Orbital selective Mott transition in multi-band systems:
slave-spin representation and dynamical mean-field theory

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We examine whether the Mott transition of a half-filled, two-orbital Hubbard model with unequal bandwidths occurs simultaneously for both bands or whether it is a two-stage process in which the orbital with narrower bandwidth localizes first (giving rise to an intermediate ‘orbital-selective’ Mott phase). This question is addressed using both dynamical mean-field theory, and a representation of fermion operators in terms of slave quantum spins, followed by a mean-field approximation (similar in spirit to a Gutzwiller approximation). In the latter approach, the Mott transition is found to be orbital-selective for all values of the Coulomb exchange energy (Hund) coupling J when the bandwidth ratio is small, and only beyond a critical value of J when the bandwidth ratio is larger. Dynamical mean-field theory partially confirms these findings, but the intermediate phase at J = 0 is found to differ from a conventional Mott insulator, with spectral weight extending down to arbitrary low energy. Finally, the orbital-selective Mott phase is found, at zero-temperature, to be unstable with respect to an inter-orbital hybridization V, and replaced at small V by a state with a large effective mass (and a low quasiparticle coherence scale) for the narrower band.

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I. INTRODUCTION

The Mott metal-insulator transition plays a central role in the physics of all strongly correlated electron materials. At a qualitative level, localization of the electrons can occur when the kinetic energy gain (typically given by the bare bandwidth) is smaller than the cost in on-site repulsive Coulomb energy (U) in particular, in the study of simplified models such as the one-band Hubbard model. In real materials however, such as transition metal oxides, several orbital components are involved. Crystal-field effects and the Coulomb exchange energy (J) affect the energy of on-site atomic states, which no longer depend only on the total local charge as in the orbitally degenerate case. Furthermore, the inter-site hopping amplitudes can be significantly different for different orbital components (due e.g. to their relative orientations). It is therefore essential to understand how these effects can affect the Mott transition, and whether qualitatively new effects are possible when the orbital degeneracy is lifted.

Recently, this question has attracted a lot of attention. In their study of Ca$_{2-x}$Sr$_x$RuO$_4$, Anisimov et al. suggested that a partial localization could take place, in which some orbital components (with broader bandwidth) are conducting, while others (with narrower bandwidth) are localized (see also Ref. 7). Following this proposal, several studies have been performed in the model context, with controversial results. Lichtenstein, Liebsch, and others challenged the existence of such an “orbital-selective Mott transition” (OSMT), on the basis of DMFT calculations. Koga and coworkers, on the other hand, did find an OSMT within their DMFT calculations, and suggested that a unique transition is found only if J = 0. A symmetry argument was put forward to explain this finding.

In this paper, a clarification of this problem is attempted, using DMFT and another, complementary approach. The latter is based on a representation of fermion operators in terms of slave quantum spins, specifically forged to address multi-orbital models (Sec. III). A mean-field approximation based on this representation, similar in spirit to the Gutzwiller approximation, provides a fast and efficient method in order to investigate the Mott transition in a wide range of parameters (Sec. IV). In Sec. V, a detailed study of the previously unexplored regime in which one of the bands is much narrower than the other and J = 0 is presented, using exact diagonalizations and quantum Monte Carlo methods in the DMFT framework. Finally (Sec. VI), the effect of an inter-band hybridisation is considered.

II. MODEL

The model considered in this paper is a tight-binding model for two bands, coupled by local interactions. The Hamiltonian reads $H = H_0 + H_{int}$, where $H_0$ is the non-interacting part:

$$H_0 = - \sum_{m=1,2} \sum_{\langle ij \rangle, \sigma} t_m d_{im\sigma}^\dagger d_{j\sigma} + h.c. + \sum_{i,m,\sigma} (\epsilon_m - \mu) d_{ima}^\dagger d_{ima},$$

in which $d_{ima}^\dagger$ ($d_{ima}$) creates (annihilates) an electron on the site $i$, in the orbital $m$, with spin $\sigma$. The $\epsilon_m$'s are crystal-field levels and $\mu$ is the chemical potential, kept here for generality. In most of the paper however, we
shall focus on the case of zero crystal-field splitting ($\epsilon_1 = \epsilon_2 = 0$) and half-filling of each band (i.e. one electron per site in each orbital, which corresponds to $\mu = 0$ given our normalization of the interaction term). At the end of the paper, we shall also consider the possibility of a non-zero inter-orbital hybridization.

The full interaction, in the case of degenerate bands in a cubic environment\textsuperscript{12,13} reads:

$$
H_{\text{int}} = U \sum_{im} \tilde{n}_{im\uparrow} \tilde{n}_{im\downarrow} + U' \sum_{i\sigma} \tilde{n}_{i\sigma\uparrow} \tilde{n}_{i\sigma\downarrow}
+ (U' - J) \sum_{i\sigma} \tilde{n}_{i\sigma\uparrow} \tilde{n}_{i\sigma\downarrow}
- J \sum_i \left[ d_{i1\uparrow}^\dagger d_{i1\downarrow} d_{i2\uparrow} d_{i2\downarrow}^\dagger + d_{i1\downarrow}^\dagger d_{i1\uparrow} d_{i2\downarrow} d_{i2\uparrow}^\dagger \right]
- J \sum_i \left[ d_{i1\downarrow}^\dagger d_{i1\uparrow} d_{i2\downarrow} d_{i2\uparrow}^\dagger + d_{i2\downarrow}^\dagger d_{i2\uparrow} d_{i1\downarrow} d_{i1\uparrow}^\dagger \right],
$$

(2)

where $\tilde{n}_{im\sigma} = n_{im\sigma} - 1/2$. Following Castellani et al.\textsuperscript{12,13}, the reduction of the Coulomb interorbital Coulomb interactions $U'$ as compared to the interorbital $U$ is related to the Hund’s coupling $J$ by:

$$
U' = U - 2J
$$

(3)

In the case of vanishing Hund’s rule coupling $J = 0$ the interaction vertex ($= U (n_1 + n_2 - 2)^2/2$) thus depends only on the total charge, while if $J \neq 0$ the inter-orbital interaction is weaker than the intraorbital one and becomes sensitive to the spin configuration.

### III. SLAVE-SPIN MEAN-FIELD THEORY

#### A. Slave-spin representation

In this section, we introduce a new representation of fermion operators in terms of constrained ("slave") auxiliary fields, which proves to be particularly convenient in order to study the multi-orbital Hamiltonian above. The main idea at the root of any slave-variable representation\textsuperscript{12,13} is to enlarge the Hilbert space and to impose a local constraint on each site, and addressing orbital-dependent properties. The basic observation behind this scheme is that the two possible occupancies of a spinless fermion on a given site, $n_d = 0$ and $n_d = 1$, can be viewed as the two possible states of a spin-1/2 variable, $S^z = -1/2$ and $S^z = +1/2$. This representation has been widely used in the case of hard-core bosons. In the fermionic context however, one needs to assure anticommutation properties, and this is done by introducing an auxiliary fermion $f_i$, with the additional local constraint:

$$
f_i^\dagger f_i = S^z + \frac{1}{2}
$$

(4)

In this manner, one obtains a faithful representation of the Hilbert space, which reads:

$$
|0\rangle = |n_f = 0, S^z = -1/2\rangle
$$

(5)

$$
|1\rangle \equiv d_i^\dagger |0\rangle = |n_f = 1, S^z = +1/2\rangle
$$

(6)

This constraint eliminates the two unphysical states $|n_f = 0, S^z = +1/2\rangle$ and $|n_f = 1, S^z = -1/2\rangle$. This representation is easily extended to the multi-orbital case, by treating each orbital and spin species in this manner. Hence a set of $2N$ spin-1/2 variables $S^z_{im\sigma}$ and auxiliary fermions $f_{im\sigma}$ are introduced ($m = 1, \ldots, N$ is the number of orbitals), obeying the local constraint on each site:

$$
\tilde{n}_{im\sigma}^f = S^z_{im\sigma} + \frac{1}{2}
$$

(7)

This constraint can e.g. be imposed with Lagrange multipliers fields $\lambda_{im\sigma}(\tau)$.

