Extended regime of coexisting metallic and insulating phases in a two-orbital electronic system

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We investigate the metal-to-insulator phase transition driven by electronic interactions in the quarter-filled Hubbard-Kanamori model on a cubic lattice with two orbitals split by a crystal field. We show that a systematic consideration of the non-local collective electronic fluctuations strongly affects the state-of-the-art picture of the phase transition provided by the dynamical mean field theory. Our calculations reveal a region of phase coexistence between the metallic and the Mott insulating states, which is missing in the local approximation to electronic correlations. This coexistence region is remarkably broad in terms of the interaction strength. It starts at a critical value of the interaction slightly larger than the bandwidth and extends to more than twice the bandwidth, where the two solutions merge into a Mott insulating phase. Our results illustrate that non-local correlations have crucial consequences on the electronic properties in the strongly correlated regime, even in the simplest multi-orbital systems.

There are two main mechanisms responsible for the formation of an insulating phase in electronic materials: a gap at the Fermi energy in the non-interacting band structure and the many-body localization induced by strong electronic interactions, as for instance the Mott scenario [1, 2]. The interplay between these different mechanisms can strongly affect the degree of electronic correlations and therefore the phase diagram for the material [3]. Both these effects are especially important when a subset of doubly- or triply-degenerate localized orbitals appears in the electronic spectrum at Fermi energy. Usually, the charge distribution on neighboring atoms lifts this degeneracy, which results in a local splitting of the orbitals called crystal field splitting. Strong electronic correlations may greatly renormalize the electronic spectral distribution, thus affecting the orbital splitting [4–7]. The crystal field splitting also has a strong influence on the Mott transition in several materials, as it favors orbital polarization and orbital selective phenomena [8–17].

The dynamical mean field theory (DMFT) [18] provides the state-of-the-art theoretical description of the Mott transition in realistic materials [19, 20]. For instance, this method captures the coexistence of metallic and insulating phases that accompanies the Mott transition in both, single-band [21–27] and multi-orbital [28–32] systems. However, in some cases DMFT is insufficient, because this theory accounts only for local correlation effects. Considering even short-range correlations beyond DMFT significantly modifies the coexistence region and drastically reduces the critical value of the interaction [26]. Long-range correlations can have even more dramatic consequences [33]. Therefore, an important leap towards an accurate theoretical description of correlated materials would be to understand the effect of non-local collective electronic fluctuations on the spectral function. Unfortunately, computational and methodological issues have hindered the detailed investigation of this problem in multi-orbital systems so far. Indeed, most of the available theoretical methods are either limited to a weakly correlated regime [34–40], or do not take into account all desired physical ingredients, such as long-range correlations [41, 42] or spatial magnetic fluctuations [43–52]. Attempts to go beyond these assumptions lead to expensive numerical calculations and thus are rather rare [53–60].

In this work, we investigate the effect of non-local fluctuations on the Mott transition in a two-orbital Hubbard-Kanamori model with the crystal field splitting and the density-density approximation for the interaction. This model is relevant for investigating the low-energy physics of some transition metal oxides [9] and fulleride molecular crystals [61]. More importantly, this model is the simplest multi-orbital system, where the influence of the orbital splitting on the Mott transition was studied in details using DMFT [6]. We challenge this solution of the problem by utilizing a relatively inexpensive diagrammatic extension of DMFT [62] – the dual triply irreducible local expansion (D-TRILEX) method [63]. This approach allows one to account for the effect of the non-local collective electronic fluctuations on the spectral function in a self-consistent manner [64, 65]. We find that, despite the apparent simplicity, the considered model displays a non-trivial behavior around the Mott transition. In particular, considering the non-local electronic correlations beyond DMFT reveals an enormously broad coexistence region of metallic and Mott insulating phases that extends from approximately the bandwidth to more than twice the bandwidth in the value of the interaction.

