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Correlation-induced band suppression in the two-orbital Hubbard model

E Plekhanov^{1,2}, A Avella^{1,2,3}, F Mancini^{1,2} and F P Mancini^{1,3,4}

¹ Dipartimento di Fisica “E.R. Caianiello”, Università degli Studi di Salerno, 84084 Fisciano (SA), Italy

² Unità CNISM di Salerno, Università degli Studi di Salerno, 84084 Fisciano (SA), Italy

³ CNR-SPIN, UoS di Salerno, 84084 Fisciano (SA), Italy

⁴ Sezione INFN di Perugia, 06123 Perugia, Italy

E-mail: plekhanoff@physics.unisa.it

Abstract.

The orbital degrees of freedom are of vital importance in explanation of various phenomena. Among them is the orbital-selective Mott transition (OSMT), which is thought to occur in several materials as $\text{Ca}_{2-x}\text{Sr}_x\text{RuO}_4$ and $\text{La}_{n+1}\text{Ni}_n\text{O}_{3n+1}$. OSMT is usually studied in the infinite-dimension limit, and for the time being, it is not clear if it could survive in one-dimensional (1D) case. There exist two scenarios for the OSMT: upon increasing the interaction in a two-band system i) one of the bands becomes insulating, while the other remains metallic and ii) one of the bands becomes empty, while the other may eventually undergo a single-band Mott insulator transition. In this work, we present a preliminary study of the two-orbital Hubbard model by means of Density Matrix Renormalization Group in 1D at quarter-filling, where the second scenario seems to be realized. In particular, we study the orbital densities, double occupancies and form-factors also in the case of finite inter-orbital inter-site hopping.

1. Introduction

The crucial role of the orbital degrees of freedom in explaining several intriguing phenomena such as metal-insulator transition and magnetism in doped phthalocyanines as well as the superconductivity in heavy-fermion compounds has been recently recognized. On the theoretical side, the study of multi-orbital systems is extremely complicated and has been mainly accomplished in the infinite-dimension limit by means of the Dynamical Mean-Field Theory, although, in these systems, the spatial correlations are essential.

Another fascinating phenomenon inherent to the multi-orbital systems is the orbital selective Mott transition (OSMT). In such a transition, by tuning the strength of the Coulomb repulsion, it is possible to open a gap in some band(s), while leaving the other(s) gapless. It is thought that OSMT occurs in materials as $\text{Ca}_{2-x}\text{Sr}_x\text{RuO}_4$ [1, 2] and $\text{La}_{n+1}\text{Ni}_n\text{O}_{3n+1}$ [3, 4, 5].

The simplest multi-orbital model is the two-orbital Hubbard model, whose most general Hamiltonian reads as follows:

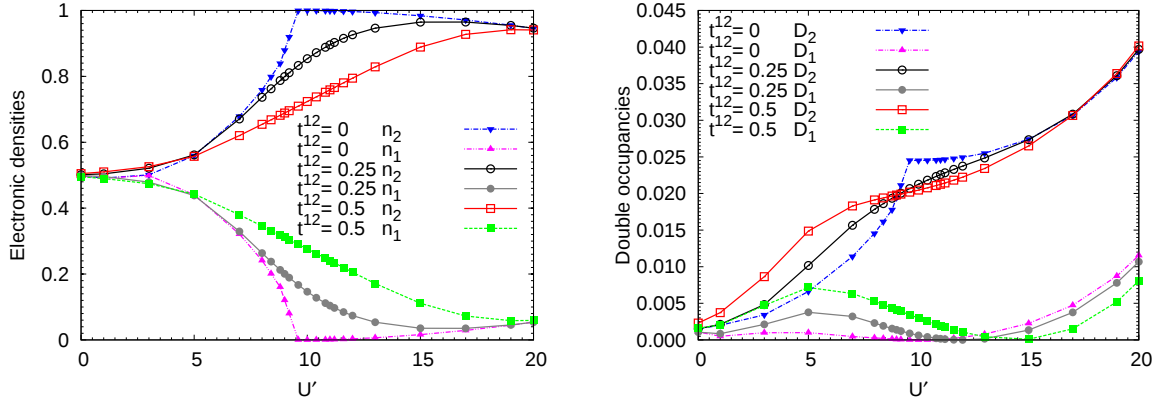


Figure 1. Left panel: U' -dependence of the average occupation number per orbital per site n_1 and n_2 at different values of inter-orbital hopping t^{12} . $U = 10$, $t^{11}/t^{22} = 0.5$, DMRG 50 sites. Right panel: The same for the average double occupancy D_1 and D_2 .

