

## Cluster Dynamical Mean Field Theory of the Mott Transition

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We address the nature of the Mott transition in the Hubbard model at half-filling using cluster dynamical mean field theory (DMFT). We compare cluster-DMFT results with those of single-site DMFT. We show that inclusion of the short-range correlations on top of the on-site correlations does not change the order of the transition between the paramagnetic metal and the paramagnetic Mott insulator, which remains first order. However, the short range correlations reduce substantially the critical  $U$  and modify the shape of the transition lines. Moreover, they lead to very different physical properties of the metallic and insulating phases near the transition point. Approaching the transition from the metallic side, we find an anomalous metallic state with very low coherence scale. The insulating state is characterized by the narrow Mott gap with pronounced peaks at the gap edge.

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The correlation driven metal-insulator transition (MIT) is one of the most fundamental problems in condensed matter physics, and continues to receive intensive attention. It is realized in numerous transition metal oxides and some organic salts, by application of the pressure or isovalent chemical substitutions [1]. The metallic state far from the transition is well described by the Fermi liquid theory, illustrating the wavelike properties of electrons in solids. In the insulating side, the electron behaves as a localized particle. Near the transition, the effective Coulomb repulsion between the carriers is of the same order as the kinetic energy term in the Hamiltonian. This regime probes the dual character of electron, namely, the particle- and wavelike character, and requires a nonperturbative method for its description.

The nature of the MIT depends strongly on the degree of magnetic frustration. In the limit of very large magnetic frustration, the insulating state is a simple paramagnetic state with local moments carrying  $\log(2)$  entropy. The metallic state is a Fermi liquid with a very heavy mass. The mass increases as the transition is approached to match the large entropy of the frustrated paramagnetic insulator. This is the essence of the Brinkman-Rice theory of the MIT, which has been substantially extended by the single-site DMFT of the Hubbard model in the paramagnetic phase [2]. The key predictions of this approach, such as the existence of a first order line ending in a second order Ising point, and numerous high temperature crossovers, have been verified experimentally [3]. The first order phase transition in a strongly frustrated situation has been confirmed by cluster-DMFT studies [4,5] and by other techniques [6].

The completely unfrustrated case is also well understood along the lines first drawn by Slater, and realized in the half-filled one-band Hubbard model with only nearest neighbor hoppings. Here, the MIT is driven by the long range magnetic ordering. The system is insulating and magnetic for arbitrarily small values of  $U$ , as a reflection of the perfect nesting of the band structure.

The character of the MIT with an intermediate degree of frustration (when the long range magnetic order is fully suppressed, but with strong short range magnetic correlations) remains an open problem. This problem can be addressed by a sharp mathematical formulation studying the *paramagnetic solution* of the cluster-DMFT equations of the Hubbard model, keeping the short range correlations only. The early cluster-DMFT studies received conflicting answers depending on different cluster schemes and different impurity solvers [7,8]. However, by going to very low temperatures using new algorithmic developments, we completely settle this question.

*Method.*—To study this problem, we apply cellular dynamical mean field theory (CDMFT) [9,10] to the two-dimensional Hubbard model, using plaquette as a reference frame. In this formalism, the lattice problem is divided into  $2 \times 2$  plaquettes and the lattice problem is mapped to an auxiliary cluster quantum impurity problem embedded in a self-consistent electronic bath. The latter is represented by an  $8 \times 8$  matrix of impurity hybridization  $\Delta$ , which is determined by the condition

$$\Delta(i\omega) = i\omega + \mu - \Sigma_c(i\omega) - \left[ \sum_{\vec{k}} \frac{1}{i\omega + \mu - t_c(\vec{k}) - \Sigma_c(i\omega)} \right]^{-1}, \quad (1)$$

where  $\Sigma_c$  is the matrix of cluster self-energies,  $t_c(\vec{k})$  is the matrix of tight-binding hoppings expressed in terms of the large unit cell ( $2 \times 2$ ) of the cluster, and  $\vec{k}$  runs over the reduced Brillouin zone of the problem. We choose the two-dimensional square lattice with only the nearest neighbor hopping  $t$ .