Method. The Hamiltonian of the considered two-orbital model on a cubic lattice

\[ H = \sum_{j \bar{j}, l, \sigma} \epsilon_{jl} c_{jl}^\dagger (\bar{c}_{j\bar{l}\sigma} + \Delta_l \delta_{j\bar{l}}) c_{j\bar{l}\sigma} + \frac{U}{2} \sum_{j, \bar{j}, \bar{l}} n_{j\bar{l}} n_{j\bar{l}} \]

contains three contributions. The hopping \( \bar{t}_{j\bar{l}} \) between lattice
sites $j$ and $j'$ describes the electronic dispersion for each of the two orbitals $l \in \{1, 2\}$. $\Delta = 2\Delta_1 = -2\Delta_2$ is the bare crystal field splitting. The interaction $U$ between electronic densities $n_{jl} = \sum_{\sigma} c_{\sigma j l}^\dagger c_{\sigma j l}$ describes both, the intra- and interorbital Coulomb repulsion. We restrict the hopping to the nearest-neighbor lattice sites and set it to $t_{(jj')} = 1/6$ for both orbitals. Hereinafter, the energy is expressed in units of the half-bandwidth of the cubic dispersion $W/2 = 6t = 1$. Calculations are performed at quarter-filling, which corresponds to the average density of $(n) = 1$ electron per two orbitals. In order to induce the orbital polarization $\delta n = (\langle n_2 \rangle - \langle n_1 \rangle)/\langle n \rangle$, we take a relatively large value for the crystal field splitting $\Delta = 0.3$. This case was studied in details in Ref. [6] using DMFT. It was demonstrated, that local electronic correlations enlarge the orbital splitting resulting in a high degree of orbital polarization. Consequently, the single electron mostly populates the lower orbital ($l = 2$) that undergoes the Mott transition at a critical value of the interaction. A similar interplay between the orbital polarization and Mott physics is also found in actual materials such as $V_2O_3$ [9] and SrVO$_3$ [66], where it is important for the Mott transition.

In order to investigate how non-local correlations affect the DMFT scenario of the Mott transition we employ the D-TRILEX method [63], where collective electronic fluctuations are treated diagrammatically beyond DMFT. This method was derived as an approximation to the dual boson theory [67–76], one of the more commonly used diagrammatic extensions of DMFT, cf. [55, 60, 77–90]. D-TRILEX method stands out for lowered complexity and its capability of correctly reproducing the results of more elaborate theories [64]. The computational simplicity of this approach allows for applications to multi-orbitals systems [91, 92].

If the system exhibits strong magnetic fluctuations, as frequently happens at half-filling, the Mott transition usually lies inside the antiferromagnetic (AFM) phase. In this case, addressing the Mott transition requires to perform calculations in a symmetry broken phase, which is problematic. Going away from half-filling suppresses the magnetic fluctuations and allows one to access the Mott transition from the paramagnetic phase. According to our calculations, the highest critical temperature for the Néel transition for the considered quarter-filled model lies below $T = 0.06$. For this reason, we set the inverse temperature to $T^{-1} = 15$, which ensures that the system is located outside the AFM phase but close to its boundary to observe strong magnetic fluctuations. We perform DMFT calculations using the w2dynamics package [93]. The D-TRILEX solution is based on the numerical implementation described in Ref. [92]. The local density of states (DOS) is obtained from corresponding local Green’s functions via analytical continuation using the ana_cont package [94].

