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Effects of non-local spin fluctuations in the orbital-selective Mott transition

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Abstract. Employing the extended dynamical mean field theory (EDMFT) and the quantum Monte Carlo (QMC) method, we investigate the effect of the spatial fluctuations in the two-band Hubbard model with anisotropic bandwidth in the vicinity of the Mott metal-insulator transition. At half filling, we demonstrate that while the inclusion of the non-local spin-spin interaction amounts to enhancing the correlation and suppressing the metallic character, the orbitally selective Mott transition (OSMT) remains stable for various strengths of the non-local correlation. The same is true when the system is doped away from half filling. The OSMT phase is evidenced at low dopant concentration and the simultaneous metallic phase emerges at overdoped regime. From the analysis of the self energy, it follows that the nature of the metallic phase upon doping violates the Fermi liquid character and persists at considerably large doping. Our theory also offers a new perspective for the investigation of the non-local fluctuation in the multi-orbital system within the single-site scheme.

1 Introduction

One of the most fundamental aspects of the physics of the strongly correlated electron systems is the Mott transition; the transition from metallic onto the insulating phase upon the variation of the pressure or the addition of doping. Much of today's understanding of this behavior has been based on the single-band Hubbard model which is known to be the simplest representation of the correlated system yet constitutes of the non-trivial many body problems. In this model, there are two well-known descriptions for the metal-insulator transition (MIT) namely the Gutzwiller approximation and the Mott-Hubbard scheme. The former corresponds to the regime where the scale of the kinetic energy is larger than that the electron-electron interaction while the latter describes the opposite case. Both approaches, however, fail to provide a full account of the evolution of the Mott transition that generally requires a non-perturbative treatment. An important step in the study of the Mott transition is marked by the development of the dynamical mean field theory (DMFT) that unifies both weak and strong coupling description. In this scheme, the MIT mechanism is shown to be disentangled from any magnetic ordering and the effects of correlation are manifested in the dynamical local fluctuation. The lattice Hamiltonian can be thus mapped onto its corresponding impurity system which is supplemented by the self-consistent equations [1].

The single band Hubbard model is, however, inadequate for describing the electronic structure of most of the transition metal oxides that exhibit multiple orbital structures at low energy. It has been long suggested that the interplay of the orbital effects and the electronic correlation is a key factor responsible for various intriguing properties such as the colossal magnetoresistance in the manganese oxide or the superconductivity in the iron pnictides (see e.g. [2–4]). The orbital degeneracy has been also realized to play a crucial role in the nature of Mott transition of several d- or f-bands such as the ruthenates oxide $Ca_{2-x}Sr_xRuO_4$ that consists of multiple bands with anisotropic bandwidth [5,6]. In this system, the metal insulator transition is suggested to be orbitally dependent meaning that there is a possible coexistence of the localized and the itinerant character as a function of the Coulomb interaction [7].

Theoretical investigation of the novel Mott transition in the ruthenates, has been extensively performed in the last few years by various schemes e.g. the DMFT, the slave spin particle and the combination between the local density approximation and the DMFT (LDA+DMFT) [7–15]. The anisotropic multiorbital system is typically represented by three- or two-band Hubbard Hamiltonian that takes account of the Hund's coupling. The contribution of the spin-flip and the pair terms on the other hand is neglected and is argued to play a minor role. In these works, the OSMT is evident at half filling as a function of U/W where the gap in the narrow band coexists with the finite spectral weight in the wide band. The origin of this

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behavior has been argued to be related to the interplay between the correlation and the bandwidth which results in the different strength of the correlation of each band. The same behavior was recently shown to hold also when the system is driven away from half filling, at low doping concentration. It is demonstrated that while the wide band indicates the metallic character upon doping, the narrow band remains pinned at the insulating state [16–18].

The nature of the OSMT is, however, not yet fully clarified and there have been conflicting results among theories and with experiments (see e.g. [19–21]). It is argued recently that the correlation of the wide band should be more substantial than that the other band following the fact that there is a strong mass renormalization and disappearance of the Fermi sheet of the d_{xy} band at $x = 0.2$ [20]. A new LDA+DMFT calculations on Ca_2RuO_4 have also indicated the absence of OSMT when the concentration of doping is changed [21]. Further studies are therefore needed to better understand the underlying mechanism of OSMT and to resolve these discrepancies. From a theoretical perspective, one of the most crucial tasks is to investigate various aspects that have been abandoned in the previous works using the mean field approximation. An interesting example in this context is the contribution of the non-local correlation which is known to play an essential role in various correlated systems.

