_2\rangle}{\sqrt{2}},$$

$$E_{\pm 2} = -U + 3J/2 \mp J_P.$$

These three doublets become the sixfold degenerate ground state when $J \to 0$. The 1,3-particle states are then

$$|\psi_{\pm 3}\rangle = |\Uparrow\Downarrow_1\rangle \frac{|\Uparrow_2\rangle \pm |\Downarrow_2\rangle}{\sqrt{2}}, \quad E_{\pm 3} = \lambda_1,$$

$$|\psi_{\pm 4}\rangle = |O\rangle_1 \frac{|\Uparrow_2\rangle \pm |\Downarrow_2\rangle}{\sqrt{2}}, \quad E_{\pm 4} = -\lambda_1,$$

$$|\psi_{\pm 5}\rangle = \frac{|\Uparrow_1\rangle \pm |\Downarrow_1\rangle}{\sqrt{2}} |\Uparrow\Downarrow_2\rangle, \quad E_{\pm 5} = \lambda_2,$$

$$|\psi_{\pm 6}\rangle = \frac{|\Uparrow_1\rangle \pm |\Downarrow_1\rangle}{\sqrt{2}} |O\rangle_2, \quad E_{\pm 5} = -\lambda_2,$$

and finally, there are two (empty and quadruple occupancy) states at the top of the ladder

$$|\psi_7\rangle = |\Uparrow\Downarrow\rangle_1 |\Uparrow\Downarrow\rangle_2, \quad E_7 = \lambda_1 + \lambda_2 + 3U - 3J/2,$$

$$|\psi_8\rangle = |O\rangle_1 |O\rangle_2, \quad E_8 = -\lambda_1 - \lambda_2 + 3U - 3J/2.$$

No Hund's rule coupling. The hybridization causes transition among atomic states. In the case of no Hund's coupling we can block diagonalize H_S into several sectors and diagrammatically represent it as shown in Fig. 2. Therefore, the calculation can be reduced from 16×16 to 5×5. The larger the level repulsion, the lower the ground state energy in each sector. The fact that the slave-spins decouple into several sectors brings about the possibility of ground-state crossings between various sectors as the parameters a_1 and a_2 are varied. Here, however, it can be shown that sector C has the lowest ground state energy for arbitrary parameters.

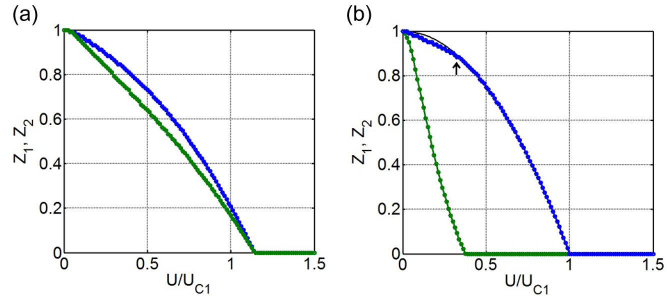

FIG. 3. Wave function renormalizations Z_1 (blue) and Z_2 (green) as a function of U/U_{C1} in the absence of Hund's rule coupling $J = 0$. The states at the bottom row correspond to doubly occupied sites. The middle-row states have occupancy of 1 or 3 and the states at the top row correspond to zero or four-electron fillings. (a) Moderate bandwidth anisotropy $t_2/t_1 = 0.5$ shows locking. (b) Large bandwidth anisotropy $t_2/t_1 = 0.15$ can unlock the bands and cause OSM transition (OSMT). We also reproduce the kink in the wider-bandwidth (blue) band as the narrow band transitions to the Mott phase [27], marked with an arrow. In the OSM phase, the wave function renormalization of the wider band follows the Brinkman-Rice formula (solid line).

Numerical minimization of the free-energy leads to Fig. 3 which reproduces the results of [27]. For $t_2/t_1 > 0.2$ the metal-insulator transition happens at the same critical U for the two bands and we refer to it as the *locking phase*, whereas for $t_2/t_1 < 0.2$ the critical U for the bands are different $U_2 < U_1$ and we refer to it as *orbital selective Mott (OSM) phase*.

In order to have the result analytically tractable we do one further simplification and that is to project out the zero and quartic occupancies per site, by dropping the high energy state at the apex of sector C. We expect such an approximation to be valid close to the Mott transition of the wider band, but invalid at low U. As a result sector C decouples into two smaller sectors $C_\pm$, each equivalent to a two-level system with the level repulsions

$$\alpha_\pm = \sqrt{a_1^2(3/2 + \sqrt{2}) + a_2^2(3/2 - \sqrt{2})} \pm \sqrt{a_1^2(3/2 - \sqrt{2}) + a_2^2(3/2 + \sqrt{2})}. \tag{22}$$

The ground state energy of the slave-spin sector is determined with α_+ inserted in the E_S expression (13) (after an inert $-U/4$ energy shift). Note that this ground state has the Z_2 symmetry $a_1 \leftrightarrow a_2$ of the Hamiltonian H_S. $E_S(\alpha_+)$ as a function of $(a_1^2 - a_2^2)/(a_1^2 + a_2^2)$ is minimized for $a_1 = a_2$. Discarding empty and filled states corresponds to the truncating part of the Hilbert space and thus leads to reduced wave function renormalization at $U \sim 0$. In Fig. 4 we have compared our analytical solution to that of the exact result. When $a_2 = 0$, Eq. (22) gives $\alpha \to 2a_1$ as in the single-band case and therefore, the same critical interaction $U_{C1} = 16|\mathcal{J}_1|$ is obtained. But for symmetric bands $a_1 = a_2$, it gives $\alpha = 2\sqrt{3}a$. Following similar analysis as