We now explain how to rewrite the original Hamiltonian\textsuperscript{12} in terms of the slave spins and auxiliary fermions. We consider first for simplicity the case $J = 0$, since the case $J \neq 0$ requires an additional approximation, as discussed later. For $J = 0$, the interaction involves only the total electron charge on a given site, and therefore reads:

$$
H_{\text{int}}^{J=0} = \frac{U}{2} \sum_i \left( \sum_{m\sigma} \tilde{n}_{im\sigma} \right)^2 = \frac{U}{2} \sum_i \left( \sum_{m\sigma} S^z_{im\sigma} \right)^2
$$

(8)

In order to express the non-interacting part of the Hamiltonian, we need to choose an appropriate representation of the creation operator of a physical electron, $d^\dagger_{im\sigma}$. However, this method introduces many variational parameters. On the opposite, S.Florens and one of the authors introduced a very economical representation of the N-orbital Hubbard model with $SU(N)$ symmetry based on a single slave variable, taken to be the phase conjugate to the total charge on a given lattice site (slave rotor representation\textsuperscript{16,17}). However, this method is not appropriate when the orbital symmetry is broken, as in the present work.
There is some freedom associated with this, since different operators in the enlarged Hilbert space spanned by the slave-spin and auxiliary fermions can have the same action on the physical (constrained) Hilbert space. We have not used the obvious possibility $d^1 \rightarrow S^+ f^\dagger$, $d \rightarrow S_- f$. This representation is correct in the physical Hilbert space (i.e., when the constraint is treated exactly), but it can be shown that additional mean-field approximations based on this representation will ultimately lead to a problem with spectral weight conservation because $S^+$ and $S^-$ do not commute. Instead, we have chosen the representation $d^1 \rightarrow 2S^x f^\dagger$, $d \rightarrow 2S^y f$, which is identical to the previous one on the physical Hilbert space, and involves commuting slave-spin operators. With this choice, the non-interacting part of the Hamiltonian reads:

$$H_0 = -\sum_m t_m \sum_{\langle ij \rangle, \sigma} 4S^z_{im\sigma} S^z_{jm\sigma}(f^\dagger_{im\sigma} f_{jm\sigma} + h.c.)$$

$$+ \sum_{i, m\sigma} (\epsilon_m - \mu)f^\dagger_{im\sigma} f_{im\sigma}$$

At this stage, no approximation has been made, provided the constraint is treated exactly.

### B. Mean-field approximation

Approximations will now be introduced, which consists in three main steps: i) treating the constraint on average, using a static and site-independent Lagrange multiplier $\lambda_{m\sigma}$ ii) decoupling the auxiliary fermions and slave-spin degrees of freedom, and finally iii) treating the slave-spin Hamiltonian in a single-site mean-field approach. This last step is quite independent of the two previous ones, and can be rather easily improved on, as done in [12].

After the first two steps, one obtains two effective Hamiltonians:

$$H^f_{eff} = -\sum_m t^f_{m} \sum_{\langle ij \rangle, \sigma} (f^\dagger_{im\sigma} f_{jm\sigma} + h.c.)$$

$$+ \sum_{i, m\sigma} (\epsilon_m - \mu - \lambda_m)f^\dagger_{im\sigma} f_{im\sigma}$$

$$H^S_{eff} = -\sum_m 4J^f_{m} \sum_{\langle ij \rangle, \sigma} S^x_{im\sigma} S^x_{jm\sigma}$$

$$+ \sum_{i, m\sigma} \lambda_m (S^z_{im\sigma} + \frac{1}{2}) + H_{int}[\{S^z_{im\sigma}\}]$$

with

$$H_{int}[\{\hat{S}_{im\sigma}\}] = U/2 \sum_i (\sum_{\sigma} S^z_{im\sigma} S^z_{im\sigma})^2$$

for $J = 0$. In these expressions, $t^f_{m}$ and $J^f_{m}$ are effective hoppings and slave-spin exchange constants which are determined from the following self-consistency equations:

$$t^f_{m} = 4t_m \langle S^z_{im\sigma} S^z_{jm\sigma} \rangle$$

$$J^f_{m} = t_m \langle f^\dagger_{im\sigma} f_{jm\sigma} + f^\dagger_{jm\sigma} f_{im\sigma} \rangle$$

The free fermion Hamiltonian describes the quasiparticle degrees of freedom. Their effective mass is set by the renormalisation of the hopping: $t^f_{m}/t_m = 4 \langle S^z_{im\sigma} S^z_{jm\sigma} \rangle$. The quasiparticle weight is associated with a different quantity, namely:

$$Z_m = 4 \langle S^z_{im\sigma} \rangle^2$$

Note that it depends in general on the orbital, a key feature for the physics that we want to address with this technique. Both the renormalisation of the mass and the quasiparticle weight are self-consistently determined from the solution of the quantum spin Hamiltonian, which describes the charge dynamics. As clear from [12], metallic behaviour for orbital $m$ corresponds to long-range order in $S^z_m$, while Mott insulating behaviour corresponds to $\langle S^z_m \rangle = 0$.

At this stage, the slave-spin degrees of freedom are still described by a quantum spin Hamiltonian on the lattice, and we therefore make the additional approximation (iii) of treating this model on the level of a single-site mean-field. We thus have to solve the single-site spin Hamiltonian:

$$H_s = \sum_{m\sigma} 2h_m S^z_{m\sigma} + \sum_{m\sigma} \lambda_m (S^z_{m\sigma} + \frac{1}{2}) + H_{int}[\hat{S}_{m\sigma}]$$

in which the mean-field $h_m$ is determined self-consistently from:

$$h_m = 2zJ^f_m \langle S^z_{m\sigma} \rangle$$

where $z$ is the coordination number of the lattice. This equation can be combined with (12) to yield:

$$h_m = 4 \langle S^z_{m\sigma} \rangle \frac{1}{N} \sum_k \epsilon_{km} \langle f^\dagger_{km\sigma} f_{km\sigma} \rangle$$

In this expression, the fermionic expectation value is to be calculated with the quasiparticle Hamiltonian. Within this single-site mean-field approximation however, the renormalisation of the hopping becomes identical to the quasiparticle residue since $\langle S^z_{im\sigma} S^z_{jm\sigma} \rangle$ factorizes into $\langle S^z_{im\sigma} \rangle^2$. As a result, the quasiparticle Hamiltonian reads:

$$H^f_{eff} = \sum_{k,m\sigma} (Z_m \epsilon_{km} + \epsilon_m - \mu - \lambda_m)f^\dagger_{km\sigma} f_{km\sigma}$$

with $\epsilon_{km} \equiv -t_m/z \sum_{i,n,n(i)} e^{-k(i-j)}$ the Fourier transform of the hopping. Equations (13, 14, 16, 17) self-consistently determine the variational parameters $h_m$, $\lambda_m$ and $Z_m = 4 \langle S^z_{m\sigma} \rangle^2$. They are the basic mean-field equations based on the slave-spin representation, which will be used below. Solving these equations requires to diagonalize the single-site spin Hamiltonian, corresponding to a $4^N \times 4^N$ matrix.

Let us finally discuss the case of a non-zero Hund’s coupling $J \neq 0$. The first three terms in (12) are easy to treat in the slave-spin formalism, since they involve only density-density interactions and are thus directly
expressed in terms of the Ising components of the slave spins. They read:

\[
\frac{U'}{2} \sum_i \left( \sum_{m, \sigma} S_{i m \sigma}^z \right)^2 + \frac{J}{2} \sum_{i, m} \left( \sum_{\sigma} S_{i m \sigma}^z \right)^2 - \frac{J}{2} \sum_{i, \sigma} \left( \sum_m S_{i m \sigma}^z \right)^2
\]

(18)

In contrast, the “spin-flip” and (intra-site) “pair-hopping” terms (last two terms in (2)) are more difficult to deal with, since they involve both slave-spin and auxiliary fermions operators. As a result, four-fermion terms are introduced which require additional mean-field decouplings. For simplicity, we choose to mimic the effect of these terms by replacing them by operators which have exactly the same effect on the slave-spin quantum numbers of the Hilbert space, namely:

\[
\begin{align*}
&-J \sum_i \left[ S_{i1\uparrow}^+ S_{i1\downarrow}^+ S_{i2\uparrow}^- S_{i2\downarrow}^- + S_{i1\downarrow}^+ S_{i1\uparrow}^- S_{i2\uparrow}^+ S_{i2\downarrow}^+ \right] \\
&-J \sum_i \left[ S_{i1\uparrow}^+ S_{i1\downarrow}^- S_{i2\uparrow}^- S_{i2\downarrow}^+ + S_{i2\uparrow}^+ S_{i2\downarrow}^- S_{i1\uparrow}^- S_{i1\downarrow}^+ \right], \quad (19)
\end{align*}
\]

