Dynamical Cluster Approximation Study of the Anisotropic Two-Orbital Hubbard Model

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We investigate the properties of a two-orbital Hubbard model with unequal bandwidths on the square lattice in the framework of the dynamical cluster approximation (DCA) combined with a continuous-time quantum Monte Carlo algorithm. We explore the effect of short-range spatial fluctuations on the nature of the metal-insulator transition and the possible occurrence of an orbital-selective Mott transition (OSMT) as a function of cluster size N_c. We observe that for $N_c = 2$ no OSMT is present, instead a band insulator state for both orbitals is stabilized at low temperatures due to the appearance of an artificial local ordered state. For $N_c = 4$ the DCA calculations suggest the presence of five different phases which originate out of the cooperation and competition between spatial fluctuations and orbitals of different bandwidths and an OSMT phase is stabilized. Based on our results, we discuss the nature of the gap opening.

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The correlation driven metal-insulator transition in two-dimensional (2D) correlated systems is still poorly understood. While the behavior of 2D one-band systems at half filling seems to be settled, this is not the case for multi-orbital systems. In one-band systems, long range correlations or local order in small size clusters caused by perfect nesting (Slater physics) [1–4] open a gap in the weak-coupling regime, whereas in the strong-coupling regime the on site Coulomb repulsion is the driving force for the gap opening (Mott physics) [5]. On the other hand, even though multiorbital models are better suited to describe real materials [6] and display rich phase diagrams [7–9] as well as interesting physics like the orbital-selective Mott transition (OSMT) [10,11], they are still under debate. The reason for that is their more complex structure compared to the one-band model due to the orbital degrees of freedom, crystal field splitting effects, and the Hund's rule exchange coupling. This situation gives us a strong motivation to investigate the two-orbital system.

The OSMT has recently been intensively studied in the context of a weakly correlated band coexisting and interacting with a more strongly correlated one in a two-orbital system [12–20]. Issues like (1) the importance of full or Ising-type Hund's rule coupling [12,14,16,18], (2) the consequences of anisotropic Hund's rule coupling [19], (3) the role of the ratio of the two bandwidths [15], (4) the inclusion of the hybridization between bands [13], (5) the effect of crystal field splitting [17], and (6) the extension to the three-band case [21] have already been addressed. Nevertheless, the importance of spatial fluctuations has not yet been explored since most calculations have been performed within the single-site dynamical mean field theory (DMFT) [22,23] where spatial fluctuations are completely ignored. On the other hand, it has already been noticed that even in a single-band case, inclusion of spatial correlation will qualitatively change the scenario of the Mott metal-insulator transition [4,24,25]. Therefore, it is crucial to address the effect of spatial fluctuations on the OSMT and the phase diagram.

Very recently, Bouadim *et al.* [20] studied the OSMT by means of a determinant quantum Monte Carlo method (DQMC) on the square lattice and showed that an itinerant band can coexist with a fully localized band in a two-orbital Hubbard model as long as long range antiferromagnetic correlation is absent. However, since the DQMC calculation was based on a simplified model where one of the two orbitals is constrained to be fully localized, it still remains unclear whether the OSMT survives in the system with spatial fluctuations or not. Moreover, since previous DMFT [12–19] and a slave spin mean field calculation [21] are based on the Bethe lattice, it is interesting to move in the direction of real systems by studying the case of a two-dimensional model on the square lattice with the Fermi level at a van Hove singularity at half filling.

In this Letter we concentrate on the nature of the gap opening and the OSMT in a two-dimensional system. The anisotropic two-orbital Hubbard model on the square lattice at half filling is the simplest model which can describe the OSMT including spatial fluctuations. The Hamiltonian is given as

$$H = -\sum_{\langle ij\rangle m\sigma} t_m c^{\dagger}_{im\sigma} c_{jm\sigma} + U\sum_{im} n_{im\uparrow} n_{im\downarrow} + \sum_{i\sigma\sigma'} (U' - \delta_{\sigma\sigma'} J_z) n_{i1\sigma} n_{i2\sigma'}, \quad (1)$$