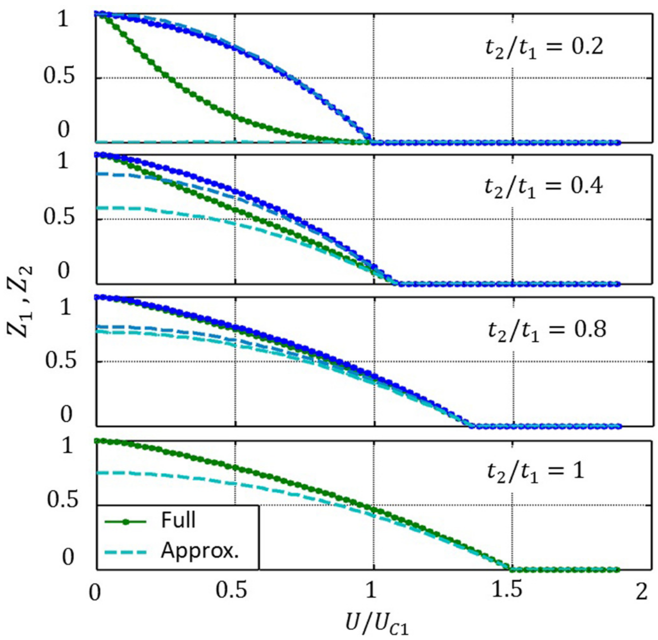

FIG. 4. A comparison of numerical minimization of the free energy vs the analytical two-level system. Discarding the empty and full occupancy states leads to underestimation of Z as $U \to 0$ but close to the Mott transition the approximation is accurate.

before, the free energy is $a^2/|\mathcal{J}| - 2\alpha^2/U$ and we obtain $U_C = 24|\mathcal{J}| = 1.5U_{C1}$ in agreement with [27,29].

Locking vs OSM phase. We formulate the locking vs OSM question as the following. Under what condition $a_1 > 0$ but $a_2 = 0$ can be a minima of the free energy? As mentioned before, setting $a_2 = 0$, α in Eq. (22) reduces to the one-band $\alpha \to 2a_1$. Therefore, the Mott transition for the wide band happens at the same critical U as before. To have a nonzero a_1 solution, we must have $U < U_{c1}$. The point $a_2 = 0$ always satisfies $dF/da_2 = 0$. To ensure that it is the energy minima we need to check that the second derivative is positive:

$$\left.\frac{d^2F}{da_2^2}\right|_{a_2=0} = \frac{1}{|\mathcal{J}_2|} - \frac{5}{|\mathcal{J}_1|} > 0, \tag{23}$$

which gives the condition $|\mathcal{J}_2/\mathcal{J}_1| < 0.2$.

We can better understand the transition by using an order parameter. The trouble with the expression of α is that it cannot be Taylor expanded when a_1 and a_2 are both small. However, we may assume $a_2 = ra_1$, with r playing the role of an order parameter which replaces a_2, and write down $\alpha(a_1,a_2) = a_1\alpha(r)$ where $\alpha(r) = \alpha_+(a_1 \to 1, a_2 \to r)$. A finite r close to the transition implies locking, whereas $r = 0$ or $r = \infty$ implies OSM phase. Close to the transition of both bands $\alpha \approx 0$ justifying an expansion of Eq. (13) in the form $E_S \approx -2\alpha^2/U + 8\alpha^4/U^3$ and Eq. (18) becomes

$$F(a_1,r) = \frac{a_1^2 W}{2|\mathcal{J}_1|} + O(a^4), \quad W_x(r,u) = 1 + xr^2 - \frac{\alpha^2(r)}{4u}.$$

Here $x \equiv |\mathcal{J}_1/\mathcal{J}_2|$ and $u \equiv U/U_{C1}$. The metal-insulator transition for a_1 happens when the mass coefficient W changes sign. For negative W, $a_1^2 > 0$ and we still have to minimize the free energy with respect to r. At small r, we can expand $\alpha(r) \approx 2 + 5r^2$. To zeroth order in r, the W-sign change happens at $u = 1$. Another transition from $r = 0$ to $r > 0$ happens when the corresponding mass term $(x - 5/u)r^2$ changes sign, giving the same critical bandwidth ratio $x_c = 5$ as we had before. So we have two equations $W(r,u) = 0$ and $\partial_r W(r,u) = 0$. The function W is plotted in Fig. 5 and the transition from locking $r > 0$ to OSM phase $r = 0$ is shown.

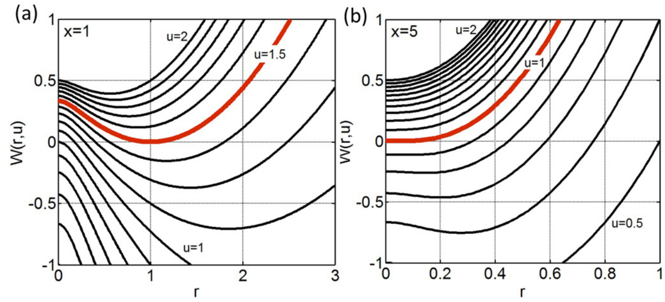

FIG. 5. The coefficient $W(r,u)$ is shown for various u as function of $r = a_2/a_1$. Equations $W = 0$ and $\partial_r W = 0$ are satisfied at the minimum of the red curve, which is (a) at a finite $r = 1$ in the Locking phase $|\mathcal{J}_1| = |\mathcal{J}_2|$ and (b) zero $r = 0$ in the OSM phase $|\mathcal{J}_1| \geqslant 5|\mathcal{J}_2|$.

Large Hund's coupling. In the presence of Hund's coupling the slave-spin Hamiltonian is modified to the diagram shown in Fig. 6.