Despite the fact that these terms connect the physical and unphysical parts of the Hilbert space (and therefore would strictly vanish if the constraint was implemented exactly), it is reasonable to expect that they will qualitatively describe the physics of the spin-flip and pair-hopping terms when the constraint is treated on average, because their action on the slave-spin quantum numbers is the correct one. Hence, we shall use the following representation of the interacting part of the hamiltonian for \( J \neq 0 \):

\[
H_{\text{int}} \approx \frac{U'}{2} \sum_i \left( \sum_{m, \sigma} S_{i m \sigma}^z \right)^2 + \frac{J}{2} \sum_{i, m} \left( \sum_{\sigma} S_{i m \sigma}^z \right)^2 - \frac{J}{2} \sum_{i, \sigma} \left( \sum_m S_{i m \sigma}^z \right)^2 - J \sum_i \left[ S_{i1\uparrow}^+ S_{i1\downarrow}^- S_{i2\uparrow}^- S_{i2\downarrow}^+ + S_{i1\downarrow}^+ S_{i1\uparrow}^- S_{i2\uparrow}^+ S_{i2\downarrow}^- \right] \\
- J \sum_i \left[ S_{i1\uparrow}^+ S_{i1\downarrow}^- S_{i2\uparrow}^- S_{i2\downarrow}^+ + S_{i2\uparrow}^+ S_{i2\downarrow}^- S_{i1\uparrow}^- S_{i1\downarrow}^+ \right]
\]

(20)

C. Benchmarks

In this section, we perform some benchmarks of the slave-spin representation and mean-field theory.

1. Atomic limit (\( J=0 \))

In the \( J=0 \) case we check explicitly that the atomic limit (i.e. \( t_m = 0 \)) of the degenerate N-band model with \( SU(2N) \) symmetry is correctly reproduced. Indeed our equations simplify drastically in this limit (\( t_m = h_m = 0 \)), leaving only the \( \lambda_{m\sigma} = \lambda \) to be determined. The constraint equation (7) reads in this case:

\[
n_F(\mu - \lambda) = Z^{-1} \sum_{Q=0}^{2N} N_Q \exp\left(-\beta\left[\frac{U}{2}(Q - N)^2 + \lambda Q\right]\right)
\]

(21)

where \( n_F(\epsilon) \) is the Fermi function, \( Z = \sum_{Q=0}^{2N} N_Q \exp\left(-\beta\left[\frac{U}{2}(Q - N)^2 + \lambda Q\right]\right) \) and \( Q \) is the total number of particles. Solving numerically this equation for \( \lambda \) leads to the correct “Coulomb staircase”, as shown in Fig. 1, as long as \( T \ll U \). At high temperatures the fact that we have imposed the constraints only in average limits the accuracy, but in practice \( T \ll U \) is not a severe limitation.

![Fig. 1: (color online). Filling vs chemical potential for a two-orbitals impurity (atomic limit of a particle-hole symmetric Hubbard model), \( U = 2, \beta = 50 \); within the slave spin mean field (full line) and exact result (dashed line). The Coulomb staircase is correctly reproduced up to temperatures of order \(~ U\).

2. N-orbital Hubbard model with \( SU(2N) \) symmetry and large-N limit

Here, we apply the slave-spin mean-field approximation to the N-orbital model (\( m = 1, \cdots, N \)), in the case where all bands have the same hopping, with \( J = 0 \). The results for the quasi-particle weight as a function of \( U \), at half-filling, are displayed on Fig. 2. A transition into a Mott phase is found for \( U > U_c(N) \). The exact large \( N \) behaviour of \( U_c(N) \) in the limit of infinite coordination (DMFT) is known to be linear in \( N \), the slope being \( U_c/N = 8|\tilde{\epsilon}| \), where \( \tilde{\epsilon} \equiv \int_{-\infty}^{0} d\epsilon D(\epsilon)|\epsilon| \). This slope is correctly reproduced by the slave-spin mean-field approximation, indicating that this approximation becomes more accurate as \( N \) is increased.

One can actually calculate analytically the critical value of the coupling within this approach, for arbitrary \( N \), by performing a perturbative expansion around the
atomic limit for small $h_m$. This yields:

$$U_c = 8(N + 1)|\bar{c}|$$ (22)

which coincides with the numerical determination in the inset of Fig. 2. We also note that (22) is precisely the result of the Gutzwiller (slave-boson) approximation in the multi-orbital case.

D. Comparison with slave bosons and slave rotors

As suggested by the fact they yield identical values of $U_c$, the slave-spin mean-field theory has many similarities with the Gutzwiller approximation (GA). In fact, as shown on Fig. 3, the whole dependence of $Z$ on $U$ is identical to that of the GA.

The slave spin representation has several advantages over the slave-boson representations that can be used to formulate the GA. One advantage is that the number of variables is smaller: $2N$ spin-1/2 degrees of freedom instead of $2^N$ slave bosons (one associated to each state in the Hilbert space, in the absence of symmetries). Another advantage is that the number of unphysical states is smaller than in slave boson representations, because the Hilbert space spanned by the $2N$ quantum spins is finite by construction, while the Hilbert space associated with the slave bosons in the absence of the constraint is an infinite-dimensional one. This might be useful in considering finite-temperature properties and the entropy of the model.

A similar remark applies when comparing the present slave-spin representation to the slave-rotor representation recently developed by S. Florens and one of the authors. The slave spin representation has several advantages over the slave-boson representations that can be used to formulate the GA. One advantage is that the number of variables is smaller: $2N$ spin-1/2 degrees of freedom instead of $2^N$ slave bosons (one associated to each state in the Hilbert space, in the absence of symmetries). Another advantage is that the number of unphysical states is smaller: $2^N$ instead of $2N$.

Since it introduces only one slave variable. Specifically, a (slave) quantum rotor and auxiliary fermions are introduced on each site such that:

$$d_{im\sigma}^i = f_{im\sigma}^i e^{i\theta_i}, \quad d_{im\sigma} = f_{im\sigma} e^{-i\theta_i}$$ (23)

where the phase is conjugate to the local charge, corresponding to the local constraint:

$$\sum_{im\sigma} (f_{im\sigma}^i f_{im\sigma} - \frac{1}{2}) = \hat{L}_i$$ (24)

in which $\hat{L}_i = 1/\partial i\theta_i$ is the conjugate momentum to the phase. It is clear from these expressions that there is a close similarity between the slave-spin and slave-rotor formalisms. Two important differences must be noted: (i) a single slave-rotor variable is introduced for all orbitals and (ii) the Hilbert space of the unconstrained rotor is infinite-dimensional, containing an infinite tower of charge states $|l\rangle$ which are physical only for $|l| \leq N$. As a result, mean-field approximations in which the constraint is treated only on average are less accurate when the contribution of these unphysical charge states becomes sizeable. This is particularly true in the weak-coupling limit. On Fig. 3 we compare the slave-spin and slave-rotor result for the quasiparticle residue in the one-band case, in order to illustrate this effect.

On the whole, slave-rotors and slave-spins offer two useful representations, the former being very economical and well suited to situations in which not only the total local charge is involved (e.g. in Coulomb blockade problems), while the latter is well suited to the investigation of orbital-dependent properties, as in the present article. Both methods are easy to implement at a very low numerical cost, hence allowing for a fast and efficient investigation of the phase diagram and phase transitions in a wide range of parameters.

