Local order and the gapped phase of the Hubbard model: A plaquette dynamical mean-field investigation

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Abstract – The four-site “DCA” method of including intersite correlations in the dynamical mean-field theory is used to investigate the metal-insulator transition in the Hubbard model. At half-filling a gap-opening transition is found to occur as the interaction strength is increased beyond a critical value. The gapped behavior found in the 4-site DCA approximation is shown to be associated with the onset of strong antiferromagnetic and singlet correlations and the transition is found to be potential energy driven. It is thus more accurately described as a Slater phenomenon (induced by strong short-range order) than as a Mott phenomenon. Doping the gapped phase leads to a non–Fermi-liquid state with a Fermi surface only in the nodal regions and a pseudogap in the antinodal regions at lower dopings $x \lesssim 0.15$ and to a Fermi-liquid phase at higher dopings.

Understanding the “Mott” or correlation-driven metal insulator transition is one of the fundamental questions in electronic condensed-matter physics [1,2]. Interest increased following P. W. Anderson’s proposal that the copper oxide based high-temperature superconductors are doped “Mott insulators” [3].

Clear theoretical pictures exist in the limits of strong and weak coupling. In strong coupling, insulating behavior results from the “jamming” effect [1] in which the presence of one electron in a unit cell blocks a second electron from entering; we term this the Mott mechanism. At weak coupling, insulating behavior arises because long-range [5] or local [6,7] order opens a gap; we term this the Slater mechanism. (Anderson [8] has argued that in 2d the strong-coupling regime provides the appropriate description of the low-energy behavior for all interaction strengths, but this view is controversial and does not address the question of interest here, namely the physical origin of the novel low-energy physics.) Many materials [2] including, perhaps, high-temperature superconductors [8] seem to be in the intermediate-coupling regime in which theoretical understanding is incomplete.

The development of dynamical mean-field theory, first in its single-site form [9] and subsequently in its cluster extensions [10–14] offers a mathematically well-defined approach to study metal-insulator transitions. The method, while approximate, is non-perturbative and provides access to the intermediate-coupling regime. In this paper we exploit new algorithmic developments [15,16] to obtain detailed solutions to the dynamical mean-field equations for the one-orbital Hubbard model in two spatial dimensions. This, the paradigmatic model for the correlation-driven metal-insulator transition, is defined by the Hamiltonian

$$H = \sum_{p,\alpha} \varepsilon_p c_{p,\alpha}^\dagger c_{p,\alpha} + U \sum_i n_{i,\uparrow} n_{i,\downarrow}$$ (1)

with local repulsion $U > 0$. We use the electron dispersion $\varepsilon_p = -2t(\cos px + \cos py)$. The dynamical mean-field approximation to this model has been previously considered [9,12,17–21]; we comment on the differences to our findings below and in the conclusions.
The dynamical mean-field method approximates the electron self-energy $\Sigma(p, \omega)$ by
\[
\Sigma(p, \omega) = \sum_{a=1\ldots N} \phi_a(p) \Sigma_a(\omega). \tag{2}
\]

The $N$ functions $\Sigma_a(\omega)$ are the self-energies of an $N$-site quantum impurity model whose form is specified by a self-consistency condition. Different implementations of dynamical mean-field theory correspond to different choices of basis functions $\phi_a$ and different self-consistency conditions [13,14]. In this paper we will use primarily the “DCA” ansatz [10] although we have also used the CDMFT method [11,21] to verify our results and make comparison to other work. In the DCA method one tiles the Brillouin zone into $N$ regions, and chooses $\phi_a(p) = 1$ if $p$ is contained in region $a$ and $\phi_a(p) = 0$ otherwise. The “cluster momentum” sectors $a$ correspond roughly to averages of the corresponding lattice quantities over the momentum regions in which $\phi_a(p) \neq 0$.

We present results for $N=1$ (single-site DMFT) and $N=4$. Because we are interested in the effects of short-range order, the restriction to small clusters is not a crucial limitation: while the precise parameter values at which the transition to insulating behavior occurs depend on the cluster size, the basic relation we establish between correlations and the insulating behavior does not, and the 4-site cluster is computationally manageable so a wide range of information can be extracted.

