Electronic properties of the degenerate Hubbard Model: 
A dynamical mean field approach

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(March 21, 2022)

We have investigated electronic properties of the degenerate multi-orbital Hubbard model, in the limit of large spatial dimension. A new local model, including a doubly degenerate strongly correlated site has been introduced and solved in the framework of the non-crossing approximation (NCA). Mott-Hubbard transitions have been examined in details, including the calculation of Coulomb repulsion critical values and electronic densities of states for any regime of parameters.

An increasing interest for strongly correlated electronic systems has been induced by the discovery of high temperature superconductors and giant magnetoresistance. Despite a large amount of papers on this fascinating field, a complete physical understanding of strongly correlated electronic systems remains a major problem of condensed matter theory. Even the simplest Hamiltonian describing such systems, given by the Hubbard model, is still an unsolved challenging problem.

The seminal work of Metzner and Vollhardt has shown the importance of large spatial dimensions. Taking the limit $D \to \infty$ leads to significant simplification of the many body problem while retaining essential dynamical features of low dimensional situations. An important amount of studies has been done within this approach, mapping the lattice problem onto a self-consistent Anderson single impurity model. This mapping becomes exact in the limit of infinite spatial dimension. For a review, see Ref. [1]. Most of this work has been done focusing on the original one-band Hubbard model, which is the simplest model to describe the electron-electron interaction-driven metal-insulator transition (MIT).

However, orbital degeneracy in known to play a crucial role in correlated systems. The degeneracy of the $d$ band is two in $V_2O_3$ and three in $LaTiO_3$. Orbital degree of freedom is relevant to explain some very interesting properties like colossal magneto-resistance, MIT in alkali-doped fullerenes, and for any physical property involving orbital ordering.

Many theoretical approaches have been proposed to describe the effect of strong Coulomb interaction in systems with orbital degeneracy, using the slave-boson method, the variational method, and the limit of high spatial dimension. Some results of these works concerning the transition criteria and the order of the MIT are substantially different. An unified theory describing degenerate Hubbard model is still missing. Concerning high spatial dimension approaches, quantum Monte-Carlo (QMC) and a generalized iterated perturbation theory (IPT) have been proposed. Imaginary time results, high computational time and fundamental difficulties at low temperature can be a limit for QMC calculations. The generalization of the IPT, developed in Ref. [16], presents the advantage of being able to deal with particle-hole asymmetric problems. However, this approach is essentially a perturbation theory with respect to the correlation strength, which is the highest energy scale of the system. The non-crossing approximation (NCA) was shown to be in excellent agreement with quantum Monte Carlo calculations for the DMFT of the one-orbital case, even far away from half-filling.

Here, we present a new approach based on the NCA within the dynamical mean field theory (DMFT).

The starting Hamiltonian is given by the two-orbital degenerate Hubbard model

$$H = \sum_{<i,j>,a,b} t_{ij}^a c_{ia,a}^+ c_{ja,b} + \frac{U}{2} \sum_{i,a} n_{ia} n_{ia - \sigma}$$

$$+ \frac{U}{2} \sum_{i,a \neq b, \sigma} n_{ia} n_{ib} + \frac{U - J}{2} \sum_{i,a \neq b, \sigma} n_{ia} n_{ib}$$

$$- \frac{J}{2} \sum_{i,a \neq b, \sigma} c_{ia}^+ c_{ia - \sigma} c_{ib - \sigma} c_{ib}$$

(1)

where the sum $<i,j>$ is the sum over nearest neighbor sites of a Bethe lattice and $a,b = 1,2$ is the band index. $c_{ia}^+$ (respectively $c_{ia}$) denotes the creation (respectively annihilation) operator of an electron at the lattice site $i$ with spin $\sigma$ and orbital index $a$ and $n_{ia}$ is the occupation number per spin and per orbital. The on-site Coulomb repulsion $U$ and the exchange parameter $J$ are assumed to be independent of orbital. In addition we will neglect the last term in the Hamiltonian and the hopping between different orbitals $t_{ij}^a = -t_0 \delta_{ab}$. Doing such approximations leads to the same Hamiltonian studied previously by quantum Monte Carlo (QMC).