In recent years, there have been some attempts to address the effect of the non-local correlation in the anisotropic two-band system. Bouadim et al. studied the Kondo lattice Hamiltonian which incorporates the on-site Coulomb interaction [22]. They imagined a system in which one of the band has been fully localized while the other remains itinerant. The model is solved by using the determinant quantum Monte Carlo (DQMC) on the lattice of size 8×8. Their main finding is that the OSMT robust at half filling following the fact that the single-particle spectral function of the itinerant band exhibits a metal-insulator transition as a function of local interaction. This argument is supported by the results of the CDMFT which is combined with the continuous time quantum Monte Carlo (QMC) [23,24]. Here, the OSMT is observed at half filling for cluster size $N_c = 4$ and the calculated phase diagram resembles those obtained by DMFT. In addition to this, it is also pointed out that the stability of the OSMT phase depends on the size of the cluster. For $N_c = 2$, MIT occurs simultaneously on both bands which is argued due to the strong antiferromagnetic fluctuations.

Since both DQMC and CDMFT calculations were performed at considerably small lattice/cluster size, it remains difficult to draw a general conclusion on the stability of the OSMT phase in the presence of the spatial correlation. This is due to the fact that the choice of the coarse graining and the cluster size may bias the interpretation of the underlying physics involved. This is evident in the single-band two dimensional Hubbard model studied by cluster DMFT for various cluster sizes. It is demonstrated that the quasiparticle peak collapses gradually as a function of cluster size and the gap will be realized at large cluster regardless of the magnitude of the Coulomb coupling. The MIT is thus argued as a result of the synergism between the short-ranged order and the formation of the local moment [25]. Whether the same is true for the multiple orbitals system, is presently unknown and requires further investigation.

Motivated by the above observations, in the present work, we discuss the role of spatial fluctuation in the anisotropic two-band system from a new perspective using the extended dynamical mean field theory (EDMFT). In this scheme, the contribution of the non-local correlation enters from the inter-site interaction and the whole lattice problems can be evaluated in the framework of the single-site impurity problem [26–29]. This approach allows one to systematically study the stability of the OSMT phase at different strength of the spatial fluctuation by varying the energy scale of the non-local interaction or the type of the inter-site interaction. The present work therefore provides a more refined interpretation on the role of the spatial fluctuation and also demonstrates a new alternative for the treatment of the non-local correlation in the multiorbital system.

The organization of the paper is as follows. We discuss in the next section the reference model and the method of solution. This is then followed by the presentation of the main results started at half-filling and then doped insulating state. The last section contains concluding remarks.

2 Model and method

We consider the two-band Hubbard model with band-specific hopping amplitude t_α and the Ising type Hund's coupling J which is a minimal model for the description of the orbital selective Mott transition (OSMT). In the present case, the Hubbard Hamiltonian is supplemented by the inter-site spin interaction with coupling I from which the non-local contribution enters in the EDMFT approximation. With this caveat in mind, the extended two-band Hubbard Hamiltonian in the standard notation reads

$$H = -\sum_{ij\alpha\sigma} t_{ij\alpha} c^\dagger_{i\alpha\sigma} c_{i\alpha\sigma} + U \sum_{i\alpha} n_{i\alpha\uparrow} n_{i\alpha\downarrow} + \sum_{i\sigma\sigma'} (U' - \delta_{\sigma\sigma'} J) n_{i1\sigma} n_{i2\sigma'} + \sum_{i\neq j\alpha} I_{ij\alpha} \mathbf{S}_{i\alpha} \cdot \mathbf{S}_{j\alpha} \quad (1)$$

where U and U' denote the on-site and the inter-band interactions. Here, the orbital and the spin index are noted by α and σ respectively.

The derivation of the EDMFT equations in the multi-orbital system can be done straightforwardly by following the steps outlined in references [26–30]. In what follows, we first express the single-site effective action in the absence of the long-range order formation (i.e. paramagnetic phase). By using the standard cavity method and introducing the Hubbard-Stratonovich field $\phi_{\alpha\gamma}$ (γ denotes the bosonic modes) to decouple the inter-site spin interaction

one readily obtains

$$\begin{aligned} S_{eff} = &- \int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \sum_{\alpha\sigma} c^\dagger_{\alpha\sigma}(\tau_1)\mathcal{G}^{-1}_{0\alpha\sigma}(\tau_1-\tau_2)c_{\alpha\sigma}(\tau_2) \\ &+ \int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \sum_{\alpha\gamma} \phi_{\alpha\gamma}(\tau_1)\chi^{-1}_{0\alpha\gamma}(\tau_1-\tau_2)\phi_{\alpha\gamma}(\tau_2) \\ &+ \int_0^\beta d\tau U \sum_\alpha n_{\alpha\uparrow}(\tau)n_{\alpha\downarrow}(\tau) \\ &+ \int_0^\beta d\tau \sum_{\alpha\gamma} \phi_{\alpha\gamma}(\tau)\mathbf{S}_\alpha(\tau) \\ &+ \sum_{\sigma\sigma'} \left[U' - \delta_{\sigma\sigma'}J\right] n_{1\sigma}(\tau)n_{2\sigma'}(\tau). \end{aligned} \tag{2}$$

where $\mathcal{G}_0$ is the dynamical Weiss field that takes account of the temporal fluctuations of the hopping of electrons between the local and the rest of the sites while $\chi_{0\gamma}$ corresponds to the two-particle bath that represents the bosonic fluctuations generated by the local moments at all other sites