$$H = - \sum_{\langle ij \rangle \alpha \beta \sigma} t^{\alpha \beta} \left(c_{i\alpha\sigma}^\dagger c_{j\beta\sigma} + h.c. \right) + U \sum_{i\alpha} n_{i\alpha\uparrow} n_{i\alpha\downarrow} \quad (1)$$

$$+ \left(U' - \frac{J}{2} \right) \sum_i (n_{i1\uparrow} + n_{i1\downarrow}) (n_{i2\uparrow} + n_{i2\downarrow}) - 2J \sum_i \sum_{k=1}^3 S_{i1}^k S_{i2}^k + J \sum_i \left[p_{i1} p_{i2}^\dagger + p_{i2} p_{i1}^\dagger \right].$$

Here $t^{\alpha\beta}$ parametrizes intra- (t^{11} and t^{22}) and inter- orbital (t^{12}) hoppings between nearest-neighbor (NN) sites, U and U' are the on-site inter- and intra-orbital Coulomb repulsions, respectively, while J is the direct exchange interaction. Rotational symmetry imposes that $U = U' + 2J$. Finally, $c_{i\alpha\sigma}^\dagger$ creates an electron with spin σ in the α -orbital of site i , $S_{i\alpha}^k \equiv \frac{1}{2} \sum_{ab} \sigma_{ab}^k c_{i\alpha a}^\dagger c_{i\alpha b}$ is the electron spin operator in the α -orbital of site i , being σ_{ab}^k the Pauli matrices, and the pair operator $p_{i\alpha}$ and the electron density operator $n_{i\alpha\sigma}$ are defined as follows: $n_{i\alpha\sigma} = c_{i\alpha\sigma}^\dagger c_{i\alpha\sigma}$, $p_{i\alpha} = c_{i\alpha\uparrow} c_{i\alpha\downarrow}$.

In the present manuscript, we use finite-size Density Matrix Renormalization Group (DMRG) method [6] to investigate the zero-temperature properties of the Hamiltonian (2). We consider chains of 50 sites with open boundary conditions. In the DMRG decimation procedure, we retain up to $M = 300$ lowest eigenstates of the density matrix, which amounts to have a truncation error on the sum of the density matrix eigenstates not larger than 10^{-5} .

2. Results

It is well known that the (OSMT) occurs at commensurate fillings ($n = 1$, $n = 2$ electrons per site). In particular, in one-dimensional (1D) case, by means of the product-wave-function renormalization-group technique, the existence of two Mott states in the Hamiltonian (2) at quarter- and half- filling for $t^{12} = 0$, $U = 10$ and $t^{11}/t^{22} = 0.5$ has been shown in Ref. [7]. It was found therein that the quarter-filling case corresponds to a complete narrow orbital suppression (NOS), while in the half-filling case there appears a true OSMT state. In the present manuscript we concentrate on the case of a quarter-filled system ($n = 1$) and explore the evolution of NOS upon introducing a finite inter-orbital hopping t^{12} . We have also studied the $t^{12} = 0$ case, already analyzed in Ref. [7], in order to compare our finite-size algorithm with their bulk one, as well as to have our own $t^{12} = 0$ reference line. In Fig. 1, we present our results for average electron

