Effect of Hund’s exchange on the spectral function of a triply orbital degenerate correlated metal

P. Lombardo, A. - M. Daré, R. Hayn
Laboratoire Matériaux et Microélectronique de Provence, CNRS UMR 6137, Université de Provence, Bât. IRPHE, 49 rue Joliot-Curie, BP 146, 13384 Marseille Cedex 13 France
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We present an approach based on the dynamical mean field theory which is able to give the excitation spectrum of a triply degenerate Hubbard model with a Hund’s exchange invariant under spin rotation. The lattice problem can be mapped onto a local Anderson model containing 64 local eigenstates. This local problem is solved by a generalized non-crossing approximation. The influence of Hund’s coupling $J$ is examined in detail for metallic states close to the metal insulator transition. The band-filling is shown to play a crucial role concerning the effect of $J$ on the low energy dynamics.

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I. INTRODUCTION

The Mott metal insulator transition (MIT) has been the subject of many experimental and theoretical studies over the past decades. Among correlated materials where the Coulomb repulsion between electrons is strong enough to overcome their kinetic energy, we find many $3d$ transition-metal oxides (see ref. [1]) and alkali-doped fullerides.

The influence of orbital degeneracy on the properties of strongly correlated electronic systems has been the subject of numerous recent studies. It has been shown unambiguously that the orbital degrees of freedom are of primary importance for understanding the nature of the Mott MIT. More recently, the interesting and controversial possibility of an orbital selective MIT in a multiorbital system has been investigated. 

Hund’s coupling plays an important role in these systems but reliable dynamical quantities are not available for a spin and orbital rotational invariant Hund’s coupling. Very recently a new approach using an extension of Wilson’s numerical renormalization group (NRG) has been proposed. 

In the present paper, we introduce into the triply degenerate orbital model a non zero Hund’s coupling parameter $J$ and we take into account its full expression including the so-called spin-flip term. The only neglected term is the orbital flip contribution or pair-hopping term between different orbitals.

Even the simplest lattice model for correlated electrons, the one-band Hubbard model presents strong difficulties and approximations are necessary to solve it. The dynamical mean field theory (DMFT) provides a solution in the limit of large spatial dimension. Within the DMFT framework, a correct description of the Mott-Hubbard metal insulator transition is possible for the one-band Hubbard model. In a previous work we have proposed an approach based on the DMFT which was able to deal with the doubly degenerate Hubbard model with a vanishing Hund’s coupling. Metal insulator transitions for integer total occupations per site $n = 1$, $n = 2$ and $n = 3$ were observed, with different values for the critical parameters on the transition lines. Besides, the transfer of spectral weight between different bands was interpreted in terms of microscopic dynamical processes. Here, in order to give a more realistic description of the spectral function of a correlated metal with several orbital degrees of freedom close to the MIT, we propose a generalization of our previous approach. Also, we develop a systematic description of the effects of degeneracy, of the Hubbard interaction and the Hund’s coupling on the triply degenerate model.

The triply degenerate model is relevant for transition-metal oxides or other transition-metal compounds where the cubic crystal field splits the $3d$ level into the $e_g$ and the $t_{2g}$ manifolds whenever it is the $t_{2g}$ manifold which is partially occupied. An example is VO$_2$ (see ref. and references therein). It shows a transition from metallic to semiconducting behavior for $x$ close to 1 and the $V^{2+}$ ion provides three electrons to the $t_{2g}$ orbitals. In that special case, however, not only correlation but also disorder effects seem to be very important, even for the stoichiometric samples. Other examples are the heavy fermion compound LiV$_2$O$_4$ which remains metallic up to very low temperature and LiTi$_2$O$_4$ which is superconducting below $T = 13.7$ K. Our approach is also relevant for MgTi$_2$O$_4$ (see ref. and references therein) which is metallic above $T = 260$ K.

