Electronic correlations in Hund metals

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To clarify the nature of correlations in Hund metals and its relationship with Mott physics we analyze the electronic correlations in multiorbital systems as a function of intraorbital interaction U, Hund's coupling J_H and electronic filling n. We show that the main process behind the enhancement of correlations in Hund metals is the suppression of the double-occupancy of a given orbital, as it also happens in the Mott-insulator at half-filling. However, contrary to what happens in Mott correlated states the reduction of the quasiparticle weight Z with J_H can happen on spite of increasing charge fluctuations. Therefore, in Hund metals the quasiparticle weight and the mass enhancement are not good measurements of the charge localization. Using simple energetic arguments we explain why the spin polarization induced by Hund's coupling produces orbital decoupling. We also discuss how the behavior at moderate interactions, with correlations controlled by the atomic spin polarization, changes at large U and J_H due to the proximity to a Mott insulating state.

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The Mott transition is one of the most dramatic manifestations of electronic correlations [1, 2]. In the single orbital Hubbard model at half-filling the system becomes insulating at a critical interaction U_c to avoid the cost of doubly occupying the orbital. Away from half-filling metallicity is recovered. Nevertheless atomic configurations involving double occupancy are avoided inducing strong correlations between the electrons. Charge fluctuations are suppressed and bad metallicity is observed.

In multiorbital systems the Mott transition happens not only at half-filling but at all integer fillings [3]. The crucial role of Hund's coupling J_H on electronic correlations has been recognized only recently [4–14]. J_H modifies U_c in a doping dependent way [4, 8] and promotes bad metallic behavior in a wide range of parameters [7, 9].

Within the context of iron superconductors, which accomodate 6 electrons in 5 orbitals when undoped, the term Hund metal was coined to name the correlated metallic state induced by Hund's coupling at moderate interaction U[15]. Originally Hund metals were described as strongly correlated but itinerant systems which are not in close proximity to a Mott insulating state and have physical properties distinctly different from doped Mott insulators [10]. On the other hand, a number of authors [16–22], have described iron superconductors as doped Mott insulators due to the doping dependence of correlations observed: there is both experimental and theoretical evidence of an enhancement of correlations with hole-doping as the half-filling Mott insulator, with 5 electrons in 5 orbitals, is approached[16–26].

Orbital dependent correlations, named orbital differentiation, have been observed in some iron superconductors [16, 19, 21, 23, 26–28] and are known to play an important role in ruthenates[29]. It has been emphasized that Hund's coupling decouples the orbitals [8, 23, 30–32], leads to orbital differentiation and even to an orbital selective Mott transition [8, 30, 31]; however, the origin of such decoupling is not well understood.

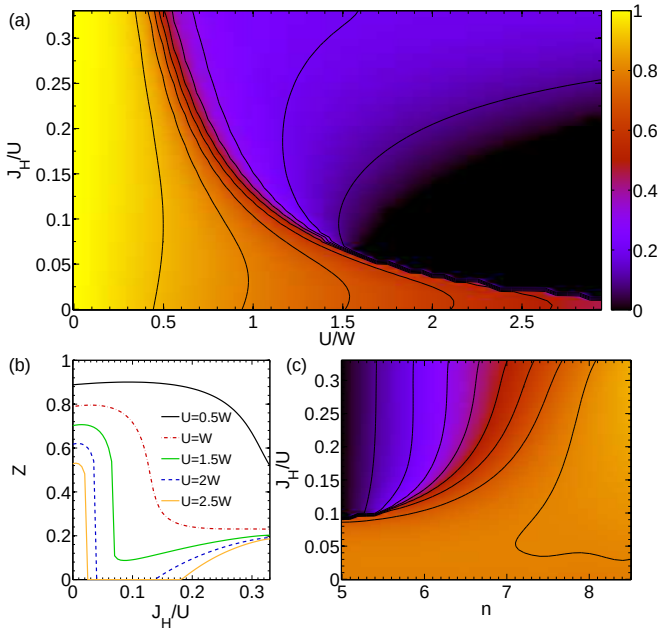

FIG. 1: (Color online) (a) Quasiparticle weight Z vs intraorbital interaction U and Hund's coupling J_H for 6 electrons in 5 orbitals, the filling of undoped iron superconductors. U and J_H are in units of the bare bandwidth W and U. A strongly correlated metallic region with small Z, in violet, appears in a wide range of parameters. The Mott insulating state is in black. The region in yellow-orange is metallic with moderate correlations. (b) Z vs J_H for the system in (a) and selected U. (c) Z vs electronic filling n and J_H with $U = W$ for a 5-orbital system. The strong suppression of Z with J_H seems connected to the $n = 5$ half-filled Mott insulator.