where t_m for orbital $m = (1, 2)$ denotes the hopping integrals between nearest-neighbor (NN) sites i and j, U and U' are intraorbital and interorbital Coulomb repulsion in-

tegrals, respectively, and $J_z n_{i1\sigma} n_{i2\sigma}$ for spin σ is the Ising-type Hund's rule coupling term. In our calculations we ignore spin-flip and pair-hopping processes. We also set $t_1/t = 0.5$ (narrow band), $t_2/t = 1.0$ (wide band), $J_z = U/4$ and $U' = U/2$. For this model we employ the dynamical cluster approximation (DCA) method with cluster sizes $N_c = 2$ and 4. The DCA method [26–28] can not only overcome the problem of the single-site DMFT method [22,23], where Mott physics rather than Slater physics is emphasized in the paramagnetic phase due to the lack of spatial fluctuations, but it is also computationally cheaper than lattice calculations. We use a weak-coupling continuous-time quantum Monte Carlo algorithm as an impurity solver [29,30]. We shall present results on the spin-spin correlations, double occupancy, self-energy, and density of states (DOS).

First, let us discuss the results obtained from the DCA with a two-site cluster ($N_c = 2$). It is known that, for a one-band system at low temperatures, the formation of a local singlet state driven by Slater physics is responsible for the gap opening. In the two-band system orbital fluctuations are present. Because of the Hund's rule coupling and the Coulomb interaction, ferromagnetic (FM) correlation between orbitals and antiferromagnetic (AFM) correlation between sites develop. In order to check for these correlations we measure the on site (intersite) interorbital spin-spin correlations $\langle S^z_{i,1} S^z_{i,2}\rangle$ ($\langle S^z_{i,1} S^z_{i+1,2}\rangle$) as a function of U/t. The results are shown in Fig. 1(a).

As the Hund's rule coupling $J_z = U/4$ is increased, the on site interorbital FM correlations (positive sign) and intersite interorbital AFM correlations (negative sign) are enhanced for both temperatures $T/t = 0.3$ and $T/t = 0.1$. At high temperatures $T/t = 0.3$ the on site interorbital FM correlations are stronger than the intersite interorbital AFM correlations which can be attributed to the fact that thermal fluctuations suppress the AFM correlations. At $T/t = 0.1$ both correlations are of the same magnitude. This behavior suggests the appearance of a local ordered state in the low temperature regime. In order to verify whether this state, in analogy to the one-band model, is responsible for the gap opening as described by Slater physics, we calculate the temperature dependence of double occupancy for both orbitals. If Slater physics is dominant, as the temperature is decreased the formation of the local order which reduces the potential energy $U\langle n_\uparrow n_\downarrow\rangle$ should cause the gap opening. In Fig. 1(b) we present the double occupancy as a function of temperature T/t for $U/t = 2.4$. The double occupancy in both bands decreases with decreasing temperature and it shows a more abrupt drop near $T/t = 0.2$. This behavior gives strong evidence of Slater physics, and the band insulator in both orbitals should be present at zero temperature for all positive interaction strengths U/t.

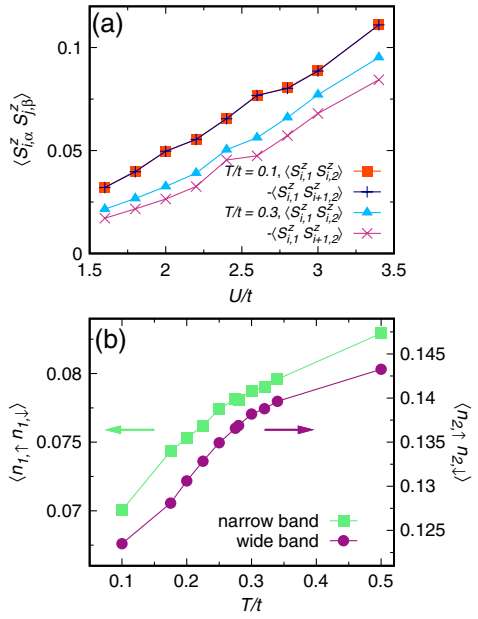

FIG. 1 (color online). (a) On site and intersite interorbital spin-spin correlations for $N_c = 2$ as a function of U/t at temperatures $T/t = 0.1$ and $T/t = 0.3$. (b) Double occupancy for $N_c = 2$ as a function of T/t for $U/t = 2.4$. Left and right axes are for the double occupancy of the narrow band and the wide band, respectively.