In our study we investigate the $t_{2g}$-derived spectral function. We find three different effects in the spectral function: (i) band effects (which are usually already well described by the local spin density approximation (LSDA)), (ii) the Hubbard satellites (at an energy scale of $U$, already well treated by DMFT of the one-band model), and (iii) multi-peak effects connected with the Hund’s coupling (energy scale $J$). It is the last aspect which is new in our approach in comparison to previous...
studies. Keeping in mind that these multi-peak effects should be important to interpret realistic spectra, we analyze nevertheless a model situation in the present work with a semi-elliptic density of states for the uncorrelated problem.

In the following section the model Hamiltonian is presented, it takes into account explicitly the effect of Hund’s coupling. This section also presents the application of the DMFT on this Hamiltonian and a method of resolution based on the non-crossing approximation (NCA). In the third section, the main results concerning spectral properties are discussed.

II. HAMILTONIAN AND SOLVING METHOD

The triply degenerate Hubbard Hamiltonian, including a non zero Hund’s coupling parameter \(J\) can be written (see for instance ref. 10) as follows:

\[
H = \sum_{i,j,a,b} t_{ij}^a c_{ia\sigma}^+ c_{ja\sigma} + \frac{U + J}{2} \left( \sum_{i,a} \delta_{n_{ia\sigma} n_{ia\sigma}} \right) + \frac{U}{2} \left( \sum_{i,a \neq b} n_{ia\sigma} n_{ib\sigma} \right) + \frac{J}{2} \left( \sum_{i,a \neq b} \delta_{n_{ia\sigma} n_{ib\sigma}} \right),
\]

where

\[
H_{\text{loc}} = \frac{U + J}{2} \left( \sum_{a,\sigma} n_{oa\sigma} n_{oa\sigma} \right)
\]

\[
+ \frac{U}{2} \left( \sum_{a \neq b,\sigma} n_{oa\sigma} n_{ob\sigma} \right) + \frac{U - J}{2} \left( \sum_{a \neq b,\sigma} n_{oa\sigma} n_{ob\sigma} \right)
\]

\[
- \frac{J}{2} \left( \sum_{a \neq b,\sigma} c_{oa\sigma}^+ c_{ob\sigma} + c_{oa\sigma}^+ c_{ob\sigma} \right).
\]

The sum \(i, j\) runs over nearest neighbor sites of a Bethe lattice and \(a, b = 1, 2, 3\) are the band indices. \(c_{ia\sigma}^+\) (respectively \(c_{ia\sigma}\)) denotes the creation (respectively annihilation) operator of an electron at the lattice site \(i\) with spin \(\sigma\) and orbital index \(a\) and \(n_{ia\sigma}\) is the occupation number operator for spin \(\sigma\) and orbital \(a\). The hopping between different orbitals will not be investigated here since \(t_{ij}^a = -\delta_{ab}\). The ref. 12 presents a general Hamiltonian for the multi orbital Hubbard model. The only term neglected in our approach is the pair-hopping term between different orbitals. The prefactors in Eq. (1) ensure the Hamiltonian is invariant under any linear combination of the \(t_{2a}\) orbitals.

Within the framework of the DMFT, by integrating out all fermionic degrees of freedom except those for a central site \(i = 0\), the lattice model can be mapped onto an effective impurity model. The corresponding Hamiltonian \(H_{\text{eff}}\) contains a local part \(H_{\text{loc}}\) and a part corresponding to the coupling to the effective medium that has to be determined self-consistently. We then write:

\[
H_{\text{eff}} = H_{\text{loc}} + H_{\text{med}},
\]

and the coupling with the effective medium is

\[
H_{\text{med}} = \sum_{k,a\sigma} \left( W_{ka\sigma}^2 b_{ka\sigma}^+ c_{oa\sigma} + H.c. \right)
\]

\[
+ \sum_{k,a\sigma} \varepsilon_{ka\sigma} b_{ka\sigma}^+ b_{ka\sigma}^c .
\]