It urges to clarify the nature of correlations in Hund metals and its relationship with Mott physics. In this paper we analyze the electronic correlations in multiorbital systems ($N = 2, 3...5$ orbitals) as a function of interactions and electronic filling n. We confirm that the doping dependent increase of correlations with J_H at moderate

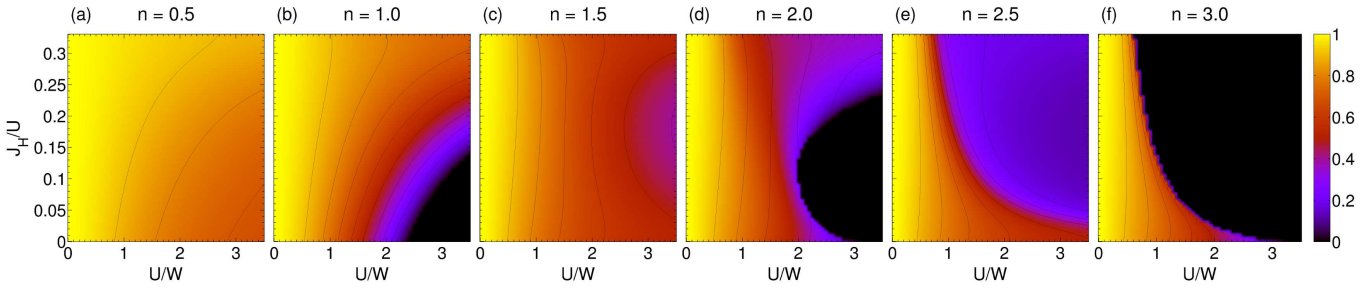

FIG. 2: (Color online) Quasiparticle weight Z vs intraorbital interaction U and Hund's coupling J_H for a 3- orbital system with electronic filling (a) $n = 0.5$, (b) $n = 1.0$, (c) $n = 1.5$, (d) $n = 2.0$ (e) $n = 2.5$ and (f) $n = 3.0$ half-filling. The Mott transition, in black, is found for the conmensurate values n=1,2,3 with different dependence on J_H. Extended metallic regions with strongly reduced Z are only found for filling close to half-filling. U and J_H are respectively given in units of the non-renormalized bandwidth W and of U. The system shows particle hole symmetry, results are also valid for electronic filling $2N - n$.

interactions is directly connected to the Mott transition at half-filling. However, contrary to what happens in correlated single-orbital systems the increase of correlations with J_H, as measured by the suppression of the quasiparticle weight Z, does not necessarily imply a suppression of charge fluctuations. We trace back this behavior to the opposite dependence of intra and interorbital charge fluctuations with Hund's coupling. With simple energetic arguments we explain the underlying phenomenology, including how the spin polarization drives the orbital decoupling. Our study unveils differences between systems with 2 electrons and those with other commensurate partial fillings. We discuss a change of behavior at large J_H and U, related to the proximity of the Mott insulator.

To address the generic features of Hund metals we consider degenerate 2D multiorbital systems with hopping t restricted to the same orbital and to nearest neighbors and bandwidth $W = 8t$. For the interactions we start from the Hubbard-Kanamori Hamiltonian [10, 33].

$$\begin{aligned} H_{\rm int} &= U\sum_a n_{a\uparrow}n_{a\downarrow} + (U' - J_H)\sum_{a<b,\sigma} n_{a\sigma}n_{b\sigma} \\ &+ U'\sum_{a\neq b} n_{a\uparrow}n_{b\downarrow} - J_H\sum_{a\neq b} c^\dagger_{a\uparrow}c_{a\downarrow}c^\dagger_{b\downarrow}c_{b\uparrow} \\ &+ J'\sum_{a\neq b} c^\dagger_{a\uparrow}c^\dagger_{a\downarrow}c_{b\downarrow}c_{b\uparrow} \end{aligned} \quad (1)$$

a is the orbital index, $\uparrow$ and $\downarrow$ the spin, $n_{a\downarrow}$ and $n_{a\uparrow}$ the electron occupancy of a given orbital with spin $\downarrow$ or $\uparrow$. We treat the interactions using a Z_2 slave spin representation [30, 34], and keep only density-density terms, see Supplemental Material (SM). That is, pair hopping and spin-flip terms do not enter into the calculation [21, 22]. The model is particle-hole symmetric with respect to half-filling. We take $U' = U - 2J_H$, with U' the interorbital interaction, as found in rotationally invariant systems [33]. Repulsive interactions require $J_H/U \leq 0.33$.

The quasiparticle weight Z provides a way to quantify the correlations between electrons. Z measures the overlap between the elementary excitations of the correlated and the non-interacting systems. It is equal to unity in non-interacting systems, decreases with increasing correlations and vanishes in Mott insulators. In Fermi liquid theory it equals the inverse of the mass enhancement. Fig. 1(a) shows in color plot the quasiparticle weight Z as a function of U and J_H for a five-orbital system with six electrons, the filling of undoped iron superconductors. Three regions can be distinguished: a metallic state with moderate correlations in yellow-orange color; an insulating Mott state at large U in black, and a strongly correlated metallic state with reduced coherence in violet. The critical U_c at which the Mott transition sets it depends non-monotonously on J_H [8]. At large values of J_H the system remains metallic even for large U [9].

The correlated metallic state, in the following Hund metal, appears at finite J_H in a wide range of parameters, including $U < W$. The way in which this region depends on the interactions reveals the crucial role played by J_H on inducing the strong correlations which seem unrelated to the $n = 6$ Mott insulating state. Similar phase diagrams are found in other cases, e.g. for 2 electrons in 3-orbitals in Fig. 2(d) and for 2 and 3 electrons in 4 orbitals and 3 electrons in 5 orbital, in Fig. S1 in SM.

Hund's coupling polarizes the spin locally. The small Z in a Hund metal is due to the small overlap between the non-interacting states and the spin polarized atomic states[5, 7, 35]. The suppression of Z is thus concomitant with an enhancement of the spin fluctuations C_S, see Fig. 3(a). Here $C_S = < S^2 > - < S >^2$ with $< S >= 0$ and $S = \sum_{a=1,\ldots,N}(n_{a\uparrow} - n_{a\downarrow})$. Arrows in Fig. 3(a) mark $J^*_H(U)$ the interaction at which the system enters into the Hund metal defined empirically as the value of J_H with the strongest suppression of Z, i.e. the most negative dZ/dJ_H value, after which Z stays finite, see Fig. S2 in SM. Above J^*_H, C_S reaches a value close to that of the Mott insulator at this filling, showing that in the Hund metal state each atom is highly spin polarized.