The ground state still belongs to sector C. In the limit of large $J/U \to 1/4$, we may ignore all the gray lines on block C and find that the ground state is that of a two-level system, Eq. (13) with the level repulsion

$$\alpha = 2\sqrt{a_1^2 + a_2^2}. \tag{24}$$

It is remarkable that the (orbital) rotational invariance of the model (even though absent in H_S) is recovered in this ground state. When the two bands have the same bandwidth, this formula predicts $U_C = U_{C1}$. Since E_S no longer depends on

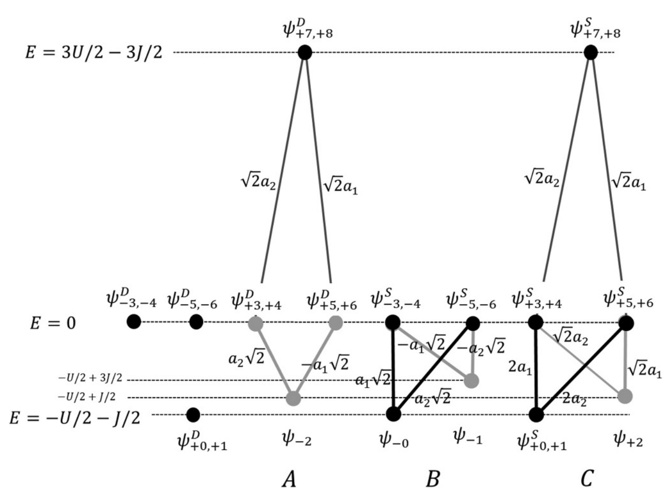

FIG. 6. Diagrammatic representation of the slave-spin Hamiltonian H_S in the two-band model at half-filling in the presence of Hund's rule coupling J. Various degeneracies are lifted by J interaction. In the limit of large Hund's coupling $J/U \to 1/4$ we may only keep sector C and neglect all the gray lines.

$a_1^2 - a_2^2$, there is no more competition between the two terms and a slight bandwidth asymmetry leads to OSM phase. This can be formulated again, following the previous section, in terms of stability of a $a_1 \neq 0$ but $a_2 = 0$ solution. We can check that

$$\left.\frac{d^2F}{da_2^2}\right|_{a_2=0} = \frac{1}{|\mathcal{J}_2|} - \frac{1}{|\mathcal{J}_1|} > 0, \tag{25}$$

which gives $|\mathcal{J}_2| < |\mathcal{J}_1|$ as the sufficient condition for OSMT, i.e., any difference in bandwidth drives the system to the OSM phase. Alternatively, by expanding the level repulsion in this case $\alpha(r) \approx 2 + r^2$ and plugging it into $W(r,u)$, we find that the critical bandwidth ratio $x_c = |\mathcal{J}_1/\mathcal{J}_2|$ is equal to one.

IV. TUNNELING BETWEEN THE ORBITALS

A very interesting question is about the fate of orbital selective Mott phase upon turning on an interorbital tunneling. The band in Mott insulating phase has one electron per site forming localized magnetic moment. There is a large entropy associated with this phase and it is natural to expect that it would be unstable toward possible ordering. A possible mechanism that can compete with magnetic ordering is the Kondo screening of the insulating band by the itinerant band, leading to conduction in the former and opening a hybridization gap in the latter band (effectively a new locking effect coming from Kondo screening). Within single-site approximation, however, the form of the renormalized coupling $\tilde{t}_{ij}^{\alpha\beta} = z_{i\alpha}^* t_{ij}^{\alpha\beta} z_{j\beta}$ implies that once an orbital goes to the Mott phase, it automatically shuts down its coupling to all other orbitals. We speculate that this effect might be responsible for the orbital selective Mott transition solution found in [18]. However, it is still a valid question whether or not the critical interactions U_C for a Mott transition are modified by interorbital tunneling, which we explore in the following.

Before treating interorbital tunneling, we discuss how the slave-spin method can be applied to the impurity problem, and its relation to the lattice.

A. Impurity vs lattice and the DMFT loop

We can also apply the slave-spin method to an impurity problem. In particular, we can use the slave-spin (as well as any other slave-particle) method as an impurity solver for the DMFT. We show in the following that the slave-spin mean-field result corresponds to such a DMFT solution with the corresponding slave-spin impurity solver. This puts the method on firm ground and allows comparison between various methods.

First, consider a generic p-h symmetric impurity model described by the Hamiltonian $H = H_0 + H_{\rm int}$ where

$$H_0 = -\sum_{k\alpha\beta} t_k^{\alpha\beta}(d_\alpha^\dagger c_{k\beta} + \text{H.c.}) + \sum_{k\beta} \epsilon_k^\beta c_{k\beta}^\dagger c_{k\beta}. \tag{26}$$

Again α,β are superindices that include both orbital and spin. We have assumed that the bath is diagonal and discarded any local "crystal field" $d_1^\dagger d_2$ for simplicity. In the simple case of single-orbital impurity $H_{\rm int} = U\tilde{n}_{d\uparrow}\tilde{n}_{d\downarrow}$. Via a substitution of Eq. (2), the hybridization term becomes $H_0 = -\sum_{k\alpha\beta} t_k^{\alpha\beta}(f_\alpha^\dagger \tau_\alpha^x c_{k\beta} + \text{H.c.})$. This problem can be written in a similar way as before $H \approx H_f + H_S$, where H_S is exactly what we had in the single-band lattice case. However, since the $f_\alpha^\dagger \tau_\alpha^x c_{k\beta}$ interaction happens only on the impurity site, we do not need the second single-site approximation here, and obtain $a_\alpha = -2\sum_{k\beta}^{\alpha\beta} t_k^{\alpha\beta}\langle f_{k\alpha}^\dagger c_{k\beta}\rangle$. In order to have a general formalism that applies to both impurity and lattice, as well as scenarios with interorbital tunneling for which $\mathcal{J}_{\alpha\beta}$ renormalizes and is difficult to compute, we regard a and z as independent variables and write the free energy of Eq. (10) as [47]

$$F(\{z,a\}) = F_f(\{z\}) + F_S(\{a\}) - \sum_\alpha a_\alpha z_\alpha. \tag{27}$$

The saddle point of F with respect to a and z gives the correct mean-field equations. F_f is the free energy of the f electron given by $F_f = -T\sum_n \text{Tr}\log[-\mathbb{G}_f^{-1}(i\omega_n)]$, where $\mathbb{G}_f^{-1}(i\omega_n) = i\omega_n\mathbb{1} - \mathbb{z}^\dagger\mathbb{\Delta}(i\omega_n)\mathbb{z}$ with $\mathbb{\Delta}(i\omega_n) = \sum_k \mathbb{t}_k^\dagger \mathbb{G}_c(k,i\omega_n)\mathbb{t}_k$, the hybridization function. The slave-spin part is given by $F_S = \text{Tr}[e^{-\beta H_S}]$, where for a single-orbital Anderson impurity, $H_S = 2a\tau^x + U\tau^z/4$, as we had in the single-band case before.