\(W_{ka\sigma}^2\) represents the hybridization between the site \(i = 0\) and the effective medium corresponding to orbital \(a\). \(\varepsilon_{ka\sigma}\) is the band energy of the same effective medium. \(b_{ka\sigma}^+\) (respectively \(b_{ka\sigma}\)) is the creation (respectively annihilation) operator of an electron in the effective medium \(a\). As in the doubly degenerate situation, the effective medium is a multi-component one that can be characterized by the effective dynamical hybridizations:

\[
\mathcal{J}^a(\omega) = \sum_{k} \frac{|W_{ka\sigma}^2|^2}{\omega + i0^+ - \varepsilon_{ka\sigma}^a}.\]

By writing the equation of motion of the Hamiltonian \(H_{\text{eff}}\) we obtain:

\[
G_{aa}(\omega)^{-1} = \omega - \varepsilon_{a} - \Sigma_{a\sigma}(\omega) - \mathcal{J}^a(\omega).
\]

Besides, on a Bethe lattice, the Green’s function presents the following property

\[
G_{aa}(\omega)^{-1} = \omega - \varepsilon_{a} - \Sigma_{a\sigma}(\omega) - t^2 G_{aa}(\omega).
\]

Therefore, the self-consistent equations of the DMFT can be simply written like

\[
\mathcal{J}^a(\omega) = t^2 G_{aa}(\omega).
\]

The local problem that has to be solved self-consistently is then formally similar to the doubly degenerate case previously investigated. However we have to deal here with a large number \(N_s\) of local impurity states \(|S_i\rangle = |\alpha_1, \alpha_2, \alpha_3\rangle\) where \(\alpha_{\sigma}\) represents the electronic occupation \((0, \uparrow, \downarrow, \uparrow \downarrow)\) of orbital \(a\) at the impurity site \(i\). Indeed, the third orbital \(a = 3\) increases \(N_s\) from 16 to 64 = 4^3. Another difficulty comes from the spin-flip term: due to this term, the basis of local states \(A = \{|S_i\rangle\}\) does no longer diagonalize \(H_{\text{loc}}\).

In the following, the 64 states that diagonalize \(H_{\text{loc}}\) will be noted \(|\bar{S}_i\rangle\). They form the basis \(A = \{|\bar{S}_i\rangle\}\). Taking into account the degeneracy of local states \(|\bar{S}_i\rangle\), it is
possible to decrease the basis dimension to 17, the corresponding states will be noted |m⟩. Indeed the 64 states can be classified in 13 generic families (third column in Table I). The kth family contains Nk local states |Sk⟩. gk indicates the number of different energies corresponding to this family. The kth family will be therefore represented by gk states |m⟩. We thus have \( \sum_{k=1}^{13} N_k = 64 \) and \( \sum_{k=1}^{13} g_k = 17 \). (For details, see Table I).

| k | label | (α1, α2, α3) | Nk | gk | (m) |
|---|---|---|---|---|---|
| 1 | 1 | (0, 0, 0) | 1 | 1 | (1) |
| 2 | 2 to 7 | (σ, 0, 0) | 6 | 1 | (2) |
| 3 | 8 to 13 | (σ, 0, 0) | 6 | 1 | (3) |
| 4 | 14 to 19 | (σ, σ, 0) | 6 | 2 | (4, 5) |
| 5 | 20 to 22 | (0, 0, 0) | 3 | 1 | (6) |
| 6 | 23 to 24 | (0, σ, 0) | 2 | 1 | (7) |
| 7 | 25 to 30 | (σ, σ, −σ) | 9 | 3 | (8, 9, 10) |
| 8 | 31 to 32 | (2, 0, σ) | 4 | 1 | (11) |
| 9 | 33 to 40 | (0, σ, σ) | 6 | 1 | (12) |
| 10 | 41 to 42 | (σ, −σ, 0) | 6 | 2 | (13, 14) |
| 11 | 43 to 44 | (0, 0, σ) | 4 | 1 | (15) |
| 12 | 55 to 60 | (0, 0, 0) | 6 | 1 | (16) |
| 13 | 61 to 62 | (0, 0, 0) | 2 | 1 | (17) |

**TABLE I:** For each family, labels of different local states are given in column 2. Column 3 displays the generic form of local state: it stands for \( N_k \) states corresponding to \( σ = + \) or \( − \), and permutation of orbitals. \( g_k \) and |m⟩ are defined in the text.