We now focus on the doping dependence of the correlations. Fig. 1(c) shows Z as a function of the electronic filling n and J_H for $U = W$, far from the $n = 6$ Mott

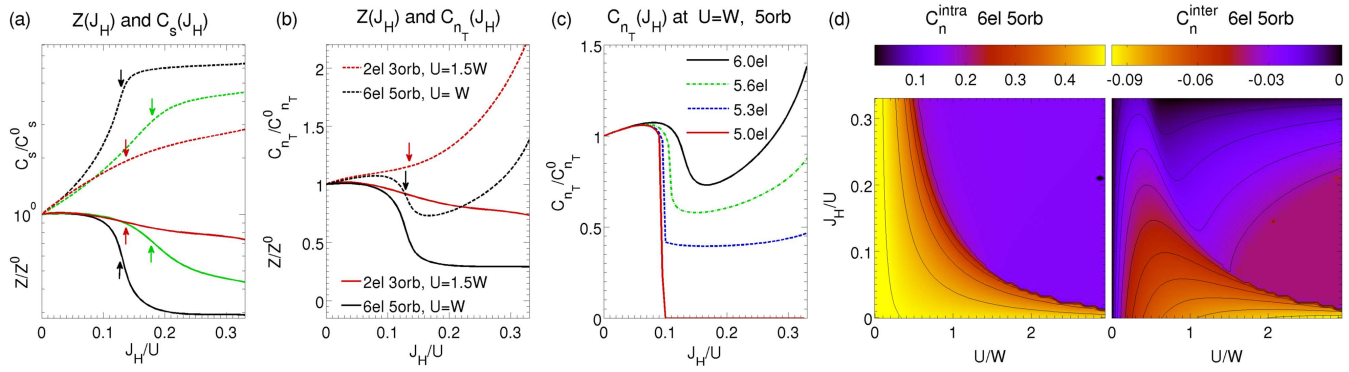

FIG. 3: (Color online)(a) Enhancement of spin fluctuations C_S and suppression of Z with J_H. $U = 1.5W$ for 2 electrons in 3 orbitals (red), $U = W$ for 6 electrons in 5 orbitals (black) and for 3 electrons in 4 orbitals (green). C_S and Z are renormalized to their $J_H = 0$ value at the given U. Arrows mark $J_H^*(U)$. The reduction of Z is concomitant to the enhancement of C_S. (b) Charge fluctuations C_{n_T} and quasiparticle weight Z vs Hund's coupling J_H renormalized to $C^0_{n_T}$ and Z^0, their value at $J_H = 0$ and the corresponding U, see legend. The enhancement of C_{n_T} while Z is suppressed differs from the behavior of Mott correlated states. (c) $C_{n_T}/C^0_{n_T}$ vs J_H for 5 orbitals with $U = W$ and different electronic fillings n. Z decreases with J_H for all values in this figure and vanishes in the Mott state at $n = 5$ (not shown). (d) Intraorbital $C_n^{\rm intra}$ and interorbital $C_n^{\rm inter}$ charge fluctuations vs U and J_H for 6 electrons in 5 orbitals. With increasing J_H, both $C_n^{\rm intra}$ and $C_n^{\rm inter}$ decrease in absolute value. In the Hund metal $C_n^{\rm intra}$ quickly saturates to its value in the Mott state while $C_n^{\rm inter}$ decreases towards zero with J_H.

transition. The strength of correlations shows a clear asymmetry with electronic filling around $n = 6$. No special feature is observed at $n = 6$ for this value of U what confirms that the $n = 6$ Mott transition is not responsible for the strong suppression of Z. On the other hand the entrance to the strongly correlated Hund metal appears at smaller J_H as n approaches $n = 5$. Connection with the Mott insulating state at half-filling is evident.

A clear doping dependence of correlations is also observed in 3-orbital systems, Fig. 2. An extended region of parameters with small quasiparticle weight, in violet, is found only for fillings relatively close to half filling $n = 3$. For smaller fillings Z depends more weakly on J_H. The dependence of the Hund metal region on the interaction parameters for filling $n = 2.5$ in Fig. 2(e), closely follows the $n = 3$ Mott insulating state, in black in Fig. 2(f).

The hallmark of Mott physics is the suppression of charge fluctuations C_{n_T} which vanish at the Mott transitions. Here $C_{n_T} =< n_T^2 > - < n_T >^2 =< (\delta n_T)^2 >$ with $n_T = \sum_{a=1,\ldots,N} n_a$, $n_a = n_{a\uparrow} + n_{a\downarrow}$, $\delta n_T = n_T - < n_T >$ and $< n_T >= n$. In single orbital systems the charge fluctuations C_{n_T} and Z have a similar doping and interaction dependence. Consequently, very often, the suppression of Z, is assumed to imply localization.