IV. ORBITAL-SELECTIVE MOTT TRANSITION WITH SLAVE-SPIN MEAN FIELD THEORY

In this section, we use slave-spin mean-field theory in order to study the two-band model with unequal hoppings. The non-interacting density of states of each band is taken to be a semi-circle (of half-width $D_1 = 2t_1$ and $D_2 = 2t_2 < D_1$), corresponding to a Bethe lattice with infinite connectivity $z = \infty$ and nearest-neighbour hoppings $t_{1,2}/\sqrt{z}$. No crystal-field splitting is introduced ($\epsilon_1 = \epsilon_2 = 0$) and we restrict ourselves to the case in which both bands are half-filled ($\langle n_1 \rangle = \langle n_2 \rangle = 1$). The model is thus particle-hole symmetric, implying that the chemical potential $\mu = 0$ and Lagrange multipliers $\lambda_1 = \lambda_2 = 0$. The parameter space was explored for $U > 0, J = 0 \div 0.5U$ i.e. $U' = U - 2J = 0 \div U$, and the ratio between the two bandwidths $t_2/t_1 = 0 \div 1.0$. For the study of the Mott transitions in this model we monitor the quasiparticle weights $Z_m = 4\langle \hat{S}_{m\sigma}^z \rangle^2$. 
Three different phases are found: at small \( U \) both bands are metallic (i.e. \( Z_m \neq 0 \)), at large \( U \) both are insulating (\( Z_m = 0 \)), and in between an “orbital selective Mott phase” (OSMP) is found in which only the band with largest bandwidth has \( Z_1 \neq 0 \), while the narrower band has \( Z_2 = 0 \).

Fig. 4 displays the phase diagram within slave-spin mean-field theory for the bandwidth ratio \( t_2/t_1 = 0.5 \). Three different phases are found: at small \( U \) both bands are metallic (i.e. \( Z_m \neq 0 \)), at large \( U \) both are insulating (\( Z_m = 0 \)), and in between an “orbital selective Mott phase” (OSMP) is found in which only the band with largest bandwidth has \( Z_1 \neq 0 \), while the narrower band has \( Z_2 = 0 \).

![Phase Diagram](image)

In the inset of Fig. 4 we reproduce for comparison the result of Koga et al. obtained within DMFT. Qualitatively, one sees that the slave-spin mean-field compares rather well to the DMFT results. There are quantitative differences in the critical values of the couplings \( U \) and \( U' \), a well known feature of Gutzwiller-like approximations. Also, the linear dependence on \( U' \) of the upper boundary of the OSMP phase is due to the simplified treatment of the spin-flip and pair-hopping terms discussed above (as indeed confirmed by the results of section IV C).

There is however one significant qualitative difference between the slave-spin results and those of Koga et al. (inset). We find that the endpoint of the OSMP phase does not lie exactly on the \( U = U' \) line. Hence, within the slave-spin mean field, the Mott transition becomes orbital-selective (OSMT) only when \( J \) exceeds a critical value. This is a rather significant finding, since for \( J = 0 \) the interacting part of the hamiltonian (\( H_{int} \)) has full \( SU(4) \) spin-orbital symmetry, while for \( J \neq 0 \) the symmetry is lower. In Ref., it was argued that indeed the enhanced symmetry of the \( J = 0 \) case prevents an orbital-selective Mott transition to occur. Our finding that a critical value of \( J \) is needed to induce an OSMT (for \( t_2/t_1 = 0.5 \)) suggests that symmetry considerations on \( H_{int} \) may not be essential to the existence of an orbital-selective transition. After all, the difference in bandwidths breaks the \( SU(4) \) symmetry from the kinetic energy part of the hamiltonian. In order to study this issue in more detail, we perform in the next section a detailed study of the \( J = 0 \) case.

### A. OSMT at \( J = 0 \)

In this section, we focus on the \( J = 0 \) case, for which \( H_{int} \) has full \( SU(4) \) symmetry, and explore the nature of the Mott transition in the full range of bandwidth ratio from \( t_2/t_1 = 0 \) to \( t_2/t_1 = 1 \).

We find that the two bands undergo a common Mott transition at a single value of \( U = U_c \) as long as the bandwidth ratio exceeds a critical threshold: \( t_2/t_1 > 0.2 \). In contrast, for \( t_2/t_1 < 0.2 \), an orbital-selective Mott phase is found, despite the enhanced symmetry of the interaction term. Fig. 4 displays our result for the phase diagram as a function of \( t_2/t_1 \) and \( U/t_1 \). All transitions are found to be second-order when \( J = 0 \). On Fig. 5 the quasiparticle weights of each band is plotted as a function of \( U \), for several values of \( t_2/t_1 \). The localization of the narrower band manifests itself as a kink in the quasiparticle weight of the wider band. As \( U \) is increased further, the wide band in turn undergoes a Mott transition. We observe that, within slave-spin mean-field, the quasiparticle weight of the wider band in the orbital-selective Mott phase coincides with that of a single-band model. This is because the slave-spin mean-field neglects charge fluctuations of the localised orbital, so that the physical behavior of the wide band becomes effectively that of a one-band model as soon as the narrow band becomes localized.

Our finding of an orbital-selective Mott transition at \( J = 0 \) when \( t_2/t_1 \) is small enough, within slave-spin mean-field theory, raises two questions. First, is this find-
ing an artefact of the slave-spin approximation or does it survive a full DMFT treatment (i.e. is it a genuine feature of the infinite-coordination model?). Second, does this invalidate the argument based on the symmetry of $H_{int}$? The first question will be addressed in detail in Sec. VIII in which a DMFT study will be performed, using exact diagonalization and Quantum Monte-Carlo techniques. We will show that indeed, a transition does exist at $J = 0$ when $t_2/t_1$ is small enough, but that the nature of the intermediate phase (OSMP) at low-energy is a rather subtle issue. In order to address the second question, let us briefly recall the symmetry argument of Koga et al. The argument relies on the gap to charge excitations in the insulating phase. When $J = 0$, charge excitations mix the two orbitals because of the enhanced SU(4) symmetry. Instead, for $J \neq 0$, the charge excitations of lowest energy are independent in each orbital sector. As a result, it is reasonable to expect (at least when the kinetic energy term is treated in a perturbative manner) that the system can sustain two different charge gaps when $J \neq 0$ while the gaps might coincide for $J = 0$. We observe however that this argument applies to the instability of the large-U Mott phase (in which both bands are gapped) when $U$ is reduced, and suggests that, for $J = 0$, the Mott gap closes at the same value of $U$ for both bands when $U/t_1$ is reduced. It does not preclude however that a transition into an intermediate phase does exist, in which the “localised” band (with the narrower bandwidth) is not fully gapped. As we shall find below, there is indeed clear evidence from the DMFT results that the orbital-selective Mott phase at $J = 0$ is not a conventional Mott insulator and that the narrow (“localised”) band does have spectral weight down to zero-energy in this phase. Obviously, the slave-spin mean-field approach is too rudimentary to be able to capture these fine low-energy aspects, but it is remarkable that it does allow us to infer correctly that an intermediate phase is indeed present.

B. Dependence of OSMT on $J$

Having clarified the situation for $J = 0$, we come back to the effect of a non-zero $J$, still within the slave-spin mean-field approximation. Fig. 7 shows how the phase diagram as a function of the bandwidth ratio $t_2/t_1$ and of $U/t_1$ is modified for $J \neq 0$. One sees that a finite $J$ enlarges the orbital-selective Mott phase and favors an OSMP. The critical ratio $(t_2/t_1)_c$ below which an OSMP exists increases significantly, e.g. $t_2/t_1 \simeq 0.55$ for $J = 0.01U$. With increasing $J$, $(t_2/t_1)_c$ tends towards 1.
Hence a common Mott transition for both bands is recovered for all values of \( J \) only when \( t_1 = t_2 \). For a given bandwidth ratio \( t_2/t_1 \), the Mott transition is orbital-selective for \( J/U > (J/U)_c \). The dependence of this critical ratio upon \( t_2/t_1 \) (i.e. the location of the endpoint of the OSMP phase) is displayed in Fig. 8. (It should be noted however that this critical ratio \((J/U)_c\) is underestimated by our simplified treatment of the pair-hopping and spin-flip term). Finally, we found that for finite \( J \), the insulator to OSMP transition remains second-order, while the metal to OSMP transition becomes first-order.

\[
H_{int} = U \sum_{im} \tilde{n}_{im\uparrow} \tilde{n}_{im\downarrow} + \left( U - 2J \right) \sum_{i\sigma} \tilde{n}_{i\sigma\uparrow} \tilde{n}_{i\sigma\downarrow} + \left( U - 3J \right) \sum_{i\sigma} \tilde{n}_{i\sigma\uparrow} \tilde{n}_{i\sigma\downarrow}.
\]

(25)

which is easily represented in terms of slave-spins as:

\[
H_{int} = \frac{U'}{2} \sum_{i} (\sum_{m,\sigma} S_{im\sigma}^z)^2 + J \sum_{i,\sigma} (\sum_{m} S_{im\sigma}^z)^2 - \frac{J}{2} \sum_{i,\sigma} (\sum_{m} S_{im\sigma}^z)^2
\]

(26)

This study is also motivated by a comparison to Quantum Monte-Carlo treatments in which the spin-flip and pair-hopping terms are not easily treated. On Fig. 8 we display the slave-spin phase diagram found for \( t_2/t_1 = 0.5 \) at zero-temperature. On sees that the OSMP shrinks dramatically (albeit the two transitions do not actually merge). This finding sheds light on the results by Liebsch in ref. 12. Because this study was based on Quantum-Monte Carlo, hence neglecting the spin-flip and pair-hopping terms, it is natural that the orbital-selective phase can be found only in a very narrow range of parameter space. The key role of spin-flip and inter-orbital pair-hopping terms for the OSMT was actually pointed out in the recent work of Koga et al. 14.