The mean-field equations with respect to z and a are, respectively,

$$a_\alpha = \frac{1}{z_\alpha}\int \frac{d\omega}{\pi} f(\omega)\omega \text{Im}\big[G_f^{\alpha\alpha}(\omega + i\eta)\big], \tag{28}$$

$$z_\alpha = \frac{dF_S}{da_\alpha}. \tag{29}$$

The first equation provides a relation between a and z that generalizes $a_\alpha = 2\sum_\beta \mathcal{J}_{\alpha\beta} z_\beta$ (see Appendix D). Having expressions for $E_S(a)$ we can eliminate a in favor of z, or vice versa, which is equivalent to a Legendre transformation. In Appendix C we apply these equations to the (single-orbital) finite-U Anderson impurity problem and show the "transition" to the Kondo phase as the temperature is lowered.

In a lattice, the free energy has the same form as Eq. (27) with the difference that $F_f = -T\sum_{k,n} \text{Tr}\log[-\mathbb{G}_f^{-1}(k,i\omega_n)]$, where the Green's function is $\mathbb{G}_f(k,i\omega_n) = [i\omega_n\mathbb{1} - \mathbb{z}^\dagger\mathbb{E}_k\mathbb{z}]^{-1}$. It can be shown that exactly the same mean-field equations are obtained if G_f in Eq. (28) is replaced with $G_f^{\alpha\alpha}(i\omega_n) \to \sum_k G_f^{\alpha\alpha}(k,i\omega_n)$. Therefore, we conclude that the two problems (lattice and impurity) are equivalent provided that the hybridization function in the impurity problem is chosen such that the impurity Green's function and the local Green's function of the lattice are equal, i.e.,

$$[i\omega_n\mathbb{1} - \mathbb{z}^\dagger\mathbb{\Delta}(i\omega_n)\mathbb{z}]^{-1} = \sum_k [i\omega_n\mathbb{1} - \mathbb{z}^\dagger\mathbb{E}_k\mathbb{z}]^{-1}, \tag{30}$$

which is the DMFT consistency equation. Therefore, slave-spin mean field is equivalent to a DMFT solution using the slave-spin method as the impurity solver. Also, note that a lattice problem in the OSM phase corresponds to an impurity problem in which the hybridization of one of the orbitals to the bath has been turned off [50]. Note that a similar discussion can be applied to other slave-boson/spin techniques. For example, the KR slave-boson has been previously applied to the Andersion impurity problem by Schonhammer [51] resulting in similar mean-field equations as we derived here.

Following the same route, the KR slave-boson mean-field solution of the lattice can be shown to be equivalent to the result of a DMFT loop with the KR slave-bosons as the impurity solver. The relation between KR slave-bosons and the slave-spins are discussed in Appendix A. See also Appendix B for a discussion of Eq. (30) at low energies.

B. Interorbital tunneling

Slave spins have been used to study iron-based superconductors [18] where the interorbital tunnelings are important. We study this tunneling effect in the specific case with *p-h* symmetry and without orbital splitting (which allows for analytic calculations). The cases that go beyond such conditions, as arising in the models for the iron-based superconductors [18], remain to be explored and are left for future work. A troublesome feature of the slave-spins is that they break the rotational symmetry among the orbitals. Within the *p-h* symmetric Bethe lattices that we study here, this rotational variation leads to ambiguities in the presence of interorbital tunnelings, as we point out here.

Let us consider a 1D chain with two orbitals $H_0 = -\sum_{n\sigma}(D^\dagger_{n\sigma}\mathbb{T}D_{n+1,\sigma} + \text{H.c.})$, with $D = (d_1\, d_2)^T$, no Hund's coupling in H_{int}, and a dispersion

$$\mathbb{E}_k = -2\mathbb{T}\cos k, \quad \mathbb{T} = \begin{pmatrix} t_{11} & t_{12} \\ t_{12} & t_{22} \end{pmatrix}. \tag{31}$$

We have chosen $t_{12} = t_{21}$ and all the elements real (and positive) to preserve the *p-h* symmetry. Strictly speaking, in 1D the mean-field factorization that led to Eq. (4) and the consequent single-site approximation are both unjustified. The choice of dimensionality, here, is only for the ease of discussion and not essential to the conclusions. As long as the dispersion matrix can be diagonalized with a momentum-independent unitary transformation (as well as any Bethe lattice, see Appendix D), the following discussion applies. Diagonalizing the tunneling matrix gives $E^\pm_k = -2t^\pm\cos k$ with

$$t^\pm = \frac{t_{11}+t_{22}}{2} \pm \sqrt{\left(\frac{t_{11}+t_{22}}{2}\right)^2 - \det\mathbb{T}}. \tag{32}$$

Including renormalization just changes $t_{\alpha\beta} \to \tilde{t}_{\alpha\beta}$. We can simply use the diagonalized form of the tunneling matrix to calculate F_0 at $T = 0$. Assuming $\det\mathbb{T} > 0$,

$$F_f = \sum_{\gamma=\pm}\int\frac{dk}{2\pi}E^\pm_k f(E^\gamma_k) \to -(\tilde{t}^+ + \tilde{t}^-)\int_{-\pi/2}^{\pi/2}\frac{dk}{\pi}\cos(k)$$
$$= -2(\tilde{t}_{11}+\tilde{t}_{22})/\pi.$$

Note that t_{12} does not enter the free energy. Inserting this expression into Eq. (27) and setting $dF/dz_i = 0$, we can remove a_i in favor of z_i. This seems to imply that there is a finite threshold (topological stability) for interorbital tunneling: as long as $\det\mathbb{T} > 0$, introducing t_{12} does not change anything in the problem and it simply drops out and OSM phase is stable against interorbital tunneling. For large t_{12} eventually $\det\mathbb{T} < 0$. So we get $t^+ > 0$ and $t^- < 0$ and the second band is inverted and F_0 becomes

$$F_f \to -2(\tilde{t}^+ - \tilde{t}^-)/\pi = -\frac{4}{\pi}\sqrt{\left(\frac{\tilde{t}_{11}-\tilde{t}_{22}}{2}\right)^2 + |\tilde{t}_{12}|^2}. \tag{33}$$

Hence t_{12} has nontrivial effects on renormalization.