Fig. 3(b) shows the evolution of C_{n_T} with J_H and compares it with that of Z, both quantities being normalized to their $J_H = 0$ value. Unexpectedly, Z and C_{n_T} depend differently on J_H. For the system with 2 electrons in 3 orbitals Z decreases and C_{n_T} increases with J_H. That is, contrary to what happens in Mott systems, the suppression of Z happens on spite of an increase of metallicity. In the 6 electrons in 5 orbitals case the strong reduction of Z comes along with a reduction of C_{n_T}. However at larger J_H, Z continues decreasing, while C_{n_T} increases. The enhancement of C_{n_T} with J_H is reduced as half-filling ($n = 5$) is approached, see Fig. 3(c). The different dependence of Z and C_{n_T} on J_H implies that in Hund metals the quasiparticle weight Z and the mass enhancement are not good measures of the charge localization.

The increase of charge fluctuations with J_H can be traced back to the suppression of interorbital correlations $C_n^{\rm inter}$. Accounting for the equivalency of all the orbitals

$$C_{n_T} = N\left(C_n^{\rm intra} + (N-1)C_n^{\rm inter}\right) \qquad (2)$$

with $C_n^{\rm intra} =< n_a^2 > - < n_a >^2 =< (\delta n_a)^2 >$ the intraorbital fluctuations, $\delta n_a = n_a - < n_a >$ and $< n_a >= n/N$. $C_n^{\rm inter} =< n_a n_b > - < n_a >< n_b >=< \delta n_a \delta n_b >$ and $a \neq b$. $C_n^{\rm intra}$, by definition positive or zero, is largest in the non-interacting limit. $C_n^{\rm inter}$ is negative for repulsive interactions and it vanishes in the absence of interactions as the charge in different orbitals is not correlated. The entrance into the Hund metal has a very strong effect on $C_n^{\rm intra}$ and $C_n^{\rm inter}$ being both strongly suppressed, see Fig. 3(d). Due to their different sign in Eq. (2) this suppression has an opposite effect in C_{n_T}. The increase of C_{n_T} with J_H is driven by the interorbital correlations which effect is enhanced by the degeneracy factor $(N-1)$ in Eq. (2). On the other hand, the suppression of C_{n_T} at J_H^* in the 6 electrons in 5 orbitals case in Fig. 3 is due to that of $C_n^{\rm intra}$. Except at half-filling, $C_n^{\rm intra}$ and $C_n^{\rm inter}$ do not vanish in the Mott insulator but their contributions cancel each other leading to zero C_{n_T}, see Fig. S3 in SM.

The phenomenology above can be understood by studying the energy of the hopping processes. Let's consider two N-orbital atoms with n electrons ($n \leq N$) and assume that inside each atom the electron spins are par-

allel to satisfy Hund's rule. An electron which hops from one atom onto the other one can end into (i) an empty orbital with spin parallel to that of the occupied orbitals with interaction energy cost $E^{\uparrow\uparrow} = U-3J_H$; (ii) an empty orbital with spin antiparallel to that of the occupied orbitals with $E^{inter\uparrow\downarrow} = U + (n-3)J_H$. (iii) an occupied orbital with $E^{intra\uparrow\downarrow} = U + (n-1)J_H$ [36]. Particle-hole symmetry considerations apply for $n > N$.

At half-filling, $n = N$, processes (i) and (ii) are blocked by Pauli exclusion principle and process (iii) controls the critical $U_c(J_H)$ for the Mott transition which strongly decreases with J_H, see Fig. 2(f). For other integer fillings and large J_H the Mott transition is controlled by process (i) and $U_c(J_H)$ increases with J_H [8], but processes (ii) and (iii) are blocked at smaller interactions.

In the metallic state the process (i) is allowed and promoted by J_H. We ascribe the entrance in the Hund metal at J_H^* to avoiding process (iii). This process is suppressed by J_H for $n > 1$ and it is directly connected to the Mott transition at half-filling. Its suppression strongly reduces the intraorbital double occupancy and $C_n^{\rm intra}$ enhancing the atomic spin polarization in the Hund metal.

Process (ii) is suppressed by J_H for $n > 3$ and promoted for $n < 3$ (as $U' = U - 2J_H$). This introduces a qualitative difference between systems with 2 electrons and those with larger integer fillings, which causes that in 2-electron systems the suppression of Z and the enhancement of C_S with J_H are smoother and favors the enhancement of C_{n_T}. Nevertheless, even when process (ii) is allowed, the suppression of process (iii) indirectly reduces the occurrence of atomic configurations with anti-parallel spins in different orbitals (not shown).

The strong supression of $C_n^{intra} =< |\delta n_a|^2 >$ at the crossover $J_H^*(U)$ reduces the interorbital charge correlations $< \delta n_a \delta n_b >$. The latter are further suppressed by the reduction of the effective interaction between the electrons in different orbitals, what produces orbital decoupling (measured by $\frac{<\delta n_a \delta n_b>}{<|\delta n_a|^2>}$): The interaction between electrons in different orbitals is U' or $U' - J_H$ depending if they have parallel or antiparallel spins, see Eq. (1). At J_H^* the occurrence of atomic configurations with parallel spin strongly increases while those involving opposite spin become less frequent, effectively reducing the interaction between electrons in different orbitals to $U' - J_H$ [37]. If J_H is further increased the decoupling is enhanced as the effective interaction $U' - J_H = U - 3J_H$ decreases. At $J_H/U = 0.33$, this interaction and $C_n^{\rm inter}$ vanish.