In Fig. 10 we display the region in \( t_2/t_1, J/U \) parameter space where the Mott transition is found to be orbital-selective, analogously to Fig 8. The critical ratio \((J/U)_c\) is found to be roughly exponential in \( t_2/t_1 \). In contrast to the case of the full hamiltonian (Fig 8), we find that no OSMT exists when \( t_2/t_1 \) exceeds a critical bandwidth ratio \( t_2/t_1 \approx 0.6 \), for any \( J/U \). Beyond this value no OSMT is found at any \( J/U \). (Note that the upper critical line at large \( J/U \) corresponds however to the unphysical case of an attractive Coulomb interaction due to \( U - 3J < 0 \)).

Finally, we emphasize that the orbital-selective Mott phase, which exists only in a very narrow range of couplings for the simplified interaction 26 at \( T = 0 \), is actually enlarged at finite-temperature, as shown in Fig. 11.

C. Role of the spin-flip and pair-hopping terms in the Hund Hamiltonian

In order to clarify the role played by the different terms of the interaction 23, we have also studied the Hamiltonian in which the spin-flip and the (on-site) inter-orbital pair-hopping terms are dropped, namely:

\[
\tilde{S}_{im\sigma}^z = \frac{1}{2} \left( \tilde{S}_{im\sigma}^+ \tilde{S}_{im\sigma}^- - \tilde{S}_{im\sigma}^+ \tilde{S}_{im\sigma}^- \right)
\]

\[
\tilde{S}_{im\sigma}^z = \frac{1}{2} \left( \tilde{S}_{im\sigma}^+ \tilde{S}_{im\sigma}^- - \tilde{S}_{im\sigma}^+ \tilde{S}_{im\sigma}^- \right)
\]

(26)

V. DYNAMICAL- MEAN FIELD THEORY FOR \( J = 0 \) AND NATURE OF THE OSMT PHASE

In this section, we study the two-band model with \( J = 0 \) using dynamical mean-field theory. Our goal is to determine whether the transition into an orbital-selective Mott phase (OSMP) found within the slave-spin approximation at small enough \( t_2/t_1 \) is indeed a robust feature, and to shed light on the possible low-energy physics of this phase. Within DMFT, the lattice model is
FIG. 9: (color online). Phase diagram ($U$ vs $U'$) for $t_2/t_1 = 0.5$ at $T = 0$ for a two-band Hubbard model without spin flip and pair hopping terms in the interaction.

FIG. 10: (color online). Critical $J/U$ for the model without spin-flip and pair-hopping as a function of $t_2/t_1$. At small ratios of the bandwidths, the system displays an OSMT above a critical $J/U$ ratio which vanishes at $t_2/t_1 = 0$. In less anisotropic systems large Hund’s coupling are needed to realize OSMPs, whereas beyond the critical bandwidth ratio of 0.6 no OMST is possible within this model.

FIG. 11: (color online). Same phase diagram as in fig. 9 but in the U-J plane at $T = 0$ and at $\beta t_1 = 40$.

The hybridisations to the effective conduction bath are self-consistently related to the local interacting Green’s functions $G_m$ through:

$$G_m(i\omega) = i\omega - t_m^2 G_m(i\omega)$$

These equations are exact for an infinite-connectivity Bethe lattice (corresponding to semi-circular non-interacting d.o.s). Particle-hole symmetry with one electron per site in each band has been assumed. We focus here on the paramagnetic solutions only. The DMFT equations will be solved in the following using both an exact diagonalisation (ED) and Quantum Monte-Carlo (QMC) technique.

**A. Exact diagonalisation study**

Within the adaptative exact-diagonization method, the effective conduction-electron bath is discretized using a finite number of orbitals $N_s$. Hence, one considers the two-orbital Anderson impurity hamiltonian:

$$H_{A1M} = \sum_{m\sigma} \epsilon_{m\sigma} a_{m\sigma}^\dagger a_{m\sigma} + \sum_{m\sigma} \sum_{l=1}^{N_s} V_{lm} (d_{m\sigma}^\dagger a_{l\sigma} + h.c) + \frac{U}{2} (\hat{n}_1 + \hat{n}_2 - 2)^2$$

The operators $a_{l\sigma}, a_{l\sigma}^\dagger$ describe the discretized conduction- bath degrees of freedom. The effective parameters $\{\epsilon_{m\sigma}, V_{lm}\}$ have to be determined self-consistently, according to (28), namely:

$$\sum_{l=1}^{N_s} \left| V_{lm} \right|^2 = t_m^2 G_m(i\omega_n)$$

The ED method becomes an asymptotically exact solver of the DMFT equations in the limit $N_s \to \infty$. In practice however, one can handle only a finite number of effective sites. For the case at hand, we used a $T = 0$ Lanczos algorithm, with $N_s = 5$ (i.e 5 effective sites per orbital). The self-consistency (30) is implemented on a Matsubara grid corresponding to a (fictitious) inverse temperature $\beta$ (taken to be in practice in the range 200 to 500, which insures a good resolution on the low-energy physics). We monitor in particular the quasiparticle weights, approximated as: $Z_m = [1 - \text{Im}\Sigma_m(i\omega_n)/\omega_n]^{-1}$ (where $\omega_n = \pi/\beta(2n + 1)$).
Our ED results for these quantities are displayed on Fig. 12 and compared to the slave-spin results, both as a function of $U$ for fixed $t_2/t_1$ and as a function of $t_2/t_1$ for fixed $U$ (inset). It is clear from this figure that, within the energy resolution which can be reached with $N_s = 5$, an orbital-selective transition is indeed observed in the DMFT(ED) results when $t_2/t_1$ is smaller than a critical value (close to 0.25), in remarkable agreement with the slave-spin mean-field. The quantitative value of the critical coupling $U/t_1$ for the localisation of the wider band is overestimated, as usual in Gutzwiller-like schemes.

The phase diagram obtained with ED, as a function of $t_1/t_2$ and $U/t_1$ is displayed in Fig. 13. Good qualitative agreement with the slave-spin mean-field is found (Fig. 5). We also studied the hysteresis properties by performing runs for increasing and decreasing values of $U/t_1$. This results in two almost parallel transition lines on Fig. 13, one corresponding to the disappearance of the metallic solution (obtained from a series of runs for increasing $U$), the other corresponding to the loss of the insulating nature of the wide band (from a series of runs for decreasing $U$). In the region between these two lines, coexistence of two types of DMFT solutions is found: for small $t_2/t_1$, one of the solutions is orbital-selective Mott and the other is fully insulating, while for larger $t_2/t_1$, one of the solutions is metallic and the other fully insulating. The actual thermodynamic transition is given by the crossing of the free energies of the two solutions. In contrast, no hysteresis has been found at the transition between the OSMP and metallic phases. This suggests that the transition from the metallic to the OSMP phase is of a very different nature than the Mott transition of the wider band. If only the gap closure is monitored, then only one transition is found at $J = 0$, in agreement with the symmetry argument of Ref. 2. As we shall demonstrate below, there is indeed strong evidence that the orbital-selective Mott phase at $J = 0$ does not display a sharp gap in either orbitals.