Integrating out the fermionic degrees of freedom leads to the single-site effective action

$$S_{\text{eff}} = -\int_0^\beta d\tau \int_0^\beta d\tau' \sum_{\sigma,a} c_{o\sigma}^+(\tau) G_{o\sigma}^{-1}(\tau - \tau') c_{o\sigma}(\tau')$$
local state $|\alpha, \beta >$ is an eigenstate of the local part of the model Hamiltonian. The corresponding local model that have to be solved is schematically represented in figure 1. The impurity site is coupled with two effective media by two effective dynamical hybridization $J^1(\omega)$ and $J^2(\omega)$.

Local states $|\alpha, \beta >$ and $|\alpha', \beta' >$ are coupled by NCA equations if one of the two following conditions are fulfilled : $|n_{\alpha 1}(\alpha) - n_{\alpha 1}(\alpha')| = 1$ and $\beta = \beta'$ or $\alpha = \alpha'$ and $|n_{\alpha 2}(\beta) - n_{\alpha 2}(\beta')| = 1$. The first and the second cases involve respectively $J^1(\omega)$ and $J^2(\omega)$.

![Two orbitals local model](image)

**FIG. 1.** Two orbitals local model. The sixteen local states $|\alpha, \beta >$ are all coupled by the orbital dependent effective medium hybridization $J^1(\omega)$ and $J^2(\omega)$.

Here are the main results of our dynamical mean field theory. The NCA approach presents the advantage to provide directly real frequencies one-particle Green’s functions. Local quantities like densities of states can therefore be computed for any regime of parameters.

![Density of states](image)

**FIG. 2.** Density of states per spin and per orbital for $U = 4 \text{ eV}$, $t = 1 \text{ eV}$ and $T = 1000 \text{ K}$. Total occupation number is $n = 0.987$. The inset shows filling dependence of low energy excitations. Solid line (respectively dotted and dashed line) is the density of states around the Fermi level for $n = 0.987$ (respectively $n = 0.992$ and $n = 0.995$).

\[ + \frac{U}{2} \int_0^\beta d\tau \left( \sum_{a\sigma} n_{oa\sigma}(\tau)n_{oa\sigma}(\tau) + \sum_{(a \neq b)} n_{oa}(\tau)n_{ob}(\tau) \right), \]

where

\[ n_{oa} = n_{oa\uparrow} + n_{oa\downarrow}. \]

Therefore, as in the one-band case, the large-$D$ version of the degenerate two-band Hubbard model is mapped onto an effective impurity model. The local correlated site is now orbitally degenerated, and two different effective media have to be considered. The corresponding Hamiltonian reads

\[ H_{\text{eff}} = H_{\text{loc}} + H_{\text{med}}, \tag{2} \]

where the local part is

\[ H_{\text{loc}} = \sum_{a\sigma} \varepsilon_d n_{oa\sigma} + \frac{U}{2} \left( \sum_{a\sigma} n_{oa\sigma} n_{oa\sigma - \sigma} + \sum_{(a \neq b)} n_{oa} n_{ob} \right), \]

and the coupling with the effective medium is

\[ H_{\text{med}} = \sum_{ka\sigma} \left( W_{ka\sigma}^0 b_{ak\sigma}^+ c_{a\sigma} + H.c. \right) + \sum_{ka\sigma} \varepsilon_k b_{ak\sigma}^+ b_{ak\sigma}. \]

The orbital dependent coupling with the effective medium is characterized by the hybridization

\[ J^\alpha(\omega) = \sum_k \frac{|W_{ka\sigma}^\alpha|^2}{\omega + i0^+ - \varepsilon_k^\alpha}. \]

From the equation of motion of this effective Hamiltonian, it follows that

\[ G_{a\sigma}(\omega)^{-1} = \omega - \varepsilon_d - \Sigma_{a\sigma}(\omega) - J^\alpha(\omega). \]

Comparing this equation to the following property of Green’s functions on a Bethe lattice

\[ G_{a\sigma}(\omega)^{-1} = \omega - \varepsilon_d - \Sigma_{a\sigma}(\omega) - i^2 G_{a\sigma}(\omega), \]

we found the self-consistent set of equations

\[ J^\alpha(\omega) = i^2 G_{a\sigma}(\omega). \]

In the following, we solve the impurity model of equation (3) using the extended version of the non-crossing approximation presented in a previous work [20]. Propagators and self-energies of the sixteen local states $|\alpha, \beta >$ are introduced, where $\alpha$ (respectively $\beta$) is the local occupation of orbital $a = 1$ (respectively $a = 2$). Each
NCA was in very good agreement with essentially exact quantum Monte-Carlo simulations for the one-band case. This approximation is then a good candidate for the investigation of the multi-band generalization of the Hubbard model.