As discussed above, at intermediate filling and interactions, around $J_H^*(U)$ the dependence of the quasiparticle weight and the fluctuations on the interactions is controlled by the establishment of the atomic polarization. On the other hand, at large J_H and U, the behavior of the locally spin polarized system becomes dominated by the decrease with J_H of the effective interaction between spin-parallel electrons and by the proximity to the Mott insulator, which happens at a larger critical interaction with increasing J_H. In particular, in the large J_H and U limit, both Z and C_{n_T} increase with J_H, see Figs. 1(b), S2 and S3. Moreover while, with increasing U, Z decreases monotonously, C_S increase for intermediate U but they start to decrease at large U and J_H see Fig. S4. This behavior, driven by the interorbital spin fluctuations, is contrary to what happens in the single-orbital Hubbard model, for which Z and C_S show an opposite dependence on U in all the range of parameters.

In conclusion, we have clarified the nature of correlations in Hund metals and its differences with those in Mott systems. In Hund metals the enhancement of correlations originate in the suppression of atomic configurations which reduce the magnetic moment, specially intraorbital double occupancy, while the hopping of electrons with spin parallel to the locally spin polarized atoms is allowed. The suppression of hopping processes involving intraorbital double occupancy links the correlations in Hund metals to the Mott transition at half-filling. However, contrary to what happens in Mott correlated systems, the reduction of the quasiparticle weight Z in Hund metals, can happen on spite of increasing charge fluctuations. Therefore in Hund metals the quasiparticle weight and the mass enhancement are not good measures of charge localization. The tendency towards orbital decoupling in the Hund metal is due to the reduction of the effective (and J_H-dependent) interaction between electrons in different orbitals produced by the predominance of atomic configurations involving parallel spins. Finally, we note that at large U and J_H the dependence of the quasiparticle weight and the spin fluctuations on the interactions reveals a crossover to a region of parameters controlled by the proximity to the Mott insulator.

The behavior discussed, together with other known properties of Hund metals [8] as the enhanced width of the Hubbard bands or the screening of the atomic moments [38] is expected to play a prominent role in iron superconductors, ruthenates and many oxides. This is confirmed by the similarity between the behavior in Fig.1 and that found with realistic models of iron superconductors[16, 23, 27]. Nevertheless the physics of these materials will be strongly influenced by the inequivalency of the orbitals[16, 19, 21–23, 27, 29] specific for each material, and not included here.

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SUPPLEMENTAL MATERIAL: SUPPLEMENTARY FIGURES

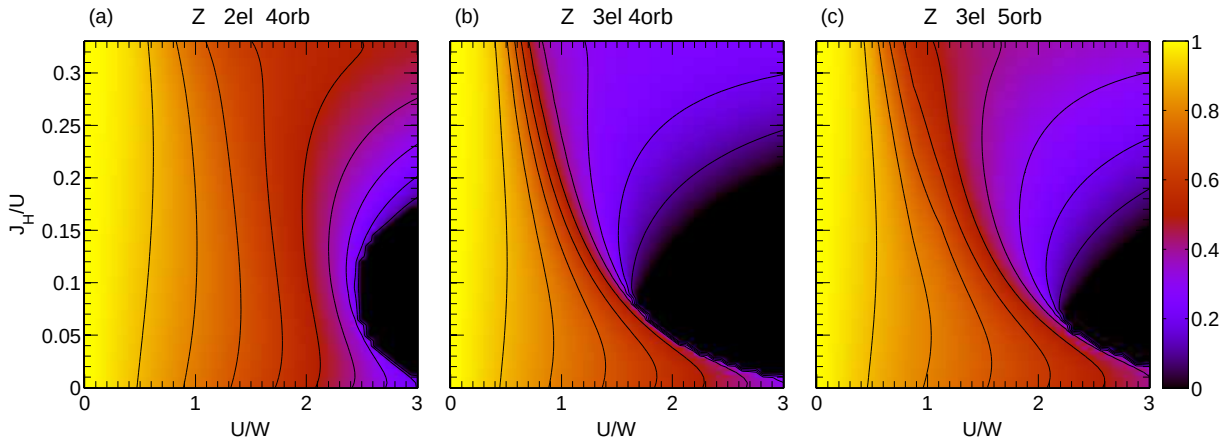

FIG. S1: (Color online) Quasiparticle weight Z as a function of intra-orbital interaction U and Hund's coupling J_H for (a) 4-orbital system with $n = 2$ electrons , (b) 4-orbital system with $n = 3$ electrons and (c) 5-orbital system with $n = 3$ electrons. U and J_H are respectively given in units of the non–renormalized bandwidth W and of U. The system shows particle hole symmetry and the results are also valid for electronic filling $2N - n$. In (a) as in Fig.2(d) both with 2 electrons the Z contour lines for $U < 2W$ are more vertical than in the other cases, i.e. weakly dependent on J_H. This is due to the different effect which for this filling has J_H on the energy of the transport processes in which one electron hops into an empty orbital with opposite spin to that the atom, see text.