![Figure 12: (color online). Quasiparticle residues at $J = 0$ in DMFT(ED) for $t_2/t_1 = 0.1$ (symbols). For comparison, the slave-spin mean-field approximation is also displayed (continuous line). Inset: same quantities as a function of $t_2/t_1$ at fixed $U/t_1 = 4.0$. (The kinks in $Z_1$ are associated with the criticality of $Z_2$.)](image)

![Figure 13: (color online). Phase diagram at $J = 0$ and $T = 0$ in ED-DMFT. The dashed line marks the disappearance of the Mott gap (downward runs). For $U$ values around 5 there is coexistence between an OSMP and - depending on the bandwidth ratio - an insulating or metallic phase.)](image)

**B. Low-energy nature of the orbital-selective Mott phase at $J = 0$, from ED and QMC**

In order to understand better the nature of the orbital-selective phase found at $J = 0$, we take a closer look at the local Green’s function for each orbital, in each phase. In order to do this, we also solved the DMFT equations using the Quantum Monte-Carlo algorithm of Hirsch and Fye22. The ED and QMC methods are quite complementary. The former applies at $T = 0$ but suffers from a limited energy-resolution due to the small value of $N_s$, while the latter is limited to finite-temperature but can be made very precise by increasing the number of time slices and the number of Monte-Carlo sweeps (we used 128 slices in imaginary time and up to $5 \times 10^5$ Monte Carlo sweeps in practice). Also, using QMC allows for a reconstruction of the spectral functions using a numerical analytic continuation based on the maximum entropy algorithm.

In Fig. 14 we display the ED results for the local Green’s functions on the Matsubara axis, for a small bandwidth ratio $t_2/t_1$ and three different values of $U$ corresponding to the insulating, metallic, and orbital-selective Mott phases. In the particle-hole symmetric case, the Green’s functions are purely imaginary on the Matsubara axis and related to the spectral function $A_m(\epsilon)$ of each orbital by:

$$\text{Im} G_m(i\omega) = -2\omega \int_0^{+\infty} \frac{A_m(\epsilon)}{\omega^2 + \epsilon^2} \text{d}\epsilon$$  \hspace{1cm} (31)

When the spectral function $A_m(\epsilon)$ has a gap, the integral in the right-hand side of (31) has no singularity.
in the $\omega \to 0$ limit, and hence $\text{Im}G_m(i\omega) \propto \omega$ at low frequency. Furthermore, $\text{Im}G_m(i\omega)$ has a minimum for $\omega$ of order $\Delta_m/2$, with $\Delta_m$ the gap in the $m$-th orbital (as can be seen by replacing $A_m(\epsilon)$ by the simplified form $1/2[\delta(\epsilon - \Delta_m/2) + \delta(\epsilon + \Delta_m/2)]$, yielding $\text{Im}G_p(i\omega) \approx -2\omega/(\omega^2 + \Delta_m^2/4))$. This is fully consistent with the ED results in the upper panel of Fig. 14, corresponding to a large value of $U/t_1 = \tau$, with both orbitals insulating and having a gap of order $U$.

In the lower panel of Fig. 14, ED results are displayed for $U/t_1 = 2$, when both orbitals are metallic. In this case, the low-frequency limit of $\text{Im}G_m(i\omega \to 0) = -\pi A_m(0)$. This is consistent with the numerical results, which also show that the Luttinger theorem is obeyed for both bands: $\pi A_m(0) = 1/t_m$.

The central panel of Fig. 14 displays the ED results for an intermediate coupling, corresponding to the orbital-selective phase. One sees that the wider band has metallic behaviour, with $A_1(\omega)$ still reaching the Luttinger value at $\omega = 0$. In contrast, $\text{Im}G_2(i\omega)$ appears to vanish as $\omega \to 0$, within the energy resolution of ED. However, in striking contrast to the upper panel (insulating phase), the minimum in $\text{Im}G_2(i\omega)$ is at a very low frequency scale which is obviously not given by $U$. This strongly suggests that $A_2(\omega)$ displays low-energy peaks very close to $\omega = 0$, and may even have spectral weight down to arbitrary low frequency.

Figure 15 compares the ED and QMC results for $\text{Im}G_{1,2}(i\omega)$ in the strongly anisotropic case $t_2/t_1 = 0.1$ for a relatively small Coulomb interaction $U/t_1 = 1.6$, easier to study with QMC. These parameters also correspond to the orbital-selective phase (Fig. 15). Very good agreement between the two methods is found, confirming the above analysis (and confirming also the Luttinger value for the wider band with greater accuracy than in ED). The corresponding spectral functions obtained by the maximum-entropy method are displayed on Fig. 15. The spectral function of the broader band is only slightly modified as compared to the non-interacting d.o.s. Small shoulders are visible, at the position of the lower and upper Hubbard bands, the Luttinger theorem is obeyed, and some of the spectral weight is transferred to higher energies as expected. The narrow-band however is obviously in a strong-coupling regime, with well-marked upper and lower Hubbard bands. The most striking features however are the two narrow peaks at low-frequency, which can be interpreted either as a split quasi-particle resonance or as the sign of a pseudo-gap (partially filled by thermal excitations since the QMC calculation is for $T/t_1 = 1/40$).

Hence, the general conclusion of this analysis is that the orbital-selective phase found for $J = 0$ at small enough $t_2/t_1$ is not a conventional Mott phase in which the (“localized”) orbital with narrower bandwidth would display a sharp gap. Instead, two narrow peaks exist near $\omega = 0$ and finite spectral weight is found down to low-energy. Our numerical data are consistent with a pseudo-gap behaviour, but a precise characterization of the low-energy nature of the phase will require further effort, using highly precise techniques at low-energy such as the numerical renormalization group. This is left for future work. Such a study should also clarify in which precise sense the narrower band is “localized” in this phase, and whether the orbital-selective transition is a true phase transition or rather a sharp crossover.
We note that this term could be eliminated by diagonalizing the non-interacting Hamiltonian. However, in the new basis, the interaction terms will be modified: terms will be generated which will have the same physical effect than a hybridization (and will involve non-local contributions in general). Indeed, as emphasized in Ref. 25, the existence of an OSMT is a basis-independent issue.

In a general two-band model, a Mott transition is signaled, when approached from the metallic side, by a low-frequency singularity in $\omega I - \Sigma(\omega) = Z^{-1}\omega + \cdots$, where $\Sigma$ and $Z$ are the self-energy and quasiparticle-weight matrices, respectively. An OSMT is characterized by $Z$ having one zero-eigenvalue while the other one remains finite. Being associated with the rank of the $Z$-matrix, it is a basis-independent notion. Our choice of basis is such that the interaction terms have the form specified above.

A. Physical considerations

Some statements about the effect of a finite hybridization can be made on general physical grounds (focusing for simplicity on the $J = 0$ case). First, for small values of $U$ when both orbitals are itinerant, it is obvious that a hybridization will not change qualitatively the low-energy nature of the metallic phase. Also, at very large $U$, when both orbitals are localized and a gap exists in both orbital sectors, we expect the presence of a gap to be a robust feature which persists in the presence of $V$. However, it is also clear that introducing $V$ into this gapped insulator allows the local moments formed in the Mott insulating state at $V = 0$ to screen each other. This occurs through the formation of on-site bonding and antibonding “molecular” levels mixing the two orbitals. As a result, the local-moment Mott insulator is expected to be replaced by a Mott insulator in which local singlets are formed on each site. The intermediate $U$ regime, in which the system is in the OSMP at $V = 0$, is more delicate. Because orbital 1 is itinerant, a Kondo screening process can take place, which will screen the local moment (formed by orbital 2 when $V = 0$). The resulting state can a priori be either a heavy-fermion metallic state involving quasiparticles with a large effective mass, or (because we are considering the half-filled case), a Kondo insulating state in which a gap is formed in the low-energy quasiparticle spectrum. Below, we study this question using the slave-spin approach and find that both phases can be obtained, depending on the value of $U$ and $V$. A larger $V$ favours the opening of a gap, as expected. Using a general low-frequency analysis, we also demonstrate that, for small values of $V$, the heavy-fermion metallic state, and not the Kondo insulating phase, is induced. We note, finally, that both the Kondo-insulating phase, and the phase obtained at large $U$ in which on-site local moments in different orbitals screen each other, have a singlet ground-state. It is therefore not obvious a priori whether these two phases are continuously connected, as found in Ref. 25, for a related (but different) model, or

VI. INSTABILITY OF THE ORBITAL-SELECTIVE MOTT PHASE UPON INTER-BAND HYBRIDIZATION

To what extent an orbital-selective Mott phase may occur in practice depends on its stability with respect to perturbations. This is an important issue in view of the fact that the Hamiltonian considered in this paper has a rather high degree of symmetry. In this last section, we consider the effect of an hybridization between the two orbitals (also recently considered in Ref. 25), i.e. of a local non-diagonal term:

$$H_{hyb} = V \sum_{i\sigma} (d_{i1\sigma}^\dagger d_{i2\sigma}^\dagger + d_{i2\sigma}^\dagger d_{i1\sigma})$$

(32)
whether a phase transition between them can exist. We return to this point at the end of this section.