Because of the spin-flip term, off-diagonal elements of \( H_{\text{loc}} \) occur for local states belonging to families \( k = 4, 7 \) and 10. \( k = 4 \) and \( k = 10 \) families can be treated in a similar way. They can be described by six (2 × 2) blocks. As for the doubly degenerate case, singlet and triplet states have to be considered here. For instance, in the two-dimensional subspace formed by \( |S_{14}\rangle = |↑, ↓, 0\rangle \) and \( |S_{15}\rangle = |↓, ↑, 0\rangle \), \( H_{\text{loc}} \) is represented by the (2 × 2) non-diagonal matrix

\[
\begin{pmatrix}
U & -J \\
-J & U
\end{pmatrix}
\]

Diagonalization leads to the first eigenstate \(|\tilde{S}_{14}\rangle = (|S_{14}\rangle + |S_{15}\rangle)/\sqrt{2} \) which corresponds to \( E_{14} = U - J \) and is the \( S^z = 0 \) component of a triplet (the corresponding \( S^z = ± 1 \) components are the states \( |σ, σ, 0\rangle \) in the \( k = 3 \) family). The second eigenstate is the singlet state \(|\tilde{S}_{15}\rangle = (|S_{14}\rangle - |S_{15}\rangle)/\sqrt{2} \) for which \( E_{15} = U + J \).

The notation is: \(|4\rangle = |\tilde{S}_{14}\rangle \) and \(|5\rangle = |\tilde{S}_{15}\rangle \).

\( k = 7 \) family is composed by two (3 × 3) blocks of the following form:

\[
\begin{pmatrix}
3U - J & -J & -J \\
-J & 3U - J & -J \\
-J & -J & 3U - J
\end{pmatrix}
\]

Considering the first block where \(|S_{25}\rangle = |↑, ↑, ↓\rangle, |S_{26}\rangle = |↑, ↓, ↑\rangle \) and \(|S_{27}\rangle = |↓, ↑, ↑\rangle \), we have the eigenstates

\[
\begin{align*}
|\tilde{S}_{25}\rangle &= -\frac{\sqrt{6}}{3}|S_{25}\rangle + \frac{1}{\sqrt{6}}|S_{26}\rangle + \frac{1}{\sqrt{6}}|S_{27}\rangle \\
|\tilde{S}_{26}\rangle &= \frac{1}{\sqrt{2}}|S_{26}\rangle - \frac{1}{\sqrt{2}}|S_{27}\rangle \\
|\tilde{S}_{27}\rangle &= \frac{1}{\sqrt{3}}|S_{25}\rangle + \frac{1}{\sqrt{3}}|S_{26}\rangle + \frac{1}{\sqrt{3}}|S_{27}\rangle,
\end{align*}
\]

with the corresponding energies

\[
\tilde{E}_{25} = 3U, \quad \tilde{E}_{26} = 3U, \quad \tilde{E}_{27} = 3U - 3J.
\]

The state \(|\tilde{S}_{27}\rangle \) plays an important role for the dynamical properties of the triply degenerate Hubbard problem. Indeed this low energy state is one component of the maximum spin multiplet \( S = 3/2 \). This fourfold multiplet is strongly stabilized by the Hund’s exchange \( J \).