On the other hand, we could have used the rotational invariance of H_{int} and done a rotation in $d_1 - d_2$ basis to band-diagonalize H_0 with the bandwidths $\mathbb{T} \to \text{diag}\{t^+,t^-\}$, before using slave-spins to treat the interactions. It is clear then that t_{12} always has nontrivial effects by modifying $t^\pm$. For example, we could start in the locking phase where $t^-/t^+ > 0.2$, and by increasing t_{12} slightly get to the OSMT phase $t^-/t^+ < 0.2$, without changing the sign of $\det\mathbb{T}$. This paradox exists for any *p-h* symmetric lattice with a diagonalizable tunneling matrix. The root of the problem is that our expression in Eq. (9) is not invariant under rotations between various orbitals. Therefore, the critical value where the OSM phase persists, is basis dependent. This ambiguity calls for the use of unbiased techniques to understand the role of interorbital tunneling on OSMT. It might be that the model we studied analytically here is a singular limit which can be avoided by breaking *p-h* symmetry and inclusion of crystal field in more realistic settings [18]. This remains to be explored in a future work.

As discussed in [25], the way to achieve rotational invariance is to liberate the f electrons that describe quasiparticles from the physical d electrons. This is achieved by a $d_\alpha \to \sum_\beta \hat{z}_{\alpha\beta} f_\beta$ representation which leads to a wave-function–renormalization matrix $z_{\alpha\beta} = \langle\hat{z}_{\alpha\beta}\rangle$ with off-diagonal elements. So far we have not been able to generalize the slave-spin to a rotationally invariant form and we leave it as a future project.

V. ON-SITE INTERORBITAL HYBRIDIZATION

Even though models for the iron-based superconductors have finite crystal level splitting and no on-site hybridization, it is interesting to introduce a hybridization between the two orbitals within the current formalism [27]. This is interesting because the on-site hybridization does not suffer from the singe-site approximation $\langle\hat{z}_{i\alpha}\hat{z}_{i\beta}\rangle \neq \langle\hat{z}_{i\alpha}\rangle\langle\hat{z}_{i\beta}\rangle$, as opposed to the interorbital tunneling and $\langle\hat{z}_{i\alpha}\hat{z}_{i\beta}\rangle$ appears as an independent order parameter, which leads to the emergence of Kondo screening as we show in this section.

We can include a term $\sum_{n,\sigma}(v_{12}d^\dagger_{n,1\sigma}d_{n,2\sigma} + \text{H.c.})$ to the Hamiltonian. In order to preserve the *p-h* symmetry, v_{12} has to be purely imaginary. The modifications to the mean-field Hamiltonians are

$$\Delta H_f = \sum_{n,\sigma}(\tilde{v}_{12}f^\dagger_{n,1\sigma}f_{n,2\sigma} + \text{H.c.}) - 2_s A_{12}Z_{12}, \tag{34}$$

$$\Delta H_S = \sum_\sigma A_{12}\tau^x_{1\sigma}\tau^x_{2\sigma}, \tag{35}$$

where $\tilde{v}_{12} = v_{12}Z_{12}$ with $Z_{12} = \langle\tau^x_{1\sigma}\tau^x_{2\sigma}\rangle$ and $A_{12} = v_{12}\sum_n\langle f^\dagger_{n,1\sigma}f_{2\sigma}\rangle + \text{H.c.}$ Z_{12} and A_{12} are are related to each other via the Hamiltonian above and they are independent of σ in the paramagnetic regime. Alternatively, we can regard them as independent and impose the mean-field equation $Z_{12} = \partial F_S/\partial A_{12}$ to eliminate A_{12} by a Legendre transformation. Assuming a small A_{12} we can compute the change in slave-spin energy using second-order perturbation theory. The result is of the form $\Delta E_S = \gamma(A_{12})^2$, where γ is (in absence of Hund's coupling) a positive constant which contains all the matrix elements and the inverse gaps $\gamma = \sum_{j\sigma\sigma'}\langle\psi_0|\tau^x_{1\sigma}\tau^x_{2\sigma}|\psi_j\rangle$

$(E_j - E_0)^{-1}\langle\psi_j|\tau^x_{1\sigma'}\tau^x_{2\sigma'}|\psi_0\rangle$, where E_j and $|\psi_j\rangle$ are the eigenvalue/states of the H_S solved in the previous section. Eliminating A_{12} in favor of Z_{12} we find that the free energy of the system is

$$F(z_1,z_2,Z_{12}) = -\frac{2_s}{\beta}\sum_{kn}\mathrm{Tr}\log\begin{pmatrix}\tilde{\epsilon}_{k1} - i\omega_n & iZ'_{12}\\ -iZ'_{12} & \tilde{\epsilon}_{k2} - i\omega_n\end{pmatrix} + E'_S(z_1,z_2) + \frac{(Z'_{12})^2}{\gamma'}. \quad (36)$$

Here E'_S is the value of $E_S(a_1,a_2) - \sum_i a_i z_i$ in the absence of hybridization v_{12} in which a_1 and a_2 are eliminated in favor of z_1 and z_2. Also, we have redefined $|v_{12}|Z_{12} \to Z'_{12}$ and $\gamma|v_{12}|^2 \to \gamma'$.