In any event, these physical arguments imply that the orbital-selective Mott phase is unstable with respect to the introduction of a non-zero hybridization, at zero-temperature. Of course, for temperatures above the Kondo scale, the physics of the OSMP can be recovered. This is an important point in view of the possible experimental relevance of the OSMP.

B. Slave-spin mean-field study

We now turn to a more quantitative study of the effect of a finite hybridization \(V\), using the slave-spin mean-field approximation. Our aim is not to establish a full phase diagram for all values of the parameters \(U\), \(J\) and \(V\), but rather to investigate whether this approach does support the physical expectations discussed above. A more extensive investigation will be presented in a future publication.

In Fig. 17, we display the quasiparticle residues \(Z_1\) (for the broad band) and \(Z_2\) (for the narrow band), as a function of \(U\) and for increasing values of the hybridization \(V\). It is seen that, starting from the OSMP in which \(Z_1 \neq 0\) and \(Z_2 = 0\) for \(V = 0\), one obtains either a phase in which both \(Z_1\) and \(Z_2\) are non-zero (i.e Kondo screening takes place), or an insulating phase in which \(Z_1 = Z_2 = 0\). This demonstrates that the hybridization is indeed a singular perturbation on both the \(J = 0\) and finite-\(J\) orbital-selective Mott phases, in agreement with the physical arguments above.

In order to check whether the Kondo-screened phase is a (heavy-fermion) metal or whether it is gapped (Kondo insulator), we have plotted in Fig. 18 the band gap of the auxiliary quasiparticles found within slave spin mean-field theory (the plot is for \(J = 0\), the \(J \neq 0\) case being similar). Note that due to the factorization of the Green’s function

\[
\langle d(\tau)_{m\sigma}d_{m\sigma}^\dagger(0) \rangle = 4\langle S^x(0)_{m\sigma}S^x(\tau)_{m\sigma}\rangle\langle f_{m\sigma}(\tau)f_{m\sigma}^\dagger(0)\rangle
\]

(33)

the physical gap in the insulating phase will be of the order of \(V\). For small and intermediate values of \(V\), the phase with \(Z_1 \neq 0\) and \(Z_2 \neq 0\) is metallic (gapless) (see Fig. 18). The orbital-selective Mott phase is replaced by a heavy-fermion regime, as shown in Fig. 17 in which the orbital with narrower bandwidth acquires a very large effective mass (corresponding to a very low quasiparticle coherence scale \(Z_2\)). This is also in qualitative agreement with our recent study of the periodic Anderson model with direct f-electron hopping. Only beyond a critical value of \(V\) is a gapped Kondo insulator found. As discussed below, this can in fact be proven generally, beyond the mean-field approximation used here.

At small to intermediate values of \(V\), the two Mott transitions associated with the OSMP at \(V = 0\) are therefore replaced by a single non-selective transition from a (heavy-fermion) metal to an insulator as \(U\) is increased. Within the slave-spin mean-field, this unique metal to insulator transition is found to be first-order, and to occur at a critical value of \(U\) which lies in between the critical interactions of the metal-OSMP and OSMP-insulator transitions.

For larger values of \(V\), the OSMP phase is replaced by a Kondo-insulating phase with \(Z_1,Z_2 \neq 0\) but a finite quasiparticle band-gap (lower plot in Fig. 17). Within slave-spin mean-field, a phase transition takes place as \(U\) is increased, towards another insulating phase with \(Z_1 = Z_2 = 0\) (corresponding to the fact that the Kondo effect does not take place when \(V\) is turned on starting from a Mott phase for both orbitals, with a large gap). As pointed out above however, this large-\(U\) insulating phase also has a singlet ground-state however, due to inter-orbital screening. Whether this phase transition is an artefact of the slave-spin mean-field or whether it is indeed present in a more accurate DMFT treatment is a question to which we shall return below.

### FIG. 17: (color online). Quasiparticle residues \(Z_1\) and \(Z_2\) within slave spins MFT, for finite \(V\). Top: \(t_2/t_1 = 0.5, J = 0.25U\) for (from right to left in the upper manifold - wide band \(\sigma\), from left to right in the lower manifold - narrow band): \(V = 0\) (OSMT system), \(V/t_1 = 0.1, 0.15, 0.2, 0.3\). Bottom: \(t_2/t_1 = 0.1, J = 0\) for (from right to left in the upper manifold - wide band \(\sigma\), from left to right in the lower manifold - narrow band) \(V = 0\) (OSMT system), \(V/t_1 = 0.05, 0.1, 0.2\). Insets show the same graph in log scale.
effect does take place as following terms in the low-frequency expansion of the self-quasiparticle residues being finite. We thus keep the following terms in the low-frequency expansion of the self-energy:

\[
\begin{align*}
\Sigma_{11}(\omega) &= \omega(1 - 1/Z_1) + \cdots \\
\Sigma_{22}(\omega) &= \omega(1 - 1/Z_2) + \cdots \\
\Sigma_{12}(\omega) &= \Sigma_{12}(0) + \cdots
\end{align*}
\] (34)

The low-energy quasiparticle band structure is then given by:

\[
[\omega - Z_1 \epsilon_1(k)][\omega - Z_2 \epsilon_2(k)] - Z_1 Z_2 [V + \Sigma_{12}(0)]^2 = 0
\] (35)

From this expression, it is easily seen that a gap is present whenever:

\[
V_{\text{eff}} > \sqrt{D_{1\text{eff}} D_{2\text{eff}}}
\] (36)

In this expression, \(V_{\text{eff}}\) is the effective hybridisation between low-energy quasiparticles, and \(D_{1\text{eff}}, D_{2\text{eff}}\) the renormalised quasiparticle half-bandwidths, given by:

\[
V_{\text{eff}} = \sqrt{Z_1 Z_2 [V + \Sigma_{12}(0)]}, \quad D_{1\text{eff}} = Z_1 D_1, \quad D_{2\text{eff}} = Z_2 D_2
\] (37)

Remarkably, \(Z_1\) and \(Z_2\) drop out from (36), and the condition for a quasiparticle band gap therefore reads:

\[
V + \Sigma_{12}(0) > \sqrt{D_1 D_2}
\] (38)

If this condition is satisfied (and \(Z_1, Z_2 \neq 0\)), one has a Kondo insulator phase, with a quasiparticle band gap given by:

\[
\Delta_g = \sqrt{(D_{1\text{eff}} - D_{2\text{eff}})^2 + 4V_{\text{eff}}^2} - (D_{1\text{eff}} + D_{2\text{eff}})
\] (39)

In the opposite case, a heavy-fermion (gapless) metallic phase is formed.

From (38), it is seen that it is the off-diagonal component of the self-energy (induced by \(V\)) which plays the key role in deciding whether a gap opens or not. From the same equation, it is also clear that a bandgap cannot open for arbitrary small \(V\). Indeed, at small \(V\), \(\Sigma_{12}\) grows at most proportionally to \(V\), and hence the left-hand side of (38) is small, while the right-hand side is finite (note that the r.h.s involves the bare bandwidths). Hence, a critical value of \(V\) is required to open a band gap and enter the Kondo insulating phase, starting from the OSMP. Note that this analysis is general and relies only on Fermi-liquid considerations, independently of the specific method used to solve the model. Note also that the situation is very different when one of the bare bands is dispersionless \((D_2 = 0)\), as is the case of the periodic Anderson models considered in [26,27]. In this case, it is clear from [26,27] that an arbitrarily small \(V\) induces the Kondo insulating state. The formation of a heavy-fermion metallic state induced by a non-zero hybridization in a generalized periodic Anderson model with \(D_2 \neq 0\) (direct f-electron hopping) was also investigated in our recent work [28].