In Table II energy eigenvalues \( E_m \) of |m⟩ states are displayed.

```
| k-family | | n_m | | E_m |
|---|---|---|---|
| 1 | 1 | 0 | 0 |
| 2 | 2 | 1 | 0 |
| 3 | 3 | 2 | U - J |
| 4 | 4 | 2 | U - J |
| 5 | 5 | 2 | U + J |
| 6 | 6 | 2 | U + J |
| 7 | 7 | 3 | 3U - 3J |
| 8 | 8 | 3 | 3U |
| 9 | 9 | 3 | 3U |
| 10 | 10 | 3 | 3U - 3J |
| 11 | 11 | 3 | 3U |
| 12 | 12 | 4 | 6U - 2J |
| 13 | 13 | 4 | 6U - 2J |
| 14 | 14 | 4 | 6U |
| 15 | 15 | 4 | 6U |
| 16 | 16 | 5 | 10U - 2J |
| 17 | 17 | 6 | 15U - 3J |
```

**TABLE II:** Energy \( E_m \) of each local state |m⟩. \( n_m \) is the total on-site occupation.

\( H_{\text{loc}} \) is diagonal in the basis \( \mathcal{A} \), the effective Hamiltonian \( H_{\text{eff}} \) can therefore be solved by using the extended version of the non-crossing approximation presented in a previous work. This approach has been used with success for various problems.

Within NCA, propagators and self-energies for the 64 local states \(|S_i\rangle \) are introduced. These propagators (and self-energies) are identical for similar local states. For instance |↑, ↑, 0⟩, |↑, 0, ↑⟩ and |↓, ↓, 0⟩ are described by the same propagator \( P_3(\omega) \) because of orbital and spin degeneracy. We have then only 17 different propagators \( P_m(\omega) \). However, all the 64 local states are needed to
express the $c_{ao\sigma}$ and the $c_{ao\sigma}^\dagger$ operators by Hubbard operators $X_{i,j} = |\bar{S}_i\rangle \langle \bar{S}_j|$. More precisely, we can write
\[
    c_{ao\sigma} = \sum_{i,j} D_{i,j}^{a,\sigma} |\bar{S}_i\rangle \langle \bar{S}_j|
\]
\[
    = \sum_{m,m'} D_{m,m'}^{a,\sigma} |m\rangle \langle m'|
\]
where $D_{i,j}^{a,\sigma}$ is a $(64 \times 64)$ matrix and $D_{m,m'}^{a,\sigma}$ is a $(17 \times 17)$ matrix. $D_{m,m'}^{a,\sigma}$ is calculated by developing the annihilation operator onto Hubbard operators and $D_{m,m'}^{a,\sigma}$ can be deduced by using the previously discussed degeneracy for local propagators $P_m(\omega)$.

In the next section we present our results for the triply orbital degenerate Hubbard model. The density of states is obtained by solving the effective DMFT model by application of the NCA.

### III. RESULTS AND DISCUSSION

In this section, we present the calculated densities of states for the triply orbital degenerate Hubbard model with a Hund’s exchange invariant under spin rotation. The DMFT results are obtained for $t = 1/\sqrt{2}$ eV, $U$ from 2 to 6 eV and for finite temperature $T = 1000$ K. We will take $J \approx U/10$ or $U/100$.

In order to understand the specific role played by Hund’s coupling, and the nature of the different bands composing the density of states, we first investigate in the following sub-section the $J = 0$ situation. The nonvanishing $J$ system will be studied in section III.B.

#### A. No Hund’s coupling

Because of the triple band degeneracy, the electronic excitation spectra present already a rich structure for $J = 0$. This is shown in figure 1 where various concentrations of charge carriers are investigated from $n = 0.9$ up to $n = 5.1$. In this triply degenerate system, six electrons can in principle coexist at each site. For some plots (labelled by a star in the figure), the Fermi level position is indicated by a small circle. These results are in agreement with previous works on the MIT for degenerate correlated systems. In the strongly correlated regime, we find an insulating state for each integer filling. For fillings close to integer values, the narrow quasiparticle structure at the Fermi level is characteristic for a strongly correlated metal. With increasing chemical potential, an important transfer of spectral weight is observed. The relative band spectral weights can be interpreted in terms of probabilities. For instance, for $n = 0.9$ the excitation spectrum is mainly composed of two bands corresponding to the lower and the upper Hubbard bands (LHB and UHB). The number of occupied electronic states of the LHB gives the probability of removing an electron from the system, like in a photoemission experiment.