The full-interacting Green's function of (2) can be expressed in terms of the self energy which becomes local in the limit of the large dimension. By denoting $\Sigma_\alpha(i\omega_n)$ as the single-particle self energy and $\Pi_{\alpha\gamma}(i\omega_m)$ for the two-particle self energy, one writes

$$\mathcal{G}_\alpha(i\omega_n) = \int_{-W}^{W} d\epsilon \frac{D_\alpha(\epsilon)}{i\omega_n + \mu - \epsilon - \Sigma_\alpha(i\omega_n)}, \tag{3}$$

$$\chi_{\alpha\gamma}(i\omega_m) = \int_{-I}^{I} d\epsilon \frac{\rho_{\alpha\gamma}(\epsilon)}{\Pi^{-1}_{\alpha\gamma}(i\omega_m) + \epsilon}, \tag{4}$$

where $\omega_n = (2n+1)\pi/\beta$ and $\omega_m = 2m\pi/\beta$ denote the Matsubara frequencies for fermions and bosons respectively. In the above equations, $D_\alpha(\epsilon)$ and $\rho_{\alpha\gamma}(\epsilon)$ denote the density of the states (DOS) for the single- and the two-particle sectors respectively which record the structure of the lattice. Having obtained these relations, it is then straightforward to show that the full-interacting Green's function and the local quantities satisfy the Dyson type equation reads

$$\mathcal{G}^{-1}_\alpha(i\omega_n) = \mathcal{G}^{-1}_{0\alpha}(i\omega_n) - \Sigma_\alpha(i\omega_n), \tag{5}$$

$$\chi^{-1}_{\alpha\gamma}(i\omega_m) = \Pi^{-1}_{\alpha\gamma}(i\omega_m) - \chi_{0\alpha\gamma}(i\omega_m). \tag{6}$$

In practice, the EDMFT approach consists of solving the effective action of equation (2) that is complemented by the self-consistent relations of equations (3)–(6). It is during this steps that the renormalization effects of the nonlocal correlation enter in the single-particle quantities. We shall further elaborate this point below.

In order to evaluate the effective action of equation (2), we employ the auxiliary field quantum Monte Carlo (QMC) within the Hirsch-Fye scheme which has been adapted to take into account the fermionic and the bosonic degrees of freedom [16,31,32]. To this end, we discretize the continuous time variable in the action of equation (2) into L time slices τ of length $\Delta\tau = \beta/L$ and then perform the discrete Hubbard-Stratonovich transformation on the density-density interaction part. The latter amounts to introducing the auxiliary Ising-like fields $s_l, l = 0, \ldots, L-1$ such that the effective action eventually depends on the fermionic variables and can be integrated out. The resulting partition function reads

$$Z = \sum_{s_{\alpha\sigma},\phi_{\alpha\gamma}} \left[\prod_\sigma \det[G^{-1}_{\alpha\sigma}(s_{\alpha\sigma}(\tau),\phi_{\alpha\gamma}(\tau))]\right] \mathscr{W}(\chi,\phi) \tag{7}$$

where $\mathscr{W}(\chi,\phi) = \exp\left[-\sum_{\tau\tau'\gamma}\phi_{\alpha\gamma}(\tau)\chi^{-1}_{0\alpha\gamma}(\tau,\tau')\phi_{\alpha\gamma}(\tau')\right]$. In the above equation, the full Green's function is given by

$$\begin{aligned} G^{-1}_{\alpha\sigma}(\tau,\tau') = \mathcal{G}^{-1}_{0\alpha\sigma}(\tau,\tau') + \delta_{\tau\tau'}\delta_{\sigma\sigma'}\sigma \Big[\delta_{\alpha\alpha'}\lambda_{\alpha\sigma}s_{\alpha\sigma}(\tau) \\ - \sum_\gamma \Delta\tau\phi_{\alpha\gamma}(\tau)\Big] \end{aligned} \tag{8}$$

where $\lambda_{\alpha\sigma} = \operatorname{arccosh}\left(\exp^{1/2\Delta\tau U_{\alpha\sigma}}\right)$ and $U_{\alpha\sigma} = U$[1]. To evaluate the interacting Green's function, we implement the Monte Carlo sampling. In our scheme, this is performed for both spin and boson fields in order to record the local and the inter-site fluctuation. The probability of receiving or rejecting the move from the initial state s,ϕ to the new configuration s',ϕ' is determined by

$$R \equiv \prod_\sigma \frac{\det G_\sigma(s',\phi')}{\det G_\sigma(s,\phi)} \frac{\exp\left[\Delta\tau\mathscr{W}'\right]}{\exp\left[\Delta\tau\mathscr{W}\right]}. \tag{9}$$

When the move is accepted, the Green's function is then updated by using the standard Dyson relation of the Hirsch-Fye algorithm for both boson and fermion.