Next, we explore the DCA for a four-site cluster ($N_c = 4$). The inclusion of next nearest-neighbor (NNN) correlations in $N_c = 4$ suppresses the local ordered state enhanced artificially in the $N_c = 2$ cluster. In addition, the system shows a weak degree of frustration because of the absence of long range correlations. In this way, the Mott physics present in the single-site systems coexists with Slater physics present in the two-site systems. Therefore we believe that the description in terms of the $N_c = 4$ clusters is closer to the real materials at finite temperature. In Fig. 2(a) we compare the on site and intersite interorbital spin-spin correlation results for $N_c = 2$ and 4 for $T/t = 0.1$. The same magnitude of both correlations for $N_c = 2$ implies the presence of a relatively strong intersite local ordered state, while the deviation of those for $N_c = 4$ indicates that the local ordered state is released due to the influence of the NNN correlations. In order to compare directly the strength of this local ordered state for $N_c = 2$ and 4, we plot NN and NNN correlations for the narrow band in Fig. 2(b). In the weak-coupling regime the NN correlation strength for $N_c = 2$ due to enhanced Slater physics is larger than that for $N_c = 4$. In the strong-coupling regime the NN correlation strength is similar for $N_c = 2$ and 4 since the insulating state for $N_c = 4$ is induced by cooperation of Mott and Slater physics. We also find strong NNN correlations for $N_c = 4$.

The competition among magnetic and orbital fluctuations as well as weak frustration for $N_c = 4$ should generate a rich phase diagram. In order to investigate this complex situation we analyze, in what follows, the on site self-energy. The imaginary part of the on site self-energy $\mathrm{Im}\Sigma(i\omega_n)$ provides information about the possible Fermi-liquid or non-Fermi-liquid behavior of the system as well as the nature of the gap opening. In Figs. 3(a) and 3(b)

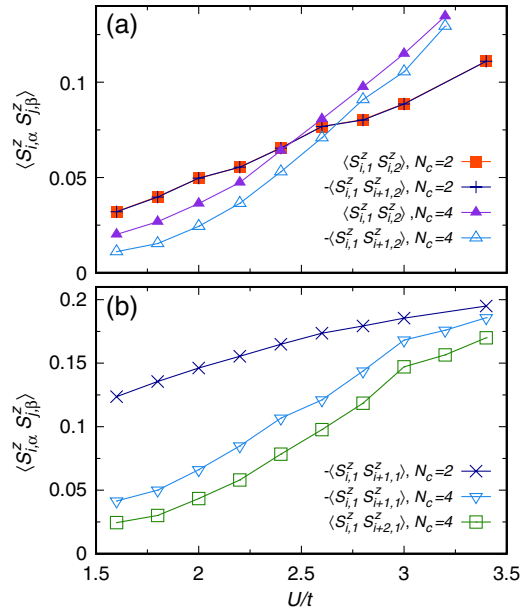

FIG. 2 (color online). (a) The on site (intersite) interorbital spin-spin correlations for $N_c = 2$ and 4 as a function of U/t at $T/t = 0.1$. (b) The narrow band (next) nearest-neighbor spin-spin (NNN, NN) correlations for $N_c = 2$ and 4 as a function of U/t at $T/t = 0.1$.