The spectral weight of the UHB gives the probability of adding an electron in an empty state (inverse photoemission). For $n$ close to 1 there is only one possibility for removing an electron, but there are five possibilities of adding an electron onto the same site. This is indicated in figure [1] for various densities: $(1,5), (2,4) \ldots$ For $J = 0$, the additional energy involved in this process is $U$, whatever the spin of the electron and the occupied orbital are.

![FIG. 1: Densities of states for various electronic occupations from $n = 0.9$ to $n = 5.1$ for the triply degenerate Hubbard model without Hund’s coupling and for $U = 6$ eV. For some fillings (labelled by a star), the Fermi level is indicated by a small circle.](image)

Densities of states for $n = 0.9, 1.9, 2.9, 3.9$ and 4.9 are displayed in figure 2 with an energy shift ensuring that all Fermi energies are at the same point. Here, the transfer of spectral weight from the LHB to the UHB is obvious. The inset shows the low energy behavior. We do not consider exactly integer values for $n$ to prevent numerical problems when the density of states at the Fermi level is very close to zero. Nevertheless, our approach is numerically well defined for filling arbitrary close to integer values, with increasing numerical efforts. For all fillings, a quasiparticle peak is clearly present, but the effective mass of these quasiparticles is strongly dependent on the number of charge carriers. The correlated system with $n = 0.9$ is much...
closer to the insulating state than the $n = 4.9$ situation. The $n = 0.9$ effective mass can be obtained from the self-energy via $m^*/m = (1 - \partial \text{Re} \Sigma(\omega)/\partial \omega)_{\omega=0}$ and is approximately seven times the $n = 4.9$ effective mass. Actually, because of electron-hole symmetry, $n = 1.1$ and $n = 4.9$ give symmetric densities of states and therefore the same effective masses for quasiparticles. Consequently, starting from $n = 1$, a 10% electron or hole doping leads to very different systems contrasting with the one band Hubbard model. For $J = 0$, we obtained a Mott metal insulator transition for each integer filling $n = 1, 2, 3, 4, 5$. This is consistent with previous theoretical works using slave-boson formalism, variational methods, and quantum Monte-Carlo dynamical mean field theory. Nevertheless, the interesting question of the order of the transition cannot be investigated by the present approach because of the NCA pathology at low temperature. Indeed, the coexistence region extending to finite doping off half-filing observed for the doubly degenerate Hubbard model has been observed only at low temperature.

**B. Non vanishing Hund’s coupling**

Keeping a spin-rotational invariant Hund’s exchange means that we have to handle explicitly the last term in expression (1). Recently, a very accurate study showing the importance of this term has been presented for the two-band Hubbard model. Indeed, a completely different behavior occurs if one replaces the rotationally invariant Hund exchange by an Ising-like one.

Here we will focus on the specific effects of the Hund’s exchange coupling on the electron dynamics for the strongly correlated metal and for the integer filling system which is insulating for large $U$. We will see that $n$ plays a crucial role.