In the $N=4$ case the impurity model is a 4-site cluster in which the Brillouin zone is divided into 4 regions, and we choose $\phi_a(p) = 1$ if $p$ is contained in region $a$ and $\phi_a(p) = 0$ otherwise. The “cluster momenta” sectors $a$ correspond to averages of the corresponding lattice quantities over the momentum regions in which $\phi_a(p) \neq 0$.

We present results for $N=1$ (single-site DMFT) and $N=4$. Because we are interested in the effects of short-range order, the restriction to small clusters is not a crucial limitation: while the precise parameter values at which the transition to insulating behavior occurs depend on the cluster size, the basic relation we establish between correlations and the insulating behavior does not, and the 4-site cluster is computationally manageable so a wide range of information can be extracted.

The Hamiltonian is
\[
H_{QI} = H_{cl} + \sum_{A,\sigma,\alpha} \left( V_A^\alpha d_A^\dagger \sigma c_A^\alpha + H.c. \right) + H_{bath}, \tag{3}
\]
\[
H_{cl} = \sum_{A,\sigma} \varepsilon_A \left( d_A^\dagger \sigma d_A^\sigma + H.c. \right) + U \sum_j n_{j,\uparrow} n_{j,\downarrow}. \tag{4}
\]

We solve the impurity models on the imaginary frequency axis using two new continuous-time methods [15,16]. Because we are studying a two-dimensional model at temperature $T > 0$ we restrict attention to phases without long-range order. The $\varepsilon_A$, $V_A^\alpha$, and $H_{bath}$ are determined by a self-consistency condition [9,14].

The $N=1$ case has been extensively studied [9]. At $N=1$, intersite correlations are entirely neglected; the only physics is the strong correlation “local blocking” effect envisaged by Mott. If attention is restricted to the paramagnetic phase, to temperature $T = 0$, and density $n = 1$ per site one finds that the ground state is metallic for $U < U_{c2} \approx 12t$ [22] and insulating for $U > U_{c2}$. The insulating phase is paramagnetic and characterized by an entropy of $\ln 2$ per site corresponding to the spin degeneracy of the localized electrons. For $U_{c1} \approx 9t < U < U_{c2}$ the insulating phase, although not the ground state, is metastable and the extensive entropy of the insulating state leads to a transition to the insulating state as the temperature is raised [9].

The antiferromagnetic solution of the single-site DMFT equations has also been extensively studied. The model considered here has a nested Fermi surface at carrier concentration $n = 1$, so at $n = 1$ the ground state is an insulating antiferromagnet at all interaction strengths $U$. The Néel temperature peaks at $U \approx 0.8U_{c2}$ [22]. This correlation strength also marks a change in the character of the transition: for $U \lesssim 0.8U_{c2}$ the expectation value of the interaction term $U n_\uparrow n_\downarrow$ decreases as the magnetic order increases. The transition is thus potential energy driven and is identified with Slater physics. However for $U \gtrsim 0.8U_{c2}$ the expectation value of the interaction term increases as the system enters the antiferromagnetic phase; the transition in this case is thus kinetic energy driven and is identified with Mott physics.

We now present results for the $N=4$ model in comparison to those obtained in the single-site approximation. Figure 1 presents the imaginary time Green function $G(R, \tau)$ at the particular values $R = 0$ and $\tau = 1/2T = \beta/2$, computed at density $n = 1$ per site for different temperatures $T$ and interactions $U$ using 1- and 4-site DCA. $G(0, \beta/2)$ is directly measured in our simulations and is related to the on-site electron spectral function $A_0(\omega)$ by
\[
G(0, 1/(2T)) = \int \frac{d\omega}{\pi} \frac{A_0(\omega)}{2 \cosh \frac{\omega}{2T}} \approx T A_0(\omega = 0). \tag{5}
\]