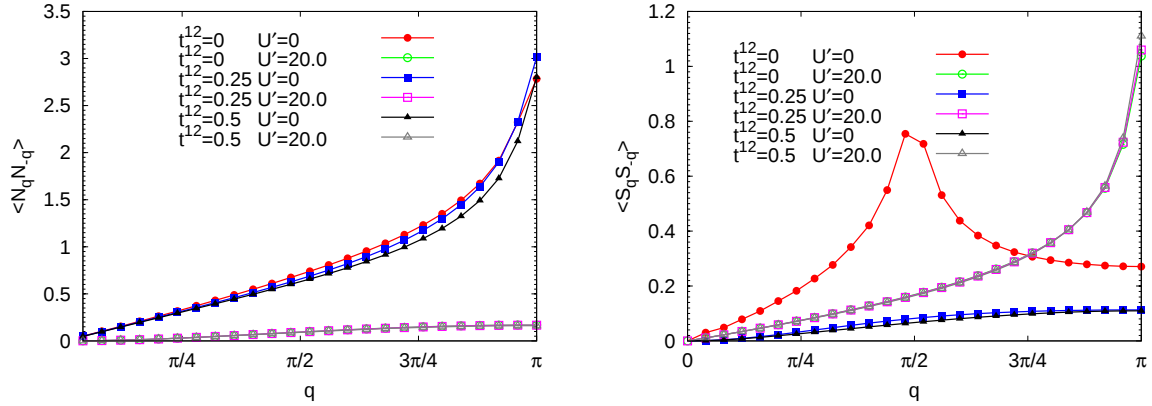


Figure 2. Fourier transforms of the density (Left panel) and spin (Right panel) static form-factors at initial ($U' = 0$) and final ($U' = 20$) points from Fig. 1 and different values of inter-orbital hopping t^{12} : $t^{12} = 0, 0.25, 0.5$. $U = 10$, $t^{11}/t^{22} = 0.5$, DMRG 50 sites.

densities and double occupancies per orbital as functions of U' at $U = 10$ and $J = (U - U')/2$. For $t^{12} = 0$, NOS occurs approximately at $U'_c = 9.4$ in qualitative agreement with Ref. [7], although in the region of $U' > U'_c$ ($J < 0$) there is a slight re-population of the otherwise empty narrow orbital. Such a re-population might be explained as the effect of the negative J Hund's exchange: the system gains more energy by populating both orbitals rather than emptying one of them. We have checked, by increasing M (not shown), that this re-population is not a DMRG artefact, and the small discrepancy between our results and those of Ref. [7] remains to be investigated. Our analysis confirm the conclusion of Ref. [7] that the quarter-filled transition is due to NOS. NOS influences inevitably the behavior of the average double occupancy per site D_i ($i = 1, 2$), as shown in the right panel of Fig.1. As U' grows for $U' < U'_c$, D_1 decreases monotonically due to the depletion of the narrow orbital. At the same time, D_2 grows due to the opposite reason and reaches the value $D_2 \approx 0.02455$ at U'_c which is very close to the Bethe-ansatz value ($D_{BA} = 0.025$ at half-filling and $U = 10$, Ref.[8]).

In order to have a deeper insight into the nature of the initial and final states involved in this transition, we have measured the static density and spin form-factors. As shown in Fig.2, in the initial state ($U' = 0$), there is a strong density correlation peaked at the wave-vector π , meaning that the density has staggered correlations. These staggered correlations are gradually suppressed at $U' > U'_c$. In such a strong-coupling regime, the wide band becomes uniformly occupied leading to an almost featureless density form-factor. The opposite picture is observed in the spin channel. At $U' = 0$ and $t^{12} = 0$, the spin form-factor exhibits a peak at $\pi/2$, implying the enhanced staggered correlations with the period of four lattice spacings, while at $t^{12} \neq 0$ the spin correlations are heavily suppressed. In the strong-coupling regime at $U' > U'_c$, only the wide orbital is active and the system resembles very much a single-band Hubbard model at half-filling. In such a case, large on-site repulsion induces strong antiferromagnetic NN correlations, as can be seen from Fig.2.

Upon switching on a finite inter-orbital hopping t^{12} , the NOS becomes incomplete, as shown in the left panel of Fig. 1. This can be understood by noting that the electrons in the narrow orbital can now reach the NN site also by making the virtual hopping through the wide orbital according to the following path: $(i, 1) \rightarrow (i + 1, 2) \rightarrow (i, 2) \rightarrow (i + 1, 1)$, where (i, α) stands for α -orbital on site i . Such an extra possibility effectively widens the narrow orbital. To better understand this widening, we have investigated the NOS when $t^{12} = 0$ and at different values of t^{11} , as shown in the left panel of Fig. 3. We have observed the full NOS for $t^{11} \lesssim 0.6$. This full