In the present work, we perform the EDMFT + QMC calculation on the Bethe lattice at and away from half filling. In the two-particle sector, we consider the RKKY type DOS that assumes the form of $\rho_\alpha(\epsilon) = \frac{1}{2I}\Theta(I_\alpha - |\epsilon|)$ [26–28,30]. We note that in contrast to the single particle DOS that consists of two different bandwidths, the magnitude of I for both bands is considered to be uniform. This is to reduce additional complexity that might arise from the interplay between the anisotropy of the two-particle DOS and the local correlation. The local interaction parameter of the Hamiltonian of equation (1) is determined by using the relation $U = U' + 2J$, with U and J are given quantities. We set the Hund's coupling at $J/W = 0.5$ and the temperature is fixed at $T/W = 0.1$, where $W = 1$ is the unit energy. The ratio between the narrow and the wide band is set as $W_2 = 2W$, where W_2 denotes the bandwidth of the wide band. In order to obtain the dynamical quantities on the real axis, the QMC data of the single and the two-particle is analytically continued by employing the maximum entropy approach [33].

[1] We assume here only the Coulomb interaction for the sake of simplicity. The inclusion of the Hund's coupling can be done straightforwardly.

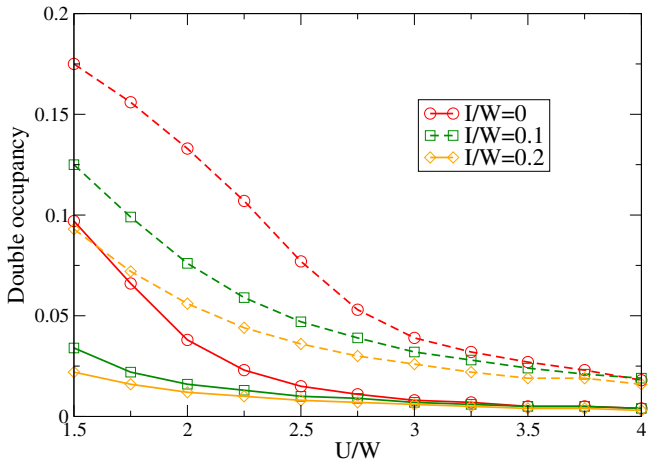

Fig. 1. (Color online) The intra-orbital double occupancy, d, of the anisotropic two-band Hubbard model at half filling for various values of the inter-site spin interaction. The solid (dashed) lines corresponds to the narrow (wide) band. Note that the lines are the guide to the eyes.

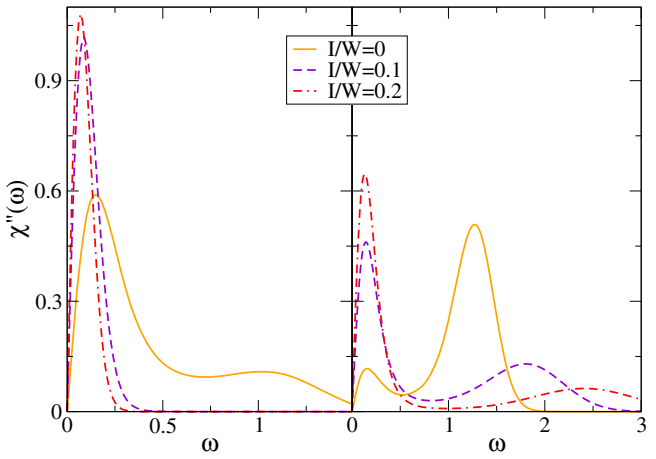

Fig. 2. (Color online) The imaginary part of the local spin susceptibility $\chi''(\omega)$ at half filling for various values of the inter-site interaction and for $U/W = 1.5$. The left and the right panel denote the narrow and the wide band respectively.