The CDMFT approach has already given numerous insights into frustrated models of kappa organics [4,11] as well as the doping driven Mott transition in the Hubbard model, when treated with a variety of impurity solvers [12]. In this Letter, the auxiliary cluster problem is solved with

the numerically exact continuous time quantum Monte Carlo (CTQMC) method [13,14].

**Results.**—Fig. 1(a) shows the phase diagram of the Hubbard model within cluster DMFT at half-filling in the absence of long range order. For interaction strength  $U < U_{c2}(T)$ , we find a metallic solution while for  $U > U_{c1}(T)$ , a Mott insulating solution exists. The two transition lines  $U_{c1}(T)$  and  $U_{c2}(T)$  cross at a second order endpoint, at temperature  $T_{\text{MIT}} \sim 0.09t$  and interaction strength  $U_{\text{MIT}} \sim 6.05t$ . It is clear that one of the most salient features of the single-site DMFT phase diagram [shown in Fig. 1(b)], namely, the existence of a first order phase transition, survives in plaquette DMFT.

Still there are substantial modifications to the single-site DMFT results when  $U/t$  is close to its critical value. Namely, (i) Strong short ranged antiferromagnetic correlations significantly reduce the value of critical  $U$  at which the second order endpoint occurs. Note that the plaquette-DMFT critical  $U$  ( $\sim 6.05t$ ) is in very favorable agreement with the Monte Carlo crossover  $U$  at which the pseudogap develops at intermediate temperatures accessible by determinantal Monte Carlo calculations (Fig. 5 in Ref. [15]). This critical  $U$  will increase if the system is more frustrated at short distance. For example, the inclusion of the next nearest hopping  $t'$  has this effect and was studied in Ref. [16]. (ii) The shape of the coexistence region, where both metallic and insulating solutions exist, is significantly different. The high temperature crossover lines (dashed line above  $T \sim 0.1t$  in Fig. 1) are similar since at high temperature the entropy of the paramagnetic insulator is of the order of  $\log(2)$  in both cluster and single-site approach. As the temperature is increased, the large entropy insulating state wins over the lower entropy metallic state. At low temperature, the situation is very different. In single-site DMFT, the metal wins at low temperature in the transition region because the emergence of the itinerant quasiparticle inside the Mott gap lowers the free energy of the strongly disordered Mott state. In the cluster case, the Mott insulator at very low temperature is very different and has small entropy due to short range singlet formation. The small entropy of this state can be confirmed by the “valence histogram” shown in the inset of Fig. 1(a). The high temperature insulating state, which has entropy of the order of  $\log(2)$ , populates many states of the plaquette with significant probability. In contrast, there is only one significant eigenvalue of the density matrix in low temperature, corresponding to the singlet state. The insulating phase at low temperature has thus very small entropy, and the bad metal has larger entropy; hence, decreasing temperature favors insulator over metal. The actual first order line (dashed line in Fig. 1(a) inside the coexistence region, where the free energy of the two phases equals) therefore bends back and critical  $U$  decreases with decreasing temperature. It is apparent that the zero temperature transition in cluster DMFT happens at  $U_{c1}$  and not at  $U_{c2}$  as in DMFT.