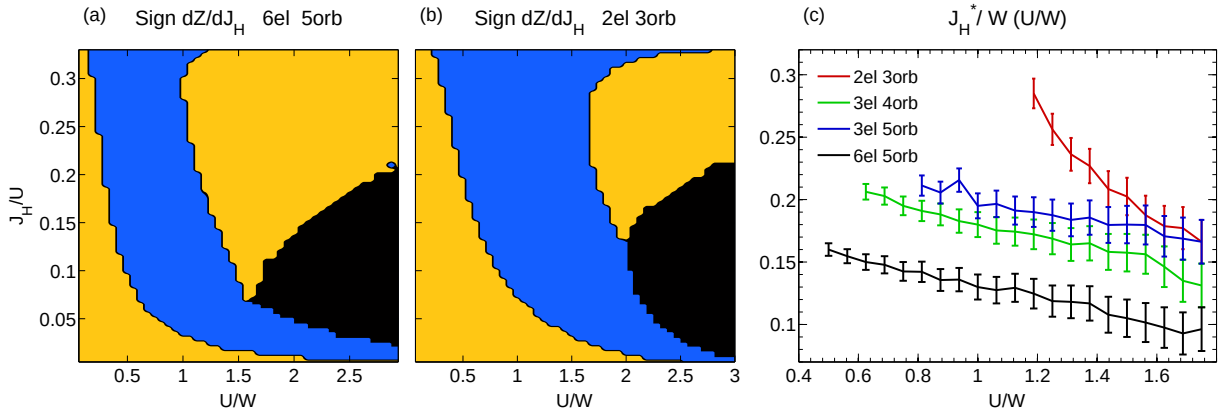

FIG. S2: (Color online)(a) and (b) Color representation for the sign of the derivative of the quasiparticle weight with Hund's coupling dZ/dJ_H for a 5-orbital system with 6 or 4 electrons in (a) and a 3- orbital system with 2 or 4 electrons in (b). Yellow is used for positive derivative, blue for negative derivative. In black, the Mott region with zero derivative. At intermediates values of U and J_H, Z is suppressed by J_H. At large U and J_H, Hund's coupling promotes metallicity and Z increases with J_H. The increase of Z with J_H found for small U and J_H is always very weak. (c) Hund's coupling J_H^* at which the strongest suppression of quasiparticle weight Z is found vs U. electrons in 4 (green) and 5 orbitals (blue) and 2 electrons in 3 orbitals (red). J_H^* and U are in units of the bandwidth W. Smaller J_H^* values are found for smaller average orbital filling $x = n/N$, except when comparing 2 electrons in 3 orbitals ($x = 0.66$) and 3 electrons in 5 orbitals ($x = 0.60$).

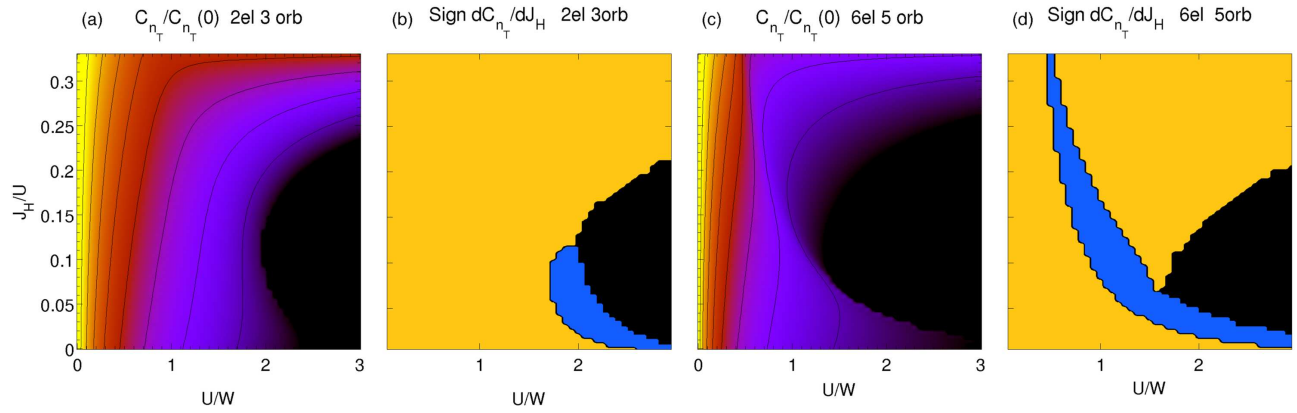

FIG. S3: (Color online) (a) and (c) Charge fluctuations C_{n_T} normalized to its value in the non-interacting case ($U = 0$ and $J_H = 0$) for 2-orbital system with 2 or 4 electrons in (a) and a 5-orbital system with 6 or 4 electrons in (c). This quantity varies between 0 and 1, facilitating the comparison with the dependence of Z on interactions in Fig. 1 and 2 of the main text. (b) and (d) Color representation for the sign of the derivative of the charge correlations with Hund's coupling dC_{n_T}/dJ_H for 2-orbital system with 2 or 4 electrons in (b) and a 5-orbital system with 6 or 4 electrons in (d), corresponding, respectively to the charge correlations in (a) and (c). Yellow is used for positive derivative, blue for negative derivative. In black, the Mott region with zero derivative. In (d) there is a region of parameters with $dC_{n_T}/dJ_H < 0$ which coincides with the region in Fig. S2(a) and Fig. 1 where the suppression of Z with J_H is strongest. In the case with 2 electrons in 3 orbitals in (b) at moderate interactions charge correlations always increase with increasing J_H, even for values of the interaction with $dZ/dJ_H < 0$.