3 Results and discussion

3.1 Half-filling

We start our analysis by considering the results of the intra-orbital double occupancy $d = \langle n_{i\alpha} n_{i\alpha} \rangle$ at half filling as depicted in Figure 1. In the absence of the inter-site spin interaction and below the critical coupling, the double occupancy of both bands decreases as a function of the Coulomb interaction. This behavior hints at the suppression of the itinerant character which can be attributed to the enhancement of the electronic correlation. As U/W increases, one readily notices that the spectral weight of the narrow band becomes minimum and beyond $U/W > 2.5$ the band undergoes a metal insulator transition. The wide band, on the other hand, remains in the metallic state and d continuously decreases as a function of the on-site interaction up to $U/W > 3.5$. The results of the double occupancy therefore suggest that the OSMT phase exists for $2.5 < U/W < 3.5$, and are in a good agreement with previous findings [7–14].

When I/W is finite, the double occupancy of both bands diminishes which thus implies the suppression of the metallic character. As can be seen, the decrease of d is more pronounced as I/W increases. The reason behind this behavior may be best understood by recalling the fact that the on-site interaction in the EDMFT is supplemented by the inter-site spin interaction from which the inter-site fluctuation enters in the approximation. This is reflected in the effective action of equation (2) and the full interacting Green's function of equation (8). Therefore, during the self consistency, the interplay between the inter-site and local correlation leads to an effective interaction that is larger than the bare Coulomb interaction. The main consequence is that the interaction among the quasiparticles is amplified and the localised character is enhanced.

This argument is substantiated by the results of the local spin susceptibility as depicted in Figure 2. For $I/W = 0$, the spin susceptibility of both bands is composed of the broad spectral weight particularly at high energy. The narrow band is distinguished from the other one by the emergence of the pronounced low-energy excitation or the paramagnon peak. This suggests that the correlation of the narrow band is more significant than that the other band. When the non-local spin interaction is switched on, one clearly observes an enhancement of the low energy excitation. The spectral weight of the wide band is adjusted in such a way that the low-energy peak becomes more noticeable while the high energy resonance is weakened. The same is also true for the narrow band in which the spectral weight is completely transferred to the low energy part and led to the pronounced paramagnon peak. One can therefore deduce that the suppression of the double occupancy in the metallic state is the reflection of the formation of the local moment which is further enhanced by the RKKY interaction.

Remarkably, the qualitative behavior of the metal insulator transition upon the inclusion of the inter-site interaction remains the same as before at $I/W = 0$. The OSMT phase emerges as a function of U/W and the insulating state shows up at strongly interacting system at large U/W. The reason for the persistence of OSMT can be understood by realizing that the inclusion of the non-local spin-spin interaction amounts to enhancing the local correlation that leads to the generation of the effective Coulomb interaction. In addition, the spatial fluctuation acts locally only on certain band and does not contribute to the correlation between the narrow and the wide band. In the EDMFT, therefore, the OSMT can be seen as a results of the interplay between the effective interaction that records the inter-site quantum fluctuations and the anisotropic bandwidth. By using this fact, one can also explain why the double occupancy becomes insensitive to the changes of the inter-site spin interaction at insulating

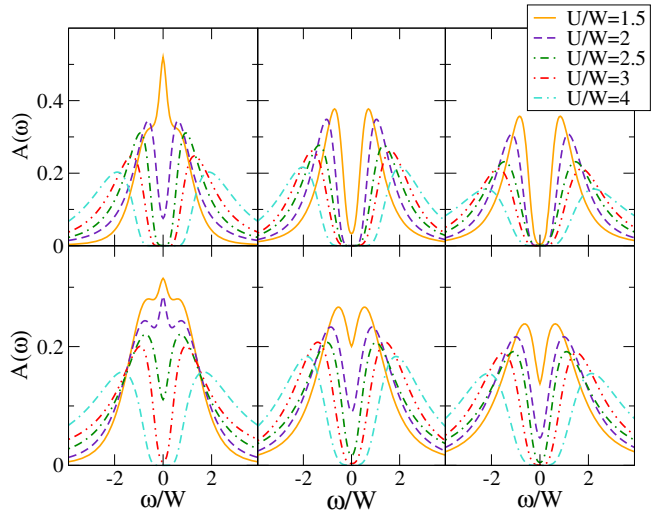

Fig. 3. (Color online) The single-particle spectral function of the extended two-band Hubbard model at half filling as a function of the Coulomb interaction U/W. Here, the magnitude of the inter-site interaction increases from the left panel to the right panel, I/W= 0, 0.1, 0.2 respectively. The upper (lower) panel corresponds to the narrow (wide) band.