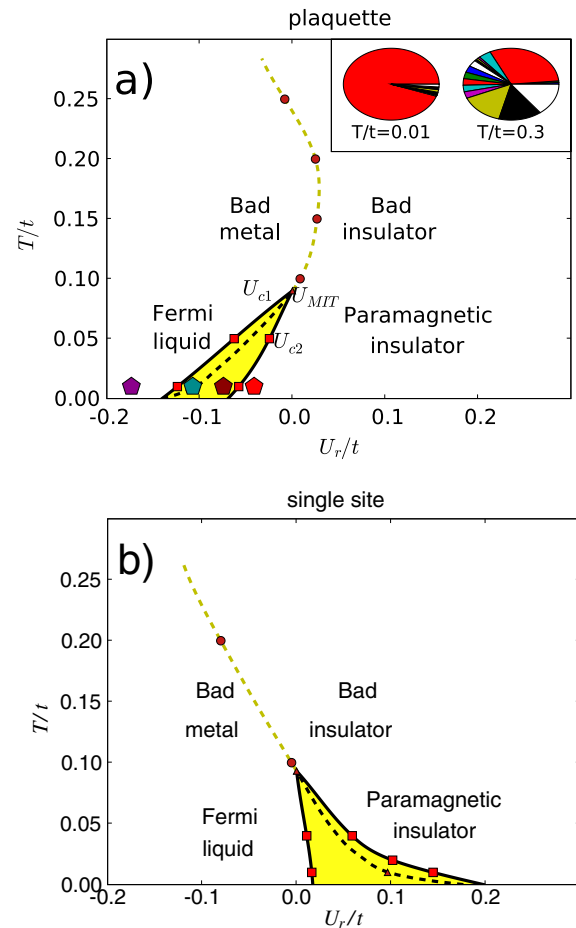


FIG. 1 (color online). (a) The phase diagram of the paramagnetic half-filled Hubbard model within plaquette CDMFT. Inset: The histogram of the two insulating states. It shows the probability for a given cluster eigenstate among the 16 eigenstates of the half filled plaquette. The singlet plaquette ground state has the highest probability. (b) For comparison, the corresponding phase diagram of the single-site DMFT (using the same 2D density of states) is shown. The coexistence region is shown as the shaded region. The dashed line marks the crossover above the critical point. The crossover line was determined by the condition that the imaginary part of the self-energy at few lowest Matsubara frequencies is flat at the crossover value of  $U$ . For easier comparison, the  $x$  axis is rescaled and the reduced value of  $U_r = \frac{U - U_{\text{MIT}}}{U_{\text{MIT}}}$  is used. The critical value of  $U$  is  $U_{\text{MIT}} = 6.05t$  in the cluster case and  $U_{\text{MIT}} = 9.35t$  in the single-site case. Pentagons in panel (a) mark the points in phase diagram for which we present the local spectral functions in Fig. 2.

While the shape of the DMFT phase diagram strongly resembles the phase diagram of the Cr-doped  $\text{V}_2\text{O}_3$ , the reentrant shape of the cluster-DMFT transition resembles more the  $\kappa$ -organic diagram [17] as pointed out in Ref. [4].

To understand the effects brought about by the short range magnetic correlations near the transition, we focus on the local spectral functions displayed in Fig. 2. As in single-site DMFT, below  $U_{c1}$  [Fig. 2(a)] the system is a normal Fermi liquid with a reduced width of the quasipar-

ticle peak ( $Z \sim 0.4$ ) and well developed Hubbard bands around  $-2.5t$  and  $2.5t$ .

The insulator in the coexistence region [Fig. 2(b)] is, however, very different than the Mott insulator in single-site DMFT. The Mott gap is small and it vanishes at  $U_{c1}$  where the insulating solution ceases to exist. At low temperature very pronounced peaks at the gap edge appear. These peaks are a clear hallmark of the coherence peaks characteristic of a Slater spin density wave.

With increasing  $U$  above  $U_{c2}$  [Fig. 2(d)] the Mott gap increases but the peaks at the gap edge remain very pronounced. Only at very large  $U$  comparable to the critical  $U$  of the single-site DMFT they lose some of their strength and dissolve into a featureless Hubbard band.

The metallic state, which competes with the insulator in the coexistence region, [Fig. 2(c)] has similar width of the quasiparticle peak as the Fermi liquid state at  $U < U_{c1}$ . Hence the quasiparticle renormalization amplitude, as extracted at finite but low temperature  $T = 0.01t$  is rather large. On the other hand, this metallic solution has somewhat reduced height of the quasiparticle peak which is mostly due to incoherent nature of the solution.

The incoherence can also be identified from the raw data on the imaginary axis. In Fig. 3 we show the imaginary self-energy for the different cluster momenta  $K$ , which can be thought as the orbitals of the multiorbital model associated with the cluster. In plaquette geometry, the self-energy is diagonal in the cluster momentum base and the on-site, nearest-neighbor, and next-nearest-neighbor self-energies can be constructed as the linear combination of these orbital self-energies [12].