**Spectral function.** To illustrate the effect of non-local correlations on the Mott transition, we compare the DOS predicted by DMFT and D-TRILEX methods. The result of these calculations is shown in Fig. 1 for three different values of the interaction $U = 1.8$, $U = 2.0$, and $U = 2.2$. First, let us focus on the quarter-filled calculations presented in the two upper rows of this Figure. We find that the results of the DMFT and D-TRILEX methods are different already at $U = 1.8$. In both cases, the DOS is metallic. The lower orbital ($l = 2$, red line) displays a three-peak structure consisting of the quasi-particle peak at Fermi energy $E = 0$ and two side peaks that correspond to lower and upper Hubbard bands (LHB and UHB). The upper orbital ($l = 1$, blue line) also exhibits the quasi-particle peak in the DOS that appears close to the Fermi energy at $E = \Delta$. However, the three-peak structure predicted by DMFT possesses a high degree of electron-hole symmetry. Instead, the DOS of obtained for the same orbital ($l = 1$) using the D-TRILEX approach resembles the DOS of a hole-doped Mott insulator with the quasi-particle peak being shifted closer to the LHB [18]. The quasi-particle peaks in the DOS of DMFT vanish simultaneously between $U = 1.8$ and $U = 2.0$, which signals the tendency towards a Mott insulating state. A further increase of the interaction decreases the electronic density at Fermi energy $A(E = 0)$. The latter
reaches zero at $U_c^* \approx 2.2$ (blue line in Fig. 2), and the DMFT solution enters the Mott insulating phase. On the contrary, the D-TRILEX solution remains metallic for the discussed values of the interaction (middle row in Fig. 1). Thus, even at $U_c^*$ it reveals pronounced quasi-particle peaks in the DOS for both orbitals. Fig. 2 shows that $A(E = 0)$ in the metallic D-TRILEX solution also decreases upon increasing the interaction. However, this solution turns into a Mott insulator only at a very strong critical interaction $U_c \approx 4.5$, which is larger than twice the bandwidth. This result seems surprising, since in the single-orbital case the non-local correlations lead to a more insulating electronic behavior [26], as correctly captured by the D-TRILEX method [63].

To explain the observed effect, we note that quarter-filling in DMFT and D-TRILEX corresponds to different values of the chemical potential. The left panel of Fig. 3 shows that at $U \geq 1.5$ the chemical potential $\mu$ of D-TRILEX (red dots) significantly deviates from the $\mu^d$ of DMFT (blue dots), and this difference increases with the interaction. We point out that D-TRILEX calculations are based on the DMFT solution of the local impurity problem that plays the role of reference system [63, 64]. We find that the quarter-filled metallic D-TRILEX solution originates from the metallic reference system that has smaller average density. Fig. 4 shows that due to $(n) < 1$ the reference system (dashed lines) remains metallic even at $U_c^*$. At the same time, the DOS predicted by D-TRILEX (solid lines) is not dramatically different from the one of the reference system. This fact suggests that the effect of non-local collective electronic fluctuations in the metallic regime consists in moving the spectral weight from above to below the Fermi energy, which brings the filling of the system to $(n) = 1$. Consequently, such redistribution of the orbital occupation decreases the orbital polarization $\delta n$ compared to DMFT, which is demonstrated in the left panel of Fig. 3.

To confirm this statement, we perform D-TRILEX calculations for the chemical potential $\mu^d$ of the quarter-filled DMFT solution. The corresponding result is shown in the bottom row of Fig. 1 and is referred to as the D-TRILEX* calculation in order not to confuse it with the metallic solution. We observe that the obtained DOS is again practically identical to the one of DMFT (bottom vs. top row in Fig. 1). However, the D-TRILEX* calculations performed in the regime $1.0 \leq U < 2.2$ where DMFT solution is metallic correspond to $(n) > 1$. Moreover, no quarter-filled D-TRILEX* solution is found near $\mu^d$ in this regime of interactions. This fact supports our previous finding that in the metallic regime non-local correlations increase the average density of the considered two-orbital system.

This physical picture changes when the DMFT solution becomes Mott insulating. We find that the corresponding D-TRILEX* solution undergoes the Mott transition at the same critical interaction $U_c^*$ as in DMFT (bottom right panel of Fig. 1). Moreover, at $U \geq U_c^*$ the average density for the D-TRILEX* solution becomes $(n) = 1$ for $\mu^* \approx \mu^d$ (bottom left panel of Fig. 3). Right panel of Fig. 3 shows that the insulating DMFT and D-TRILEX* solutions are almost fully polarized and have approximately the same value of $\delta n$, which results in electron-hole symmetric DOS for the lower orbital (top and bottom left panels of Fig. 3). Consequently, the upper orbital becomes nearly unoccupied and thus cannot strongly interact with the lower one. For this reason no transfer of the spectral weight between the orbitals by means of the non-local fluctuations occurs in the insulating regime. At $U \geq U_c^*$
the D-TRILEX $^*$ solution remains quarter-filled and Mott insulating, which is confirmed by the zero electronic density at Fermi energy (red asterisks in Fig. 2). Therefore, both, the DMFT and the D-TRILEX methods predict the Mott transition for the considered system at the same value of the critical interaction $U^*_c$. However, including non-local collective electronic fluctuations beyond DMFT allows one to additionally capture the metallic solution that coexists with the Mott insulating one up to the second critical interaction $U^*_c$.