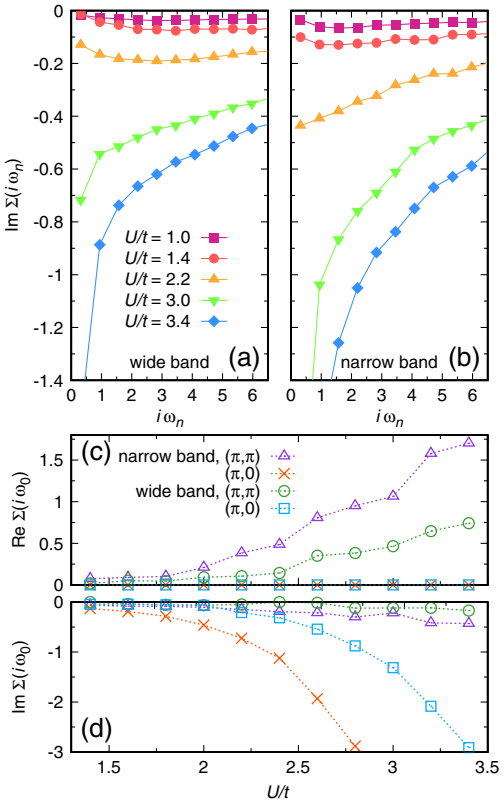

FIG. 3 (color online). The imaginary part of the on site self-energy for $U/t = 1.0, 1.4, 2.2, 3.0, 3.4$ at $T/t = 0.1$ for $N_c = 4$ (a) in the narrow band and (b) in the wide band. The real (c) and imaginary (d) part of self-energy at the lowest Matsubara frequency ω_0 for $K = (\pi, \pi)$ and $(\pi, 0)$ sectors as a function of U/t.

we present $\mathrm{Im}\Sigma(i\omega_n)$ for the narrow and wide band, respectively, at $T/t = 0.1$. According to Fermi-liquid theory, $\mathrm{Im}\Sigma(\omega)$ at $T = 0$ at $\omega \to 0$ extrapolates to 0. In the weak-coupling regions below $U/t = 1.4$ this Fermi-liquid behavior is seen in both bands. Between $U/t = 1.4$ and 1.8 Fermi-liquid behavior is still present in the wide band, while non-Fermi-liquid behavior is observed in the narrow band. The electrons begin to localize in the narrow band driven by both Slater and Mott physics, while those in the wide band are still delocalized. As the interaction is increased, non-Fermi-liquid behavior is observed in both bands. At $U/t = 2.8$, $\mathrm{Im}\Sigma(i\omega_n)$ in the narrow band diverges, which indicates the opening of a gap, while the metallic state (non-Fermi liquid) is still present in the wide band. These results evidence a OSMT. In the strong-coupling region $U/t = 3.4$ the insulating state is observed in both bands.

In what follows we shall analyze the nature of the gap opening. According to recent results obtained for the single-band plaquette Hubbard model [25], momentum sectors $K = (0, 0)/(\pi, \pi)$ and $(\pi, 0)/(0, \pi)$ undergo a metal to band insulator transition and a metal to Mott insulator transition, respectively. In Figs. 3(c) and 3(d), respectively, we present the real and imaginary parts of the self-energy at the lowest Matsubara frequency ω_0, $\mathrm{Re}\Sigma(i\omega_0)$ and $\mathrm{Im}\Sigma(i\omega_0)$, for $K = (\pi, \pi)$ and $(\pi, 0)$ in both bands. While $\mathrm{Re}\Sigma(i\omega_0)$ gives information about the energy shift of the spectral function, $\mathrm{Im}\Sigma(i\omega_0)$ introduces the scattering rate. As the interaction is increased, $\mathrm{Re}\Sigma_{(\pi,\pi)} = -\mathrm{Re}\Sigma_{(0,0)}$ increases while $\mathrm{Im}\Sigma_{(\pi,\pi)} = \mathrm{Im}\Sigma_{(0,0)}$ remains small in both bands. These results suggest a metal to band insulator transition where the gap is opened through separation of the poles away from the Fermi level. On the other hand, as the interaction increases $\mathrm{Im}\Sigma_{(\pi,0)} = \mathrm{Im}\Sigma_{(0,\pi)}$ displays a divergent behavior and $\mathrm{Re}\Sigma_{(\pi,0)} = -\mathrm{Re}\Sigma_{(0,\pi)}$ in both bands is zero due to particle-hole symmetry. Therefore, in the strong-coupling region, the gap in the $K = (\pi, 0)$ and $(0, \pi)$ sectors is only induced by the divergence of $\mathrm{Im}\Sigma(i\omega_0)$ which is a signature for Mott