Below  $U_{c1}$ , the self-energies of all four orbitals are very similar and results are close to the single-site DMFT. The

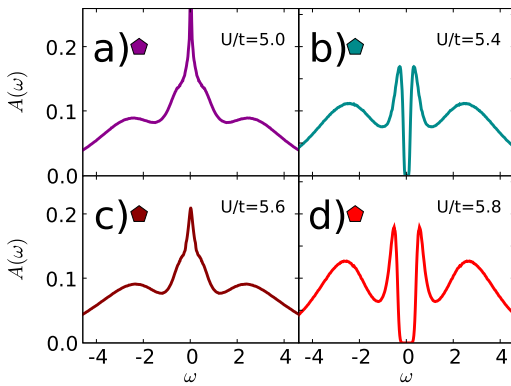


FIG. 2 (color online). The local spectral function for four representative values of  $U/ts$  and temperature  $T = 0.01t$  marked by pentagons in Fig. 1. (a) For  $U$  below  $U_{c1}$  the system is in Fermi liquid regime with rather large coherence temperature. (b) In the coexistence region, the insulating solution has a small but finite gap ( $\sim 0.2t$ ). (c) The metallic solution in the same region is strongly incoherent and the value at zero frequency decreases due to the finite scattering rate [see self-energy in Fig. 3(a)]. (d) For  $U$  above  $U_{c2}$ , the Mott gap steadily increases with  $U$ .

metallic phase in the coexistence region Fig. 3(c) has a large scattering rate in the  $(\pi, 0)$  orbital, in the orbital which contributes most of the spectral weight at the fermi level. The coherence scale in this strongly incoherent metal is thus severely reduced. The scattering rate as a function of temperature is not quadratic even at  $T = 0.01t$  and remains large  $\sim 0.2t$  at that temperature.

In Figs. 3(b) and 3(d) the Mott insulating state can be identified by the diverging imaginary part of the  $\Sigma_{(\pi,0)}(i\omega)$ . Because of particle-hole symmetry, the real part of the same quantity vanishes. Therefore, the only way to open a gap in the single particle spectrum is to develop a pole at zero frequency  $\Sigma_{(\pi,0)} \approx C/(i\omega)$ . We checked that the insulating state in the coexistence region has the characteristic  $1/(i\omega)$  behavior at very low temperature and the

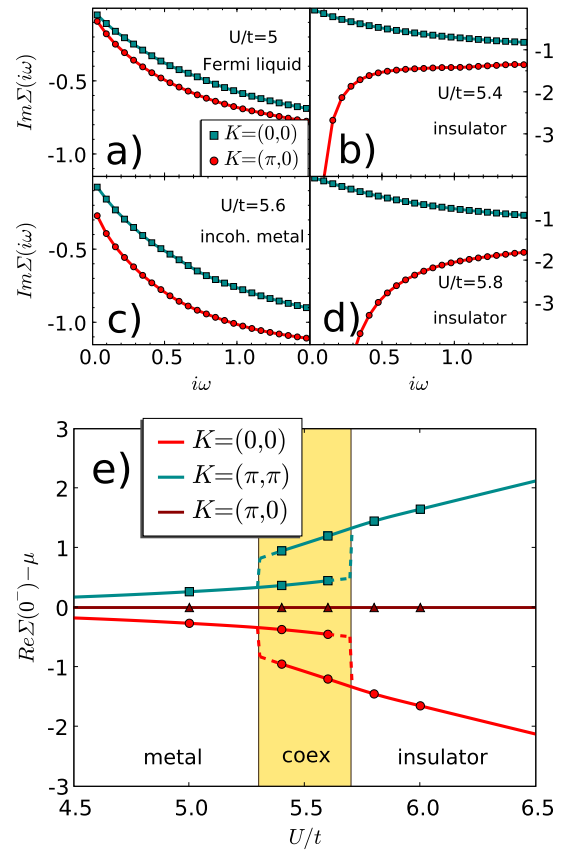


FIG. 3 (color online). Top: The imaginary part of the cluster self-energies for the same parameters as in Fig. 2. Because of particle-hole symmetry, the  $(\pi, \pi)$  and  $(0, 0)$  cluster self-energies have the same imaginary part and we show only one of them. Below the MIT shown here in (a), the momentum dependence of the self-energy is rather weak and the cluster dependence is very similar to the single-site DMFT solution. In the coexistence region, the metallic solution shown here in (c) is strongly incoherent especially in the  $(\pi, 0)$  orbital. For the insulating solutions in (b) and (d), the  $(\pi, 0)$  scattering rate diverges which opens the gap in the spectra. bottom: (e)  $\text{Re}\Sigma_K(0^-) - \mu$  as a function of  $U$ . Because of particle-hole symmetry,  $\text{Re}\Sigma_{K=(\pi,0)} - \mu$  vanishes.