Equation (36) is nothing but the free energy of a Kondo lattice at half-filling [52] with renormalized dispersions $\tilde{\epsilon}_{k1}$ and $\tilde{\epsilon}_{k2}$. In a Kondo lattice, this form of the free energy appears using Z'_{12} as the Hubbard-Stratonovitch field that decouples the Kondo coupling $\gamma'\vec{S}_2\cdot d_1^\dagger\vec{\sigma}d_1$. Here $S_2 = d_2^\dagger\vec{\sigma}d_2$ is the spin of the Mott-localized band and γ' plays the role of the Kondo coupling. As a result of this coupling, a new energy scale $T_K \sim D\exp[-1/\gamma']$ appears, with $D \sim \min(2\tilde{t}_{11},U_{C1})$, below which the Kondo screening takes place which in the p-h symmetric case gaps out both bands but away from p-h symmetry mobilizes the Mott localized band. Either way, we conclude that the orbital selective Mott insulating phase is unstable against hybridization between the two orbitals in agreement with [27]. However, even though a true selective Mottness is unstable, orbital differentiation, reflected as large difference in effective mass, can exist [16].

VI. CONCLUSION

In conclusion, we have used slave-spin mean-field method to study two-band Hubbard systems in the presence of Hund's rule coupling. We have developed a Landau-Ginzburg theory of the locking vs OSMT. We discussed the relation between slave-spins and the KR boson methods (Appendix A). We have also applied the method to impurity problems and shown a correspondence between the latter and the single-site approximation of the lattice using the DMFT loop. Finally, we have discussed the limitations of the slave-spin method for multiorbital models with both particle-hole symmetry and interorbital tunneling and shown that the orbital selective Mott phase is unstable against on-site hybridization between the two orbitals. As possible future extensions of this work, it is certainly interesting to study the nature of the Mott transition at finite temperature and seek explicit solutions of Eq. (36).

Note added in proof. After completion of this manuscript, we became aware of another work [53] which contains a Landau-Ginzburg theory of OSMT in the presence of the interorbital tunneling. The conclusions of the two works agree wherever there is an overlap.

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APPENDIX A: VARIOUS SLAVE-PARTICLE METHODS

For a one band model, KR introduces four bosons and uses the representation $\hat{z}^\dagger_\sigma = P^+[p^\dagger_\sigma e + d^\dagger p_{-\sigma}]P^-$, where $p^\dagger_\sigma$, $e^\dagger$, and $d^\dagger$ are (hardcore) bosonic creation operators for σ-spinon, holon, and doublon, respectively, and $P^\pm$ are projectors that depend on the occupations of the bosons and are introduced to normalize the probability amplitudes over the restricted set of physical states. On the other hand, an SU(2) spin-variable $\vec{\tau}_\alpha$ can be represented by two Schwinger bosons a_α and b_α satisfying the constraint $a^\dagger_\alpha a_\alpha + b^\dagger_\alpha b_\alpha = 1$ (hardcoreness), via

$$\tau^z_\alpha = b^\dagger_\alpha b_\alpha - a^\dagger_\alpha a_\alpha, \quad \tau^x_\alpha = a^\dagger_\alpha b_\alpha + b^\dagger_\alpha a_\alpha. \quad (A1)$$

On an operator level, the two methods have the same Hilbert space as depicted in Table I for the case of one orbital. Average polarization of the spin along various direction in the Bloch sphere corresponds to condensation of a and b bosons.

A trouble with the slave-spin representation is that the f quasiparticles carry the charge of the d electron and thus the disordered phase of the slave-spins (in which the f electrons still disperse beyond single-site approximation) is not a proper description of the Mott phase. As a remedy, it has been suggested [31] to replace τ^x in Eq. (2) with τ^+ and fixing the problem of nonunity of Z in the noninteracting case by applying fine-tuned projectors $\hat{z}^\dagger = P^+\tau^+P^-$. We note that this looks quite similar to KR.

For M spinful orbitals, KR requires introducing 4^M bosons (only one of them occupied at a time), whereas only $2M$ slave-spins are required (each with the Hilbert space of 2). Thus the size of the two Hilbert spaces are the same $2^{2M} = 4^M$.

APPENDIX B: GENERAL LOW-ENERGY CONSIDERATIONS

Generally, for a lattice with the Green's function

$$\mathbb{G}_d(k,\omega) = [\omega\mathbb{1} - \mathbb{E}_k - \Sigma_d(k,\omega)]^{-1}, \quad (B1)$$

at low energies we can expand the self-energy

$$\Sigma_{d,lat}(k,\omega) = \Sigma(0,0) + \vec{k}\cdot\partial_{\vec{k}}\Sigma(0,0) + \omega\partial_\omega\Sigma(0,0) + \cdots.$$

Within single-site approximation, the second term is zero. Denoting the third term as $\partial_\omega\Sigma_d \approx 1 - \mathbb{Z}^{-1}$ and assuming $\mathbb{Z} = \mathbb{z}\mathbb{z}^\dagger$ we can write

$$\mathbb{G}_d(k,\omega) \approx \mathbb{z}[\omega\mathbb{1} - \mathbb{z}^\dagger\mathbb{E}_k\mathbb{z}]^{-1}\mathbb{z}^\dagger, \quad (B2)$$

which simply means $\mathbb{G}_f(\omega) = [\omega\mathbb{1} - \tilde{\mathbb{E}}_k]^{-1}$.

TABLE I. Comparison of the Schwinger boson representation of the slave-spin (left) and Kotliar-Ruckenstein slave-bosons (right).