The phase coexistence is signalled by the appearance of two different values of the chemical potential $\mu$ and $\mu^*$ leading to the same average density $\langle n \rangle$, as demonstrated in the left panel of Fig. 3. If we follow the $\mu(U)$ curve that gives $\langle n \rangle = 1$ in the weak coupling regime (red dots), we obtain the metallic solution until it continuously turns into an insulating phase at $U^*_c$. Above this threshold, any value of the chemical potential inside the Mott gap gives the same average density, and the two solutions corresponding to $\mu$ and $\mu^*$ can be considered equivalent from there on. On the other hand, if we start from the chemical potential $\mu^*$ that corresponds to the insulating phase and decrease the interaction following the condition $\langle n \rangle = 1$, we obtain the insulating solution (red asterisks). The latter exists until the critical interaction $U^*_c$ below which no solution for $\mu^* \approx \mu^d$ is available at quarter-filling. At this value of the interaction the hysteresis loop is abruptly connected to the metallic solution with a jump. This behavior means that the function $\langle n \rangle(\mu)$ is not monotonic and exhibits a region of negative charge compressibility $\kappa = \frac{1}{\langle n \rangle^2} \frac{d\langle n \rangle}{d\mu}$. According to our calculations, the metallic and insulating D-TRILEX solutions are both characterized by $\kappa > 0$, hence they are thermodynamically stable and are separated by a region of negative charge compressibility. A similar behavior was found in DMFT solution of the Hubbard-Kanamori model for small doping around half-filling [95–99], and for different parameters using a strong-coupling expansion [97].

Conclusions. We investigated the effect of non-local collective electronic fluctuations on the Mott transition in a two-orbital quarter-filled Hubbard-Kanamori model by comparing the results of the D-TRILEX and DMFT methods. At the considered temperature, the DMFT solution of the problem remains metallic below the critical interaction $U^*_c = 2.2$, and at this value of the interaction undergoes the Mott transition. We find that the inclusion of non-local correlations by means of the D-TRILEX approach stabilizes the metallic phase up to the very large critical interaction $U^*_c = 4.5$. The D-TRILEX method also captures the Mott transition at $U^*_c$ as a second stable solution. This leads to a remarkably broad coexistence region between the metallic and the Mott insulating phases that exist at the same filling, but with different values of the chemical potential between the $U^*_c$ and the $U^*_c$ critical interactions. Our results show that already for a simple two-orbital model DMFT cannot correctly interpolate between the moderately- and strongly-interacting regimes. This fact bring an interesting evidence that non-local correlations in multi-orbital systems may lead to non-trivial effects due to the presence of additional channels for collective electronic fluctuations.

As the considered model was proposed for a low-energy description of some realistic materials [9, 61], the coexistence of metallic and Mott insulating phases could be detected experimentally, for example by measuring dielectric properties of the system [100]. One can speculate that the observed phase coexistence could be exploited in the realization of Mott-based electronic switches or transistors. The experimental realization of Mott field effect transistors (MottFET) was shown to be practically viable [66, 101, 102]. The region of negative charge compressibility between the two stable solutions could forbid the spontaneous switch between the two solutions. In this case, application of a static electric field should be sufficient to drive the transition between the metallic and Mott insulating phases, as this perturbation would effectively change the chemical potential from $\mu$ to $\mu^*$ or vice versa.

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