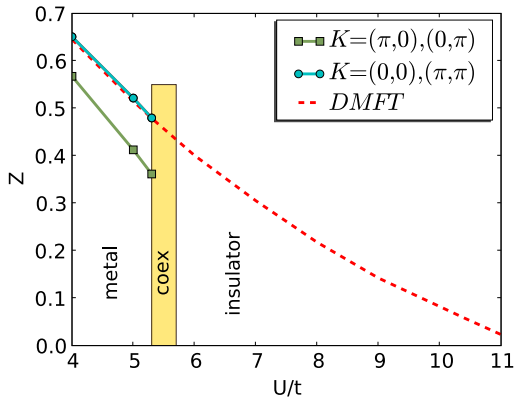


FIG. 4 (color online). The quasiparticle residue  $Z$  vs  $U/t$  for different orbitals in CDMFT. Below the transition point, the  $(0, 0)$  and  $(\pi, \pi)$  orbitals have essentially the same  $Z$  as single-site DMFT (dotted line) while the quasiparticles are more renormalized in the  $(\pi, 0)$  orbital.

coefficient  $C$  in the coexistence region decreases as  $U$  decreases. The closure of the gap at the  $U_{c1}$  transition point is confirmed by the vanishing of  $C$  at that point.

The other two orbitals expel their Fermi surfaces by a different mechanism; namely, the real parts of the self-energy are such that the effective chemical potential  $\mu_{eff} = \mu - \Sigma(0^-)$  moves out of the band. The separation of the two orbitals gradually increases as  $U$  increases, and it jumps at the critical  $U$  showing the hysteresis behavior displayed in Fig. 3(e).

The important issue in the MIT is whether the short range magnetic exchange in the Hubbard type of models allow the Brinkman-Rice scenario of diverging effective mass. In Fig. 4 we plot the quasiparticle renormalization amplitude  $Z$  of the four different orbitals of the plaquette. As shown in Fig. 4, the growth of the effective mass in cluster DMFT is cutoff by the exchange interaction and the spatial coherence is lost way before the quasiparticles acquire a large effective mass. The lattice  $Z_{\mathbf{k}}$  is a linear combination of the two values plotted in Fig. 4. The quasiparticles at  $(\pi, 0)$  and  $(0, \pi)$  are renormalized more strongly than those away from the two points. More importantly, close to  $U_{c1}$ , where the system is still coherent at  $T = t/100$ , the quasiparticle renormalization amplitude is rather large for the plaquette without frustration ( $Z \sim 0.36$ ). Very near and inside the coexistence region, the metallic state remains very incoherent at our lowest temperature  $T = t/100$ . We therefore cannot determine the low energy  $Z$  which might vanish at  $U_{c2}$  at zero temperature.

In conclusion, we used essentially an exact numerical method, CTQMC simulations, and clarified the nature of the Mott transition in plaquette-DMFT. The short range correlations which are accounted for in this study but are absent in single-site DMFT do not change the order of the Mott transition which remains first order with coexistence of metallic and insulating solution. Our cluster-DMFT

study predicts the existence of the anomalous metallic state within the coexistence region with very low coherence temperature. This regime could be relevant to the interpretation of experiments in  $\text{VO}_2$  [18] and  $\text{PrNiO}_3$  under the applied pressure [19] where an anomalous metallic state was reported. On the theoretical side, the plaquette DMFT brings new light on the nature of the interaction driven MIT. The cluster DMFT of this problem retains aspects of Mott physics, as described in single-site DMFT, and Slater physics. It does that by having two orbitals  $[(\pi, 0)$  and  $(0, \pi)]$  exhibit a Mott transition while the remaining orbitals  $[(0, 0)$  and  $(\pi, \pi)]$  undergo a band transition. This Slater-Mott transition requires momentum space differentiation and has no analog in single-site DMFT.

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