$a^\dagger_\uparrow a_\uparrow$	$b^\dagger_\uparrow b_\uparrow$	$a^\dagger_\downarrow a_\downarrow$	$b^\dagger_\downarrow b_\downarrow$	$e^\dagger e$	$p^\dagger_\uparrow p_\uparrow$	$p^\dagger_\downarrow p_\downarrow$	$d^\dagger d$
1	0	1	0	1	0	0	0
0	1	1	0	0	1	0	0
1	0	0	1	0	0	1	0
0	1	0	1	0	0	0	1

Comparing to Eq. (16), this means that the correlation functions of the slave-particles are just decoupled $\langle \hat{z}_{i\alpha}(\tau)\hat{z}^\dagger_{j\beta}\rangle \to z^*_\alpha z_\beta$ within single-site approximation, also discarding any time dynamics at low energies. For the tunneling matrix, we simply have $\tilde{\mathbb{t}} = \mathbb{z}^\dagger \mathbb{t}\mathbb{z}$. In the following we discuss such low-energy approximations on the DMFT loop. The Green's function of an impurity and a local site on a lattice are, respectively,

$$i\omega_n \mathbb{1} - \Sigma_{d,\mathrm{imp}}(i\omega_n) = \mathbb{G}^{-1}_{d,\mathrm{imp}}(i\omega_n), \tag{B3}$$

$$\mathbb{G}_{d,\mathrm{loc}}(i\omega_n) = \sum_k [i\omega_n - \mathbb{E}_k - \Sigma_{d,\mathrm{lat}}(k,i\omega_n)]^{-1}. \tag{B4}$$

Separating the interaction part of the self-energy $\Sigma_{d,\mathrm{imp}}(i\omega_n) = \Delta(i\omega_n) + \Sigma_{d,I}(i\omega_n)$, the DMFT approximation identifies $\Sigma_{d,I}(i\omega_n) = \Sigma_{d,\mathrm{lat}}(k,i\omega_n)$. Again expanding $\Sigma_{d,I}(\omega) \approx (1 - \mathbb{Z}^{-1})\omega$ we have

$$\mathbb{G}_{d,\mathrm{imp}}(i\omega_n) = \mathbb{z}[i\omega_n \mathbb{1} - \tilde{\Delta}(i\omega_n)]^{-1}\mathbb{z}^\dagger, \tag{B5}$$

with $\tilde{\Delta}(i\omega_n) = \mathbb{z}^\dagger \Delta(i\omega_n)\mathbb{z}$ in agreement with $\mathbb{G}_{f,\mathrm{imp}}(i\omega_n) = [i\omega_n \mathbb{1} - \tilde{\Delta}(i\omega_n)]^{-1}$. Using the same approximation for $\mathbb{G}_{d,\mathrm{loc}}$ leads to

$$\mathbb{G}^{-1}_{d,\mathrm{loc}}(i\omega_n) \to \mathbb{z}\sum_k [i\omega_n - \tilde{\mathbb{E}}_k]^{-1}\mathbb{z}. \tag{B6}$$

The DMFT self-consistency loop is $\mathbb{G}_{f,loc}(i\omega_n) = \mathbb{G}_{f,imp}(i\omega_n)$ or

$$\sum_k [i\omega_n - \tilde{\mathbb{E}}_k]^{-1} = [i\omega_n \mathbb{1} - \tilde{\Delta}(i\omega_n)]^{-1}. \tag{B7}$$

Within the slave-spin approach there are no interactions:

$$\Sigma_{f,\mathrm{imp}} = \mathbb{z}^\dagger \Delta(i\omega_n)\mathbb{z}, \quad \Sigma_{f,I} = 0, \quad \Sigma_{f,\mathrm{lat}} = 0, \tag{B8}$$

and Eq. (B7) is satisfied as it does for any noninteracting problem. Note that this is Eq. (30).

Rotation. Using the vector D for the d electrons, in the presence of interorbital tunneling we may sometimes be able to eliminate such interorbital tunneling by a rotation to $D = \mathbb{U}D_\pm$. Since $D = \mathbb{z}F$, we assume the same rotation in the F-space $F = \mathbb{U}F_\pm$ (otherwise they would contain interorbital tunneling) and the two $\mathbb{z}$s are related by $\mathbb{z} = \mathbb{U}^\dagger \mathbb{z}_\pm \mathbb{U}$. Assuming that $\mathbb{U}$ is a SO(2) matrix, and $\mathbb{z}_\pm$ is diagonal, we find

$$\mathbb{z} = \frac{z_+ + z_-}{2}\mathbb{1} - \frac{z_+ - z_-}{2}\begin{pmatrix} -\cos 2\alpha & \sin 2\alpha \\ \sin 2\alpha & \cos 2\alpha \end{pmatrix}, \tag{B9}$$

which has off-diagonal elements. Note that if one of the $z_\pm$ elements vanishes, e.g., $z_- = 0$, we can factorize $\mathbb{z}$:

$$\mathbb{z} = z_+ \begin{pmatrix} \cos\alpha \\ -\sin\alpha \end{pmatrix}(\cos\alpha \;\; -\sin\alpha). \tag{B10}$$

Then, it can be seen that $\mathbb{Z} = \mathbb{z}\mathbb{z}^\dagger \to z_+\mathbb{z}$ has the same form. This basically means one linear combination of f electrons is decoupled (localized) and the itinerant spinon band carries characters of both d_1 and d_2 bands. This basis dependence of the orbital Mott selectivity is again an artifact due to lack of rotational invariance.

APPENDIX C: FINITE-U ANDERSON MODEL

Here we apply slave-spins to the finite-U Anderson impurity model. The slave-spin part of the Hamiltonian is as we had in the one band case. We can use Eq. (27) to eliminate a in favor of z. In the wide band limit for the conduction band, we have $G_f(i\omega_n) = [i\omega_n - i\Delta_K \mathrm{sgn}(\omega_n)]^{-1}$ where $\Delta_K = \pi\rho t^2 z^2$, and the free energy is

$$F(z) = -2_s \int_{-D}^{D} \frac{d\omega}{\pi} f(\omega)\mathrm{Im}[\log(i\Delta_K - \omega)] + E'_S(z). \tag{C1}$$

E'_S is obtained by eliminating a from the $E_S(a) - 2_s az$ part of the free energy in Eqs. (13) and (27) and is equal to $E'_S = -\frac{U}{4}\sqrt{1-z^2}$. Here we have done a simplification to replace F_S with its zero temperature value (ground state energy) while maintaining the temperature dependence of the F_f. We expect this approximation to be valid in the large-U limit especially close to the transition. The mean-field equation with respect to z is

$$z\int_{-D}^{D} d\omega f(\omega)\mathrm{Re}\left[\frac{1}{\omega - i\Delta_K}\right] + \frac{U}{4\rho t^2}\frac{z}{\sqrt{1-z^2}} = 0. \tag{C2}$$