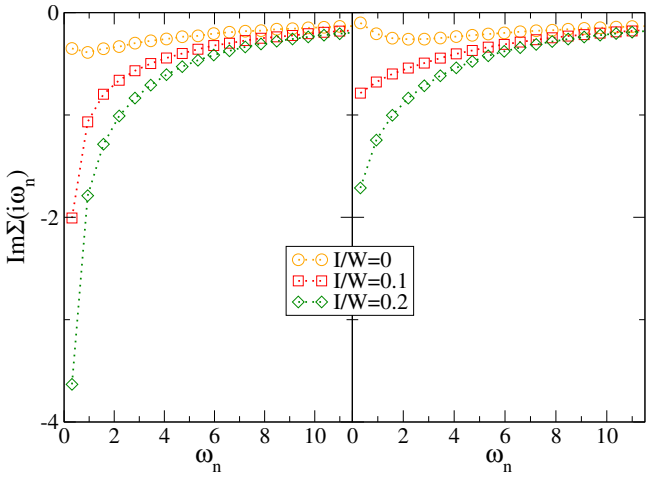

Fig. 4. (Color online) The imaginary part of the self energy as a function of the inter-site interaction on the fermionic Matsubara axis. The results are obtained at various values of inter-site coupling but at constant Coulomb interaction $U/W = 1.5$. The left and the right panel correspond to the narrow and the wide band respectively.

state. At pronounced U/W, the Coulomb interaction is the dominant energy scale such that the contribution of the inter-site interaction becomes negligible. In this regime, one sees that the effect of the bandwidth anisotropy is also overshadowed by the strong electron-electron interaction as reflected in the decrease of the splitting of the spectral weight.

To elaborate the above discussion, we present in Figure 3, the orbital-resolved single-particle spectral function for various values of the Coulomb interaction. At weakly interacting system $U/W \leq 2$ and for $I/W = 0$, both bands depict the quasiparticle peak which is a distinct signature of the metallic state. As U/W increases, the orbital selective Mott transition emerges which is marked by the simultaneous existence of the gap in the narrow band and the finite spectral weight in the wide band. Eventually, at pronounced on-site interaction, the system enters the insulating state as indicated by the simultaneous opening of gap on both bands

As the inter-site spin interaction is turned on, the spectral weight of both bands collapses such that the system almost at the onset of the insulating state. The Kondo resonance of the narrow band vanishes and the dip emerges at the Fermi level. The same is also true for the wide band, except that the spectral weight at the Fermi level is larger than that the other one. One can see that the formation of dip is further pronounced as I/W increases signaling that the itinerant character of both bands is strongly suppressed. When U/W slightly increases, the OSMT phase arises which is marked by the opening of the gap in the narrow band that coexists with the dip in the wide band. At last, at strongly interacting regime both bands show opening of gap thus signifying the emergence of the insulating state. An important question left to be answered is whether the finite spectral weight at the verge of Mott insulator truly marks the metallic state and does not an artefact associated with the analytical continuation. In order to address this issue, it is necessary to examine the imaginary part of the self energy which is plotted in Figure 4.

For $I/W = 0$, the self energy suggests for the metallic behavior which is marked by the largest spectral weight and particularly for the wide band, one observes $\mathrm{Im}\Sigma(\omega + \mathrm{i}\delta \to 0) \to 0$ at low energy. The latter is usually associated to the good metallic behavior. As can be seen, this character changes significantly upon the inclusion of the inter-site interaction where $\mathrm{Im}\Sigma(\omega + \mathrm{i}\delta \to 0)$ of both bands becomes finite and exhibits $\frac{1}{\omega+\mathrm{i}\delta}$ behavior at low energy. As expected, this behavior is further pronounced as I/W increases which can be used to explain the formation of the low dip in the spectral function. The formation of divergent like character in the imaginary part of the self energy is a clear signal that the correlation in the system is enhanced. One can thus deduce that the finite spectral weight at Fermi energy for $I/W > 0$ is a trace of the non Fermi liquid excitations with finite life time.

We can now summarize that while the inclusion of the spatial fluctuation amounts to inducing the instability in the metallic state, the OSMT phase at half filling is robust as a function of the Coulomb interaction. Our results therefore support the conclusion drawn in the previous works based on the QMC and the CDMFT calculation regarding the stability of OSMT in the presence of the non-local fluctuation. In addition to this, we have further revealed that the nature of OSMT phase remains unaltered despite the enhancement of the spatial fluctuation[2].

[2] The same trend is also observed when I/W further increases.

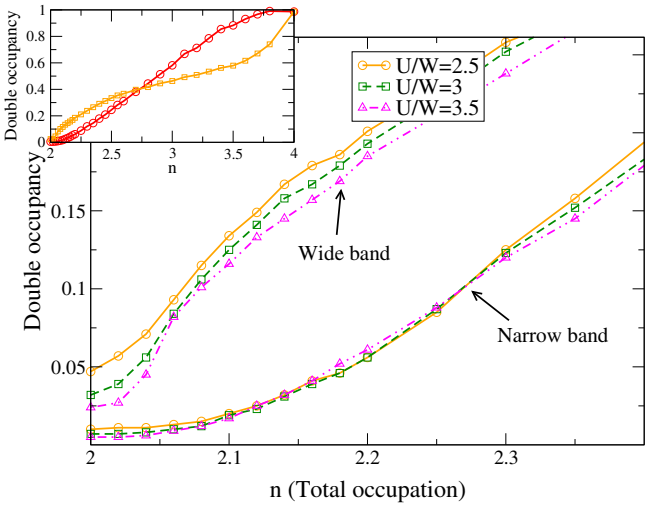

Fig. 5. (Color online) The intra-orbital double occupancy for various values of Coulomb interaction and for $I/W = 0.1$, in the range of $2 \leq n \leq 2.4$. The same is also shown in the inset for extended doping range at $U/W = 3.5$.