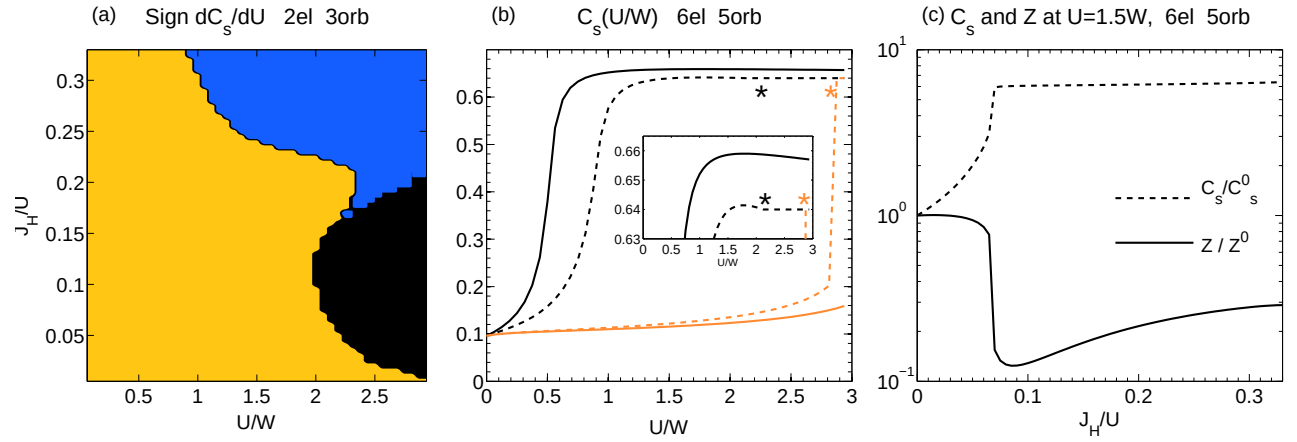

FIG. S4: (Color online) (a) Derivative of the spin correlation C_S with U for a 3-orbital system with 2 electrons. At large U and J_H, when the atoms are locally polarized, the spin fluctuations decrease with U which promotes localization. The region where this effect is found is similar to that shown in Fig. S2(b) with positive dZ/dJ_H. (b) Spin fluctuations C_S as a function of U for 6 electrons in 5 orbitals and $J_H/U = 0.30, 0.15, 0.015, 0.01$ from top to bottom. For small J_H/U C_S increases with U. C_S saturates in the Hund metal prior to the Mott transition, marked with stars. Inset: Blow up of the large J_H/U curves at large U show non-monotonous C_S with U in this region of parameters.(c) Spin fluctuations C_S and quasiparticle weight Z normalized to their value at $J_H = 0$ and the given $U = 1.5W$ as a function of J_H. At J_H^*, Z strongly decreases due to the enhanced spin polarization. However at larger values the behavior of these two quantities. C_S saturates, while Z starts increasing, due to the decrease of the effective interaction with J_H.

SUPPLEMENTAL MATERIAL: THE ISING Z_2 SLAVE-SPIN APPROACH

Approaches which use slave particles have being widely used to deal with interacting fermions. In particular, in multiorbital systems, slave–spin approaches, in Z_2 [30, 34] or $U(1)$ [27] versions, have proven to be very useful. In this work we have used the Z_2 slave-spin technique developed in [30, 34] in its single-site approximation.

In the Z_2 slave–spin approach the two possible occupancies of a spinless fermion on a given site, $n_c = 0$ and $n_c = 1$, are substituted by the two states of a pseudospin spin-1/2 variable, $S^z = -1/2$ and $S^z = +1/2$:

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

n_f is the occupation of an auxiliary fermion f, introduced

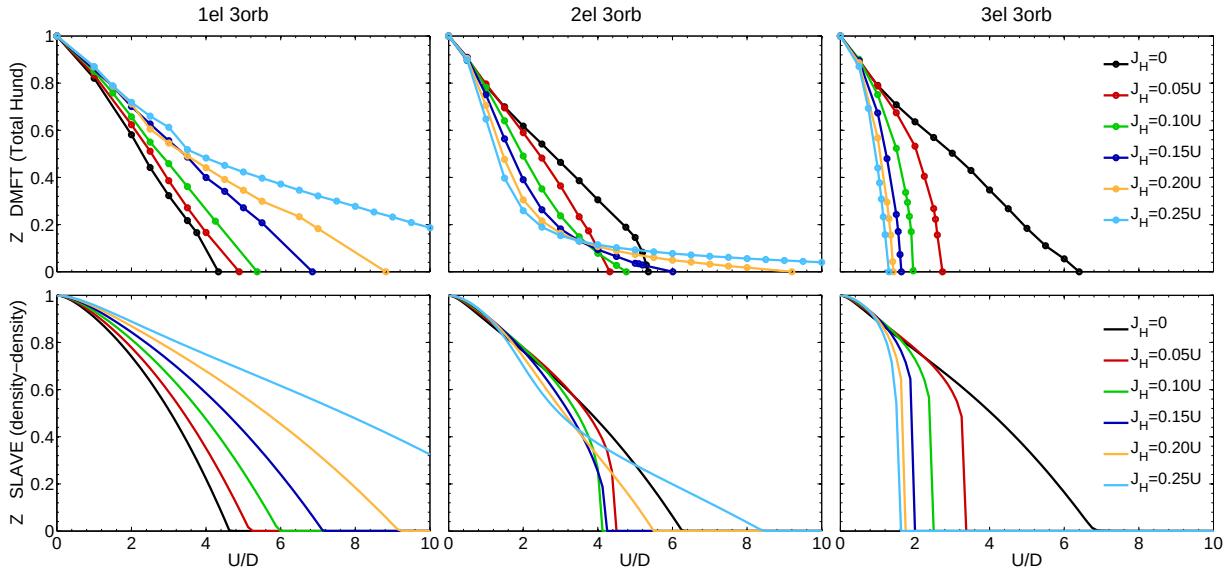

FIG. S5: (Color online) Comparison between quasiparticle weight Z of computed with DMFT and the Slave Spin method described. We show the for a model with 3 equivalent orbitals with semicircular density of states with $n = 1, 2, 3$ electrons per site. A semicircular density of states with half-bandwidth D is used in both calculations. The DMFT data, taken from [9], were computed using the complete interacting Hamiltonian including the spin–flip and the pair–hopping terms. Only the density–density part (Ising approximation) is included in the slave-spin calculation.

to satisfy the anticonmutation relations. Two unphysical states $|n_f = 0, S^z = +1/2\rangle$, $|n_f = 1, S^z = -1/2\rangle$ are generated in the procedure. To eliminate them, the local constraint $n^f = S^z + \frac{1}{2}$ has to be imposed.