The slave-spin mean field results presented above can be placed in the context of this general low-frequency analysis. Within this approach, one has:

\[
Z_1 = 4\langle S_1^z \rangle^2, \quad Z_2 = 4\langle S_2^z \rangle^2, \quad V_{\text{eff}} = 4\langle S_1^z S_2^z \rangle V
\] (40)

It is important to realize that this approach does provide an off-diagonal component of the physical electron self-energy, which, using (37), is given by:

\[
\frac{\Sigma_{12}(0)}{V} = \frac{\langle S_1^z S_2^z \rangle - \langle S_1^z \rangle \langle S_2^z \rangle}{\langle S_1^z \rangle \langle S_2^z \rangle}
\] (41)

C. General low-frequency analysis

In order to understand better the nature of both the metallic and the insulating phases to which the OSMP is driven for \(V \neq 0\), we perform here a low-energy analysis in terms of a renormalized quasiparticle band-structure (see also [11]). We focus on the case in which the Kondo effect does take place as \(V\) is turned on, resulting in both quasiparticle residues being finite. We thus keep the following terms in the low-frequency expansion of the self-energy:

\[
\begin{align*}
\Sigma_{11}(\omega) &= \omega(1 - 1/Z_1) + \cdots \\
\Sigma_{22}(\omega) &= \omega(1 - 1/Z_2) + \cdots \\
\Sigma_{12}(\omega) &= \Sigma_{12}(0) + \cdots
\end{align*}
\] (34)

FIG. 18: (color online). Gap amplitude of the auxiliary fermions (see text) and quasiparticle residues within slave spins MFT, for two values of \(V\). Top: \(t_2/t_1 = 0.1, J = 0\) for \(V/t_1 = 0.1\) (upper panel), and \(V/t_1 = 0.6\) (lower panel). The corresponding critical \(V\) for the non-interacting system is \(\sqrt{D_1 D_2} \approx 0.63\) in this case.
Note that in more conventional slave-boson approaches, the physical electron operators are related to the quasiparticles by a slave-boson condensation amplitude which is a c-number \( \langle d^\dagger_m d^\dagger_n \rangle = \sqrt{Z_m f^\dagger_n f^\dagger_m} \). As a result, \( V_{\text{eff}} = \sqrt{Z_1 Z_2} V \), and no off-diagonal component of the self-energy is present. In such slave-boson approaches, the condition for the presence of a quasiparticle band gap is therefore entirely unrenormalized by interactions and reads: \( V/\sqrt{D_1 D_2} > 1 \). This is an oversimplification which is not present in the slave-spin approach. There, the criterion for the opening of a gap reads:

\[
\frac{V}{\sqrt{D_1 D_2}} > \frac{\langle S^z_1 \rangle \langle S^z_2 \rangle}{\langle S^z_1 S^z_2 \rangle}
\]

However, despite the renormalisation of the hybridisation by the off-diagonal self-energy, we find that in practice this criterion is very close to the non-interacting one, which gives a reasonable approximation of the critical hybridisation necessary to open a band gap. We also note that, within the slave-spin approach, the insulating gap takes its bare value \( 2V \) (corresponding to the splitting between the bonding and antibonding molecular levels) as soon as \( Z_1 = Z_2 = 0 \), which is certainly an over-simplification.

Finally, we comment on the phase transitions between the different phases induced by a non-zero hybridization. At small \( V \), it is clear that there must exist a phase transition between the metallic (gapless) heavy-fermion phase and the insulating (gapped) phase, as \( U \) is increased (as indeed seen on Fig. 15 top panel). The situation is less clear at larger \( V \). There, we always expect an insulator with a singlet ground-state. However, the mechanism behind this singlet formation is rather different at smaller and larger values of \( U \). In the former case, Kondo screening dominates and the singlet is formed by screening the local moment in orbital 2 by the electrons in orbital 1. At larger \( U \), the Kondo coupling is smaller, and it is the formation of an inter-orbital molecular bonding level (due to \( V \) which is responsible for the singlet formation. Within slave-spin mean theory, we find a phase transition between these two kinds of insulator as \( U \) is increased, the latter one being signalled by \( Z_1 = Z_2 = 0 \) (Fig. 15 bottom panel). However, it is not clear whether this phase transition is a real feature or an artefact of the slave-spin approximation. In \( 25 \), Koga et al. recently suggested that these two phases should be adiabatically connected, as found also in the study of the periodic Anderson model with correlated conduction electrons \( 26,27 \) (note however that the present model is different, in that both bands have a dispersion and that an inter-orbital interaction is present). The problem is qualitatively similar (but not equivalent, because of the inter-orbital interaction) to the two-impurity Kondo problem \( 28 \), in which the inter-impurity singlet (RKKY) fixed points and the Kondo-singlet fixed points are in general adiabatically connected (except in the special case of particle-hole symmetry, where a phase transition does occur). Note that it is well known \( 28 \) that for this latter model, slave-boson approximations do lead to spurious first-order transitions. A full answer to this question is beyond the scope of this paper, and is left for a future investigation, together with a complete phase diagram as a function of interaction strength and hybridization.

VII. CONCLUSION

In this article, we have studied whether the Mott transition of a half-filled, two-orbital Hubbard model with unequal bandwidths occurs simultaneously for both bands or whether it is a two-stage process in which the orbital with narrower bandwidth localizes first (giving rise to an intermediate ‘orbital-selective’ Mott phase). In order to study this question, we have used two techniques. The first is a mean-field theory based on a new representation of fermion operators in terms of slave quantum spins. This method is similar in spirit to the Gutzwiller approximation, and the slave-spin representation has a rather wide range of applicability to multi-orbital models. The second method is dynamical mean-field theory, using exact diagonalization and Quantum Monte-Carlo solvers.

The results of the slave-spin mean-field confirms several aspects of previous studies \( 9,11 \), and in particular the possibility of an orbital-selective Mott transition. However, some of the conclusions differ from those of previous work. Specifically, the slave-spin approximation suggests that a critical value of the bandwidth ratio \( (t_2/t_1)_c \), exists, such that the Mott transition is orbital-selective for arbitrary value of the Coulomb exchange (Hund coupling) \( J \) when \( t_2/t_1 < (t_2/t_1)_c \). When \( t_2/t_1 > (t_2/t_1)_c \), \( J \) has to be larger than a finite threshold for an OSMT to take place. This suggests that the existence of an OSMT is not simply related to the symmetry of the interaction term only. In particular, an intermediate phase is found for \( J = 0 \) at small \( t_2/t_1 \).

We have studied whether DMFT confirms these findings, and found that the main qualitative conclusions on the existence of the orbital-selective phase are indeed the same, but that the nature of the intermediate phase at \( J = 0 \) is a rather subtle issue. Indeed, the narrow band does not have the properties of a gapped Mott insulator in this phase and displays finite spectral weight down to arbitrary low-energy. This is, for example, consistent with a pseudo-gap behaviour but requires further studies to be fully settled (using e.g. low-energy techniques such as the numerical renormalization group).

We note also that our study emphasizes the key role of the exchange and (on-site) inter-orbital pair hopping terms in the Coulomb Hamiltonian in stabilizing the orbital-selective phase, in agreement with Koga et al. \( 11 \).

Finally, we found that the orbital-selective Mott phase is generically unstable with respect to an inter-orbital hybridization \( V \). In the presence of such a term, two possible phases are obtained, depending on the strength of \( U \) and \( V \). Either the narrow orbital acquires a large (but
finite) effective mass, corresponding to a heavy-fermion metallic state. Or the system is an insulator with a gap. This insulator differs from the Mott insulator at \( V = 0 \) since it has a singlet ground-state. This is due to screening processes, involving both Kondo exchange and the formation of an on-site molecular (bonding) level. Whether one has in fact two different insulating phases separated by a phase transition (each phase being dominated by one of these screening processes) -as obtained by slave-spin mean-field-, or whether one has a simple crossover is an open question which deserves further study.

Of course, at intermediate temperature (above the quasiparticle coherence scale of the narrower band, but below that of the wider band), a physics similar to the orbital-selective Mott phase can be recovered even in the presence of a finite hybridization. This orbital-selective heavy-fermion state might be relevant to the physics of \( \text{Ca}_2\text{Sr}_2\text{RuO}_4 \). This is indeed supported by the recent angular magneto-resistance oscillations experiments of Balicas et al.\(^2\).

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