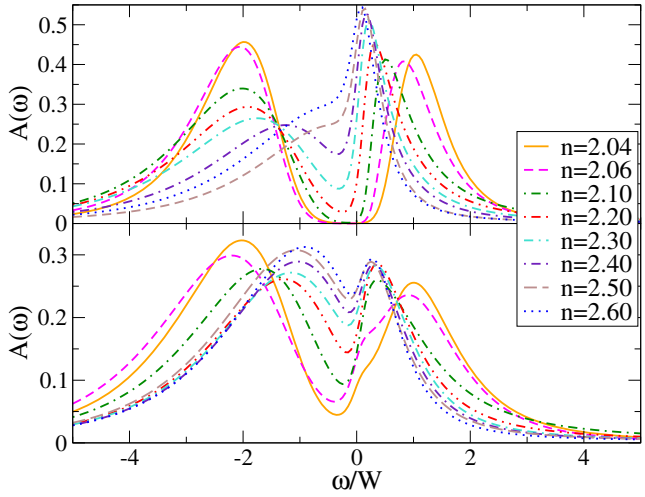

Fig. 6. (Color online) The orbital-resolved single-particle spectral function at $U/W = 2.5$ for various values of the occupation n. While the upper panel corresponds to the narrow band, the lower panel denotes the wide band.

3.2 MIT away from half filling

In this section, we extend the above analysis by looking at the possibility of OSMT phase upon doping the insulating state. Unless otherwise stated, all results presented in this section are obtained at $I/W = 0.1$ and at $T/W = 0.1$. In this regime, we have observed that the results are free from any sign problems. We first examine the intra-orbital double occupancy as a function of n as depicted in Figure 5. In our notation, n denotes the total occupation which is defined as $n = \sum_i^2 \tilde{n}_\alpha$ where $\tilde{n}_\alpha$ is the occupation of specific band. At low doping regime ($n < 2.10$), the double occupancy of the narrow band is clearly pinned at half filling, at the Mott insulating state. The wide band on the other hand increases immediately after the addition of doping thus signifying the suppression of the localisation character. One can thus summarize that, at low doping regime, the itinerant character of the wide band coexists with the insulating state of the narrow band i.e. OSMT phase. The rapid enhancement of the metallic state in the wide band upon doping strongly implies that the doping, at low concentration, is transferred only to this band. This can be understood by recalling the fact that the correlation in the narrow band remains more pronounced than that in the wide band. The vacant sites in the wide band are thus more favorable since the energy cost required to overcome the local repulsion is smaller than that the other one.

When the doping further increases, the double occupancy of both bands obviously enhances and in addition becomes comparable in magnitude (see inset of Fig. 5). The latter can be understood as a manifestation of the suppression of correlation such that the energy cost for occupying the sites in the narrow band gradually comparable to that in the wide band. This is certainly supported by the self energy data which will be further discussed below. Remarkably, as the occupation number goes beyond $n \approx 2.60$, the behavior of the double occupancy reverses such that spectral weight of the narrow band is larger than that the wide band (see inset of Fig. 5). The narrow band thus becomes more itinerant than that the other one which, as can be seen, persists up to $n = 4$. This change of character is clearly related to the availability of the states of each band at highly doped regime for the formation of double occupancy. As will be shown shortly below, the narrow band consists of intense peak at the Fermi level which reflects the large number of states in the band. Thus, as the system is further doped the fraction of doping is transferred to the narrow band and, hence, stimulates the rapid increase of the metallic character of this band.

Let us now consider the effect of doping from the perspective of the single-particle spectral function. The results are shown in Figure 6 where each spectral lines corresponds to certain value of n. At low doping regime, $n \leq 2.10$, one readily observes the coexistence of the metallic and the insulating character or the OSMT phase. Here, the single-particle gap prevails in the narrow band while a finite spectral weight around the Fermi level arises in the wide band. As doping increases, the gap in the narrow band vanishes and the spectral weight of both bands shifts to a larger value signifying the simultaneous existence of the metallic character. In this regime $2.20 \leq n \leq 2.40$ the spectral function of both bands consists of a pseudogap which implies the persistence of the strong correlation. When the system is in the overdoped regime, the pseudogap of the narrow band clearly diminishes and the spectral function gradually transforms onto single-peak structure. Here, one obviously observes the pronounced low energy peak that reveals the existence of a large number of states in the band.