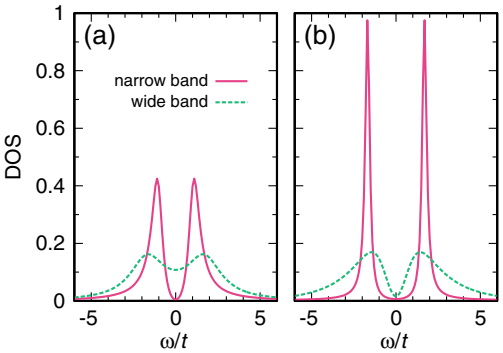

FIG. 4 (color online). Density of states at $T/t = 0.1$ and $N_c = 4$ for (a) $U/t = 2.8$ and (b) $U/t = 3.4$. We employ the Padé approximation method for the analytic continuation.

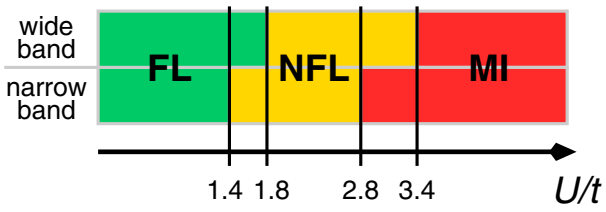

FIG. 5 (color online). The phase diagram with five phases for $N_c = 4$.

physics. These results are similar to the single-band plaquette Hubbard model results [25] but, while a first-order transition occurs in the single-band Hubbard model, the OSMT behavior is present in the two-band Hubbard model. In order to show the OSMT more clearly, we present in Fig. 4 the density of states (DOS) at $T/t = 0.1$ for the interaction values $U/t = 2.8$ [Fig. 4(a)] and $U/t = 3.4$ [Fig. 4(b)]. These interaction values have been identified as onsets for the OSMT and insulator phases, respectively. For $U/t = 2.8$ the narrow band exhibits a gap at the Fermi energy ($\omega = 0$), while the wide band has a finite DOS at $\omega = 0$. This means that for a given interaction strength U/t two stages of the Mott transition are present, with a Mott insulator in the narrow band and a metal in the wide band. At $U/t = 3.4$ both bands show a gap at $\omega = 0$. The gap in the narrow band is wider than that in the wide band. Finally, we plot the phase diagram with the identified five phases for $N_c = 4$ in Fig. 5.

In summary, we have explored the anisotropic two-orbital Hubbard model using the DCA method with cluster sizes $N_c = 2$ and 4. The DCA cluster with $N_c = 2$ for the single-band model is known to describe a system with artificially strong local order between sites and the gap opening is controlled by Slater physics. Our results show that this intersite AFM correlation is still strong in spite of orbital fluctuations, leading to a gap at low temperatures. The appearance of the insulating states can be described by Slater physics. We have also investigated within DCA the $N_c = 4$ cluster which includes NNN correlations. Unlike the $N_c = 2$ cluster, the local ordered states are not present in the weak-coupling limit. In the very weak-coupling regime Fermi-liquid behavior is present in both bands. As the interaction increases, the electrons in the narrow band weakly localize and non-Fermi-liquid behavior is observed, even though the Fermi-liquid behavior is still present in the wide band. In the intermediate region, non-Fermi-liquid behavior is observed in both bands. In the strong-coupling region the electrons in the narrow band are completely localized and those in the wide band are partially localized which can be described as the OSMT. In the very strong-coupling region both orbitals are insulating. The nature of the gap opening is that of coexisting Slater physics in the momentum sector $K = (0, 0)/(\pi, \pi)$ and Mott physics in momentum sector $K = (\pi, 0)/(0, \pi)$.

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