Useful and comprehensive information concerning electronic dynamic processes are given by these densities of states, without any size effects due to small clusters and till very low temperature.

Spin and orbital dependent densities of states \( \rho_{a\sigma}(\omega) \) are obtained from NCA Green’s functions by:

\[
\rho_{a\sigma}(\omega) = -\frac{1}{\pi} \text{Im}\{G_{a\sigma}(\omega)\}. 
\]

Figure 2 displays the density of states per spin and per orbital of the doubly degenerate Hubbard model for a total occupation number \( n = 0.987 \). Both lower and upper Hubbard bands are present. Relative spectral weights between the lower and the upper Hubbard band are given by the ratio 1/3. Quasiparticle excitations can be seen around the Fermi level. The origin of this low energy structure can be clarified in the context of NCA by observing its temperature and filling dependence [19] or by reducing the Hilbert space of available local states onto the impurity [20].

The proximity of the \( n = 1 \) metal insulator transition is confirmed by the disappearance of the low energy spectral weight. The inset shows the behavior of quasiparticle excitations just before the transition. Total occupation numbers are \( n = 0.987, n = 0.992 \) and \( n = 0.995 \).

It is interesting to compare two-bands densities of states with one-band NCA results. This is shown in figure 3, for \( U = 5 \) eV and \( n_{\text{tot}} = 0.94 \). Spectral weights are in good agreement with previous approaches like the IPT one [14]. More precisely, we found that degeneracy has a strong influence only on high energy excitations: respective spectral weights of lower and upper Hubbard bands for \( n_{\text{tot}} = 1 \) are 1 and 3 in the two-orbitals problem, instead of 1 and 1 for the same filling in the one-orbital problem. However, NCA bands structures are strongly different to IPT ones. Fine structures displayed by IPT results are not present in our approach which is confirmed by recently obtained QMC spectral functions for the multi-orbital Hubbard model in infinite dimension [22].

Figure 4 shows the general evolution with respect to the total occupation number of electron density of states per spin and per orbital, for \( U = 5 \) eV, \( t = 1 \) eV and \( T = 1000 \) K. Each curve corresponds to a given Fermi level. Quasiparticle low energy excitations can be seen around the Fermi level. Total occupation numbers \( n \) are indicated for each density of states. For integer fillings \( n = 1, n = 2 \) and \( n = 3 \), the system is an insulator. It is metallic for any other filling. The interesting transfer of spectral weight from high to low (Fermi level) energy scale will be studied in details later.
consistent with experimental observations in filling controlled oxides family such as Sr$_{1-x}$La$_x$TiO$_3$ [21].

The Fermi level dependence of total occupancy is plotted in figure 6. These results are consistent with recent QMC simulations for the multi-orbital Hubbard model [22]. When the system in an insulator, as for $U = 4$ eV in the figure, a small displacement of the Fermi level in the insulating gap does not lead to a significant variation of the total occupation number. A plot of occupation number versus chemical potential displays a plateau as soon as a MIT is crossed. Our results show that three successive MIT at integer fillings occur in the system. $n = 1$ and $n = 3$ transitions are equivalent because of the particle-hole symmetry. For a given $U$, the Mott gap of the $n = 2$ transition is smaller than the $n = 1$ gap. This is in good agreement with previous calculations leading to a larger critical $U_c$ for the $n = 2$ transition [4]. We found $U_c(n = 2) \approx 3.5$ and $U_c(n = 1) \approx 3.1$.

In summary, we have proposed a new approach based on the dynamical mean field theory for the doubly degenerate Hubbard model, combined with a generalization of the non-crossing approximation in order to solve the equivalent self-consistent local impurity problem. This impurity problem consists in a doubly degenerate local correlated site (sixteen local states) embedded in a conduction band which is orbital dependent.

We obtained a description of the integer filling metal insulator transitions consistent with previous theoretical works using slave-boson formalism, variational method and quantum Monte-Carlo dynamical mean field theory. One of the advantages of our approach is to provide the full spectrum of excitations for any regime of parameters and a clear interpretation of the quasiparticle nature. Besides, many extensions of the model Hamiltonian can be done within this framework. In future calculations, we will increase the degeneracy (some oxides, like Sr$_{1-x}$La$_x$TiO$_3$ are triply degenerate) and we will take explicitly into account the exchange interaction by introducing a non zero Hund coupling parameter $J$. We will also extend our analysis to thermodynamic and transport properties.

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