While the enhancement of the metallic behavior is also evident in the wide band at large doping concentration, the spectral weight of the band is clearly suppressed. This certainly corresponds to the fact that the wide band provides smaller number of states where the double occupation becomes probable. Thus, as argued

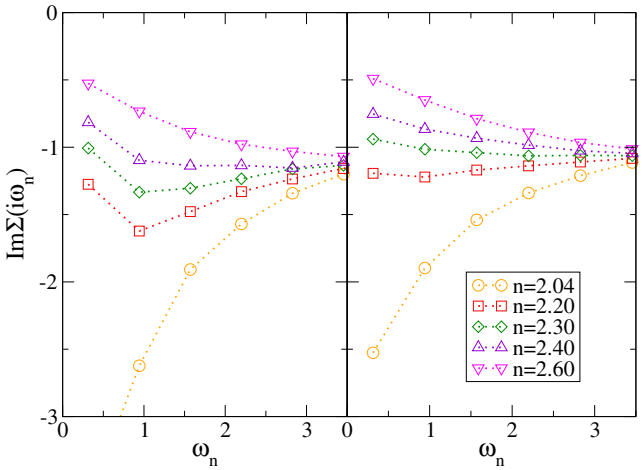

Fig. 7. (Color online) The imaginary part of the self energy for $U/W = 2.5$ as a function of occupation n. Note the results at low doping $n = 2.04$ that signifies the OSMT character. Here, the spectral weight of the wide band (right panel) is larger than that the narrow band (left panel) which can be associated to the increase of the itineracy character of the wide band.

above, in the highly doped regime, most of the doping will move to the narrow band and leads to a large number of double occupancy in this band.

In order to supplement the above-mentioned points, let us discuss the nature of metallic state upon doping by examining the imaginary part of the self energy. The results are plotted in Figure 7 for various values of n. The imaginary part of the self energy for $n \geq 2.20$ clearly suggests for the emergence of the metallic character. In this regime, the self energy of the wide band can be easily distinguised from that of the narrow band i.e. the spectral weight of the latter is smaller than that the former band. This clearly corresponds to the nature of correlation on each band which is obviously more pronounced in the narrow band. The latter can be also used to explain for the emergence of the strong pseudogap character in the single particle spectral function. Interestingly, the low energy part of the self energy $\omega \to 0$ extrapolates to finite value and therefore suggests that the correlation in the doped system remains important. The resonance in the spectral function, therefore, reflects the short-lived excitations and the metallic phase does not correspond to the Fermi liquid character.

From the above results, we can now argue that the transition from the insulating to metallic state as a function of doping is not substantially changed by the inclusion of the spatial fluctuation. The evolution of double occupancy in the present work is relatively comparable with the recent results based on the DMFT [16,17]. We have also observed that the somewhat similar will emerge when the inter-site spin interaction increases (not shown).

4 Summary and conclusions

In summary, we have analyzed the effects of the spatial fluctuation in the two-band Hubbard model with anisotropic bandwidths that incorporates the inter-site spin interaction. The Hamiltonian is solved by means of the EDMFT that has been generalized to take account of the orbital degeneracy. At half filling, our results clearly indicate that the inter-site interaction does not induce any substantial changes in the nature of MIT. The OSMT phase is evident as a function of the Coulomb interaction and both bands become insulator at large U/W. The effect of the inter-site spin interaction is shown to suppress the Kondo resonance which leads to the instability of the metallic state. While this behavior becomes more pronounced as I/W increases, the OSMT phase is prevailed. It is argued that the OSMT in the presence of the spatial fluctuation is a consequence of the interplay between the effective interaction that records the non-local quantum fluctuation and the anisotropic bandwidth.

Away from half filling, the evolution from the insulating to metallic character as a function of doping can be segmented into three different regimes. At low doping regime, the system clearly demonstrates the OSMT phase. It is shown that the wide band absorbs all additional particles/hole such that the other band remains in the insulating state. As doping increases i.e. intermediate regime, both bands become metallic with different strength of correlation. It is clearly indicated that the double occupancy of the wide band remains larger than that the other one. At overdoped regime, the nature of the correlation of both band reverses such that the narrow band becomes more metallic than that the wide band.

Taken together, our results have provided further insights on the role of the spatial fluctuation in the two-band Hubbard model with anisotropic bandwidth. We have shown that the OSMT phase persists both at half-filling and away from half filling at various strengths of the spatial fluctuation. In this work, we have also demonstrated that EDMFT offers a reasonable route for investigating the effect of spatial fluctuations in the multiorbital system.

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