In figure 3, the calculated densities of states are displayed for various values of $n : n = 0.9$, $n = 1.9$ and $n = 2.9$. They correspond to strongly correlated metals close to the insulating state. The narrow quasi-particle peak at the Fermi level is a signature of the large electronic effective mass close to the MIT. For each $n$ and for $U = 6$ eV, the calculation has been done for three values of Hund’s parameter $J = 0$, $U/100$ and $U/10$. The (a) part of the figure shows that, for $n = 0.9$, the effect of a finite $J$ value is restricted to high energy excitations of the spectrum. This can be understood by considering the energies of the local states listed in table 1. For $n = 0.9$, local states playing an important role in the electronic dynamics are those with occupations 0, 1 and 2. Larger occupations of local states are highly unlikely. The only $J$-dependent local energies are those for the two-fermion states $|3\rangle$, $|4\rangle$, $|5\rangle$ and $|6\rangle$. Transitions from singly occupied state to these states involve high energy excitations of the order of $U$. This $J$ influence restricted to high energy bands is specific to the singly occupied multi-band Hubbard model. Indeed, the physical situation is dramatically different for $n = 1.9$ and $n = 2.9$ (part (b) and part (c) of figure 3). Here, a non zero $J$ has a strong influence on high energy excitations as well as close to the Fermi level. For low energy excitations an important reduction of the spectral weight is observed, which is clearly visible in the figure insets and is in agreement with very recent results at half filling for the doubly degenerate Hubbard model with Hund’s exchange. Here, we found that this effect is also observed away from half filling. Besides, this reduction is accompanied by the emergence of a multi-peak structure around the Fermi level.
corresponding to the lifting of degeneracy of multiparticle states in table. This multi-peak effect is stronger for \( n = 2.9 \) which is consistent with the energy interval \( 3J \) between the three-fermion local states of spin 3/2 and 1/2. If we approach \( n = 3 \), the peak at around \( 3J \) diminishes such that we are left with a gap of the order of \( U \) at \( n = 3 \).

For instance, for a multi-orbital Hubbard model without Hund’s coupling and for a flat density of states, S. Florens and A. Georges found that \( U_c \) is proportional to \( n(1 - n) \). The maximum critical coupling \( U_c(n) \) for three orbitals is obtained for \( n = 3 \), the half-filled situation, where orbital fluctuations are largest. This result is consistent with previous work, in particular M.J. Rozenberg has found that \( U_c(2) > U_c(1) \) for the doubly degenerate orbital (with \( J = 0 \)) Hubbard model by using Quantum Monte-Carlo calculations.

Concerning the influence of the Hund’s coupling \( J \) on the Mott transition at \( T = 0 \), an interesting generalization of the linearized dynamical mean field theory has been proposed recently. In addition to a reduction of \( U_c \) due to \( J \), a qualitative change in the nature of the \( T = 0 \) Mott transition has been observed for any finite \( J \). The reduction of \( U_c \) has been given in details only for \( n = M \) where \( M \) is the degeneracy. Here we find important differences between the half-filled case \( n = M \) and the \( n \neq M \) situation. Besides, our approach is able to explore dynamical properties by calculating the full densities of states.

The integer filling situation is examined in figure. The stability of the metallic state is ensured by the intermediate value \( U = 2 \) eV which is smaller than the critical \( U_c \) of the MIT for different integer fillings. \( J \) takes values 0 and \( U/10 \). Here again, the effect of a non-zero \( J \) is very weak for \( n = 1 \) (part (a)) and restricted to high energy excitations. A completely different behavior occurs for \( n = 2 \) and \( n = 3 \). For \( n = 2 \) (part (b)), the introduction of a non-vanishing \( J = U/10 \) is sufficient to destroy the quasiparticle coherent peak, which is consistent with the NRG results for the two-orbital Hubbard model. This effect becomes stronger for the \( n = 3 \) situation where a pseudo-gap is observed. Such a structure with a pseudo-gap at the Fermi energy is already present at half filling in the solution for the local impurity model proposed in ref. Here we show that this critical role of \( J \), leading to a pseudo-gap criticality, can be observed away from half filling but the critical Coulomb and Hund parameters are strongly dependent on \( n \). This property has important consequences on the nature of the different MIT in degenerate systems. A multi-band Hubbard model displays a Mott transition at all integer fillings. Nevertheless, by taking into account the Hund’s exchange term, the different MIT present different low energy dynamical behavior. It has been shown in previous studies that the critical correlation strengths \( U_c \) depend on \( n \).
An appreciable decrease of the density of states at energy excitations is a light increase of spectral weight. Hund’s exchange is very weak. The only effect on the low $n = 2$ situation, the density of states at $n$ found for $J$ for a critical value stronger for the half-filled system $n$ integer occupations $n$ that $\epsilon$ states at $U$ and for a constant $F$ as a function of $J$ goes to zero for a critical value $J_c \approx 0.2$ eV but for $n = 3$ this takes place at a lower repulsion value $U = 2.4$ eV.