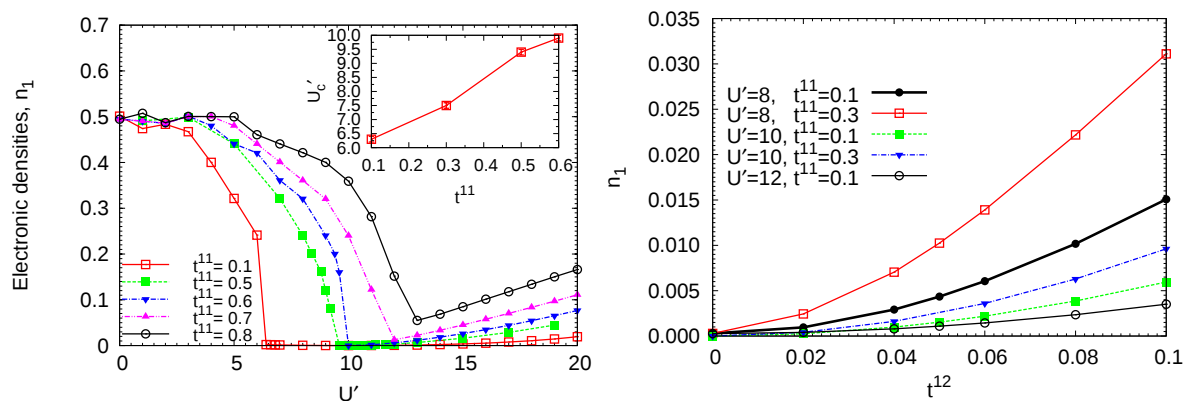


Figure 3. Left panel: U' -dependence of the narrow band occupation at $t^{12} = 0$ and different values of t^{11} . In the inset, U'_c is shown as function of t^{11} . Right panel: The narrow band occupation as function of t^{12} as the latter goes to zero at several values of U' and t^{11} .

NOS occurs at some $U'_c(t^{11})$ (shown in the inset) above which n_1 starts growing nearly linear. This situation changes drastically when $t^{12} \neq 0$. The NOS in this case is never complete even for small t^{12} , as shown in Fig. 1. In the right panel of Fig. 3 we present a study of the narrow band occupation as $t^{12} \rightarrow 0$ for different values of U' and t^{11} . We have chosen these values in such a way that there is a complete NOS at $t^{12} = 0$. It can be seen from Fig. 3 that as soon as t^{12} is finite, n_1 is never suppressed completely.

Summarizing, by using finite-system DMRG, we have studied the influence of the inter-orbital hopping t^{12} on NOS in quarter-filled two-orbital Hubbard model (2). We have found that t^{12} prevents the narrow orbital from complete suppression, by providing an additional contribution to the intra-orbital hopping. We have found that at $t^{12} = 0$, a complete NOS occurs at $U'_c(t^{11})$ for $t^{11} \lesssim 0.6$ while for greater values of t^{11} NOS is incomplete for all values of $U' \in [0, 20]$. On the contrary, our data suggest that a finite t^{12} prevents complete NOS even in case of very narrow band ($t^{11} = 0.1$). In the regime with $U' < U'_c$ we find a strong enhancement of staggered charge correlations, while in the case when $U' > U'_c$ the staggered spin correlations are favoured.

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References

- [1] S. Nakatsuji and Y. Maeno, Phys. Rev. Lett. **84** (2000) 2666.
- [2] S. Nakatsuji and Y. Maeno, Phys. Rev. Lett. **90** (2003) 137202.
- [3] K. Sreedhar, M. McElfresh, D. Perry, D. Kim, P. Metcalf and J. M. Honig, J. Solid State Chem. **110** (1994) 208.
- [4] Z. Zhang and M. Greenblatt, J. Solid State Chem. **117** (1995) 236.
- [5] Y. Kobayashi, S. Taniguchi, M. Kasai, M. Sato, T. Nishioka and M. Kontani, J. Phys. Soc. Jpn. **65** (1996) 3978.
- [6] S. R. White, Phys. Rev. Lett. **69** (1992) 2863.
- [7] S. Miyashita, Y. Yamashita, K. Yonemitsu, A. Koga and N. Kawakami, J. Phys.: Conf. Ser. **150** (2009) 042128.
- [8] F. H. L. Essler, H. Frahm, F. Göhmann, A. Klümper, and V. E. Korepin, The One-Dimensional Hubbard Model (Cambridge University Press, Cambridge, U.K., 2005).