In a multiorbital system each of the orbital and spin species have to be treated in this manner. That is, a set of $2N$ pseudospin-1/2 variables $S^z_{ia\sigma}$ and auxiliary fermions $f_{ia\sigma}$ are introduced at each site i Here $a = 1, N$ and σ are the orbital and spin indices. On each site these variables have to satisfy the local constraint:

$$n^f_{ia\sigma} = S^z_{ia\sigma} + \frac{1}{2}, \tag{S1}$$

what can be done with time-dependent Lagrange multipliers fields $\lambda_{ia\sigma}(\tau)$.

Following the prescription in[34] the physical fermions $c_{ia\sigma}$ are represented by

$$c_{ia\sigma} = f_{ia\sigma} O_{ia\sigma}\,, \qquad c^\dagger_{ia\sigma} = f^\dagger_{ia\sigma} O^\dagger_{ia\sigma}.$$

Here $O_{ia\sigma}$ is a pseudospin-1/2 operator defined as

$$O_{ia\sigma} = \begin{pmatrix} 0 & \gamma_{ia\sigma} \\ 1 & 0 \end{pmatrix}$$

with $\gamma_{ia\sigma}$ a complex number[34], see below.

To solve the interacting problem several approximations are introduced [30, 34]: (i) Only the density-density terms of the Hubbard-Kanamori Hamiltonian, Eq. (1) in the main text, are included [39], (ii) The constraint is treated on average, i.e. using a static Lagrange multiplier $\lambda_{a\sigma}$ and the Hamiltonians of the pseudospin slave variables and the auxiliary fermions are decoupled (iii) The problem is solved in a single-site mean field approximation, which render all variables site independent. After these approximations the total Hamiltonian can be written as the sum of two effective Hamiltonians, for the auxiliary fermions and the pseudospins, H_f and $H_{\rm PS}$, to be solved self-consistently at mean-field level.

The fermionic Hamiltonian for a generic multiorbital system without orbital hybridization is:

$$H_f = \sum_{a\,\sigma} \sum_{\mathbf{k}} \left(Z_{a\sigma}\,\varepsilon_{a\sigma} + \epsilon_a - \mu - \lambda_{a\sigma}\right) f^\dagger_{a\sigma}(\mathbf{k}) f_{a\sigma}(\mathbf{k}), \tag{S2}$$

where μ is the chemical potential, ϵ_a the crystal field and $\varepsilon_{a\sigma}$ is the original fermionic dispersion. In this single-site approximation the renormalization of the dispersion is given by the quasiparticle weight

$$Z_{a\sigma} = \langle O_{a\sigma}\rangle^2,$$

self-consistently determined from the solution of the pseudospin Hamiltonian.

$$\begin{aligned} H_{\rm PS} &= \sum_{a\,\sigma} h_{a\sigma} O_{a\sigma} + \sum \lambda_{a\sigma} \left(S^z_{a\sigma} + \frac{1}{2}\right) \\ &+ \frac{U'}{2}\left(\sum_{a\sigma} S^z_{a\sigma}\right)^2 + J_H \sum_a \left(\sum_\sigma S^z_{a\sigma}\right)^2 \\ &- \frac{J_H}{2} \sum_\sigma \left(\sum_a S^z_{a\sigma}\right)^2 \end{aligned}$$

where $h_{a\sigma} = \langle O_{a\sigma}\rangle \sum_{\mathbf{k}} \varepsilon_{a\sigma}(\mathbf{k}) \langle f^{\dagger}_{a\sigma}(\mathbf{k}) f_{a\sigma}(\mathbf{k})\rangle$.

In the case of a spin and orbital degenerate system without spontaneous breaking of the symmetry, as the one discussed in the main text, $\lambda_{a,\sigma}$, $h_{a,\sigma}$ and $Z_{a,\sigma}$ become orbital and spin independent and the corresponding indices can be dropped. A convenient choice for $\gamma_{i,a\sigma} = \gamma$ in this case is[34] $\gamma = \frac{1}{\sqrt{n(1-n)}} - 1$

In Fig. S5 the quasiparticle weight Z calculated within this Ising Z_2 slave–spin approach for a system 3–degenerate orbitals with n electrons per site is compared with the DMFT results from [9], which include the full rotationally invariant Hund interaction. Here we use a semicircular density of states, different to the square lattice with hopping to first nearest neighbors used in the main text. An overall agreement between the two methods is observed. The Ising slave–spin approach captures the different behaviors of Z observed for the whole range of J_H values. Quantitatively, the agreement is quite good for $n = 1, 3$ being, Z and the critical U_c for the Mott transition just slightly overestimated, as it is common in slave variable approaches and in the Gutzwiller approximation. At intermediate filling ($n = 2$) and large J_H, the suppression of Z in slave–spin approach is weaker than in DMFT. Moreover U_c is underestimated probably due to a more prominent role played in these region of parameters by the pair-hopping and spin-flip terms, neglected in the calculation. The qualitative behavior, an extended metallic region with reduced coherence, is in any case well captured.

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