Indeed, in figure 6, the dependence of the density of states at $\epsilon_F$ on $J$ is plotted for $n = 1$, $n = 2$ and $n = 3$, and for a constant $U = 2.4$ eV. For $n = 1$, the influence of Hund’s exchange is very weak. The only effect on the low energy excitations is a light increase of spectral weight. An appreciable decrease of the density of states at $\epsilon_F$ is found for $n = 2$ and $U = 2.4$ eV but the effect is much stronger for the half-filled system $n = 3$. Similarly to the $n = 2$ situation, the density of states at $\epsilon_F$ goes to zero for a critical value $J_c \approx 0.2$ eV but for $n = 3$ this takes place at a lower repulsion value $U = 2.4$ eV.

FIG. 6: Densities of states at $\epsilon_F$ as a function of $J$ for various integer occupations $n = 1$, 2 or 3, and for $U = 2.4$ eV. Note that $J$ plays an important role at half filling $n = 3$ but also away from half filling for $n = 2$.

Indeed, in figure 6, the dependence of the density of states at $\epsilon_F$ on $J$ is plotted for $n = 1$, $n = 2$ and $n = 3$, and for a constant $U = 2.4$ eV. For $n = 1$, the influence of Hund’s exchange is very weak. The only effect on the low energy excitations is a light increase of spectral weight. An appreciable decrease of the density of states at $\epsilon_F$ is found for $n = 2$ and $U = 2.4$ eV but the effect is much stronger for the half-filled system $n = 3$. Similarly to the $n = 2$ situation, the density of states at $\epsilon_F$ goes to zero for a critical value $J_c \approx 0.2$ eV but for $n = 3$ this takes place at a lower repulsion value $U = 2.4$ eV.

IV. CONCLUSION

We have proposed an approach based on the dynamical mean field theory which is able to describe important features of dynamical electronic properties of the triply degenerate Hubbard model. The self consistent local impurity problem is solved with a generalization of the non-crossing approximation. This impurity problem consists in a triply degenerate local correlated site (64 local states) embedded in an uncorrelated conduction band which is orbital dependent. As expected, for $J = 0$, we obtained a Mott metal insulator transition for each integer filling namely $n = 1, 2, 3, 4, 5$.

The influence of a Hund’s exchange invariant under spin rotation has been studied in detail. In agreement with previous works, we found that a non-zero $J$ implies a reduction of the low energy spectral weight. This effect is observed for integer as well as for non-integer fillings. In addition, we established the occurrence of multi-peak effects in the spectral function at the metallic side of the MIT. These effects give rise to structures with an energy scale $J$. An important result of our approach is the very strong dependence of all these effects on the filling. The destruction of low energy states is much more pronounced at half filling than at other fillings. Besides, for $n = 1$, this effect is not visible. Another interesting point is the occurrence of a particular value $J_m$ for which the reduction is maximum, $J_m$ increasing with $U$.

It could be interesting to include in the present model different bandwidths for different orbitals to investigate the role of Hund’s exchange in the so-called orbital selective Mott transition.22 Another possible perspective for this work is to understand how disorder in real materials can affect the results concerning Hund’s exchange influence. Finally, the pair hopping term between different orbitals (orbital-flip term) can be studied in the framework of our approach and will be the subject of a forthcoming publication, as well as a more specific treatment of realistic spectra.

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