Close to the transition, the second term is effectively like a $z/\rho J(z)$ with $J(z) \equiv (4t^2/U)\sqrt{1-z^2}$. At zero temperature the left side simplifies to

$$z\log\frac{\Delta_K}{D} + \frac{z}{\rho J(z)} = z\log\frac{\Delta_K}{T_K(z)} = 0, \tag{C3}$$

where $T_K(z) = De^{-1/\rho J(z)}$. So to have nonzero z we must have $\Delta_K = T_K$ which determines z. Also, we can go to nonzero temperature. We just replace the log term in the above expression with its finite-temperature expression from Eq. (C2):

$$z\mathrm{Re}[\tilde{\psi}(i\Delta_K) - \tilde{\psi}(D)] + \frac{z}{\rho J(z)} = 0. \tag{C4}$$

This is solved numerically and the result is shown in Fig. 7. It shows a Kondo phase $z > 0$ for $T < T^0_K$.

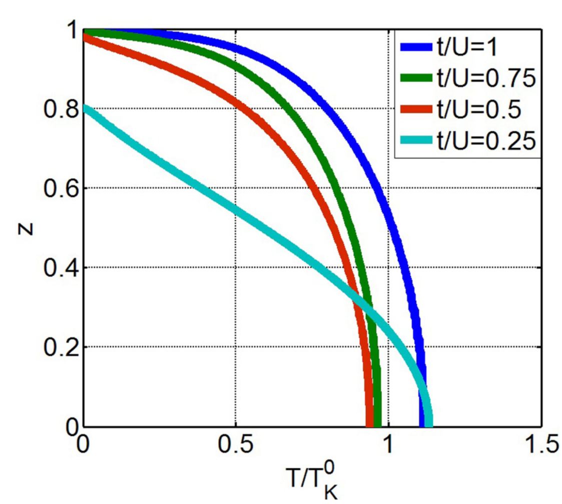

FIG. 7. The order parameter z for the Anderson model calculated from numerical evaluation of Eq. (C4). $T^0_K = De^{-1/\rho J}$, where $J = 4t^2/U$. Note that this is off with a factor of 4, an artifact of slave-spin method. We have used $D = 100U$, whereas t/U is varied.

APPENDIX D: STABILITY OF OSMT AGAINST INTERORBITAL TUNNELING IN A BETHE LATTICE

Using equations of motion, the coefficient $\mathcal{J}_{\alpha\beta}$ defined after Eq. (4) can be related to the correlation function of the electrons at the same site. The result is

$$\mathcal{J}^{\alpha\beta} = t^{\alpha\beta}\sum_{\eta}[\tilde{t}^{-1}]^{\beta\eta}\int\frac{d\omega}{2\pi}f(\omega)\omega A_{ii}^{\eta\alpha}(\omega), \quad \text{(D1)}$$

where $A_{ii}^{\eta\alpha}(\omega)$ is the $\eta\alpha$ orbital element of the local spectral function matrix. This together with $a^{\alpha} = 2\sum_{\beta}\mathcal{J}^{\alpha\beta}z^{\beta}$ leads to Eq. (27). In a Bethe lattice we can use recursive methods [54] to compute $A_{ii}^{\alpha\beta}$. When the tunneling matrix is Hermitian and there is no chemical potential or crystal field, the procedure is especially simple. We diagonalize the renormalized tunneling matrix $\tilde{\mathfrak{t}} = U\tilde{\mathfrak{t}}^{D}U^{-1}$. Then the retarded and the spectral functions are

$$\mathbb{G}^{R}(\omega) = \tilde{\mathfrak{t}}^{-1}U\mathbb{\Lambda}(\omega)U^{-1}, \quad \mathbb{A}(\omega) = U\mathbb{A}^{D}(\omega)U^{-1}, \quad \text{(D2)}$$

where diagonal matirix $\mathbb{\Lambda}$ contains λ elements that satisfy $\lambda_i + \lambda_i^{-1} = \omega/\tilde{t}_D^{i}$ with the retarded boundary condition. $\mathbb{A}^{D}$ is diagonal matrix of semicircular density states whose width are given by the eigenvalues of $\tilde{\mathfrak{t}}$. By plugging this into Eqs. (D2) and (D1) and using

$$\int\frac{d\omega}{2\pi}f(\omega)\omega\mathbb{A}_{ii}^{D}(\omega) = -0.2122\times 2|\tilde{\mathfrak{t}}^{D}|,$$

we see that if the eigenvalues of the matrix $\tilde{\mathfrak{t}}$ all have the same sign, then $U(|\tilde{\mathfrak{t}}^{D}| = \tilde{\mathfrak{t}}^{D})U^{-1} = \tilde{\mathfrak{t}}$. This is the generalization of the protection of OSM phase against interorbital tunneling, discussed in the 1D case in the paper. For the case of two bands,

$$\det\tilde{\mathfrak{t}} > 0 \quad \Rightarrow \quad \mathcal{J}^{\beta\alpha} = -0.2122\times 2t^{\beta\alpha}\delta^{\beta\alpha},$$
$$\det\tilde{\mathfrak{t}} < 0 \quad \Rightarrow \quad \mathcal{J}^{\beta\alpha} = -0.2122\times 2t^{\beta\alpha}R^{\alpha\beta}, \quad \text{(D3)}$$

i.e., for $\det\tilde{\mathfrak{t}} > 0$, the $\mathcal{J}$ matrix does not have any off-diagonal elements and the diagonal elements are proportional to the bare diagonal hoppings (as before), but if $\det\tilde{\mathfrak{t}} < 0$, there is a matrix $R = U\langle\tau^{z}\rangle U^{-1}$ inside the $\mathcal{J}$ matrix which does depend on renormalization.

Again in this problem, one could have done the rotation in d_{α} sector before using the slave-spins, in which case, interorbital tunneling would have an effect and could cause OSM transition. Therefore, the stability found above is basis dependent. This ambiguity is absent when p-h symmetry is broken and the tunneling matrix cannot be diagonalized independent of the momentum [18].

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