The last approximate equality applies for sufficiently small $T$ and shows that the behavior of $G(0, \beta/2)$ provides information on the existence of a gap in the system. For
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$N = 1$ and $U \lesssim 10t$ $G(0, \beta/2)$ increases as $T$ decreases, indicating the development of a coherent Fermi-liquid state. In the 4-site DCA results a transition is evident as $U$ is increased through $U^* \approx 4.2t$: for $U < U^*$ $A(0)$ increases slowly as $T$ is decreased, as in the single-site model, but for $U > U^*$, $A(0)$ decreases, signalling the opening of a gap. The very rapid change across $U = U^*$ is consistent with a first-order transition, as found in the careful CDMFT analysis of Park et al. [21]. The critical $U$ is seen to be essentially independent of temperature indicating that the entropies of the metallic and non-metallic states are very similar. The end point of the first-order transition is at about $T = 0.25t$ which is approximately the Néel temperature of the single-site method, at $U = 4t$ [23].

Figure 2 shows as the solid line the local electron spectral function computed by maximum entropy analytical continuation of QMC data for $U = 6t$ and doping $x = 0$. Dashed line: spectral function in the $P = (0, \pi), (\pi, 0)$-momentum sector. Dotted and dash-dotted lines: $P = (0, \pi), (\pi, 0)$ and local spectral functions obtained by performing the DCA momentum averages of the standard SDW mean-field expressions for the Green function, with gap $\Delta = 1.3t$.

Figure 3 shows as the solid line the local electron spectral function computed by maximum entropy analytical continuation of QMC data for $U = 6t$ and $n = 1$. Analytical continuation is well known to be an ill-posed problem, with very small differences in imaginary time data leading in some cases to very large differences in the inferred real-axis quantities. A measure of the uncertainties in the present calculation comes from the difference between the spectra in the positive-energy and negative-energy regions, which should be equal by particle-hole symmetry. We further note that the gap is consistent with the behavior shown in fig. 1. The local spectral function exhibits a characteristic two-peak structure found also in CDMFT calculations [21]. The dotted line gives the spectral function for the $P_x$-sector, corresponding to an average of the physical spectral function over the region $(\pi/2 < p_x < 3\pi/2), (-\pi/2 < p_y < \pi/2)$; this is seen to be the origin of the gap-edge structure.

We present in fig. 3 the temperature dependence of the double-occupancy $D = \langle n^2 \rangle$ computed using the 1-site and 4-site DCA for a relatively weak and a relatively strong correlation strength. In the single-site approximation antiferromagnetic correlations are absent in the paramagnetic phase and become manifest below the Néel temperature; the difference between paramagnetic and antiferromagnetic phases therefore gives insight into the physics associated with the antiferromagnetic correlations. For the weaker interaction strength $U = 5t$, the development of Fermi-liquid coherence as $T$ is decreased in the paramagnetic phase means that the wave function adjusts to optimize the kinetic energy, thereby pushing the interaction term farther from its extremum and increasing $D$. At this $U$ the magnetic transition is signaled by a rapid decrease in $D$, indicating that the opening of the gap enables a reduction of interaction energy, as expected if Slater physics dominates. For the larger $U = 10t$ in the
single-site approximation we see that $D$ is temperature independent in the paramagnetic phase because for this $U$ and temperature the model is in the Mott insulating state (a first-order transition to a metallic state would occur at a lower $T$). The antiferromagnetic transition is signalled by an increase in $D$ because in the Mott state the transition to antiferromagnetism is kinetic energy driven.

Turning now to the 4-site calculation we see that at $U = 5t$ a decrease in $D$ sets in below about $T^* = 0.23t \approx 0.8T^*_N$-site. $T^*$ is also the temperature below which $G(0, \beta/2)$ begins to drop sharply. This indicates that the opening of the gap is related to a reduction of interaction energy, implying a “Slater” rather than a “Mott” origin for the phenomenon. For $U = 10t$ we see a gradual increase in $D$ as $T$ is decreased, reflecting the Mott physics of kinetic energy gain with increasing local antiferromagnetic correlations.

To further understand the physics of the transition we examine which eigenstates $|n_{cl}\rangle$ of $H_{cl}$ are represented with high probability in the actual state of the system. We define $F_{n_{cl}} = \langle n_{cl}|\hat{\rho}|n_{cl}\rangle$ with $\hat{\rho}$ the cluster reduced density matrix obtained by tracing the partition function over the bath states. One particularly interesting state is the “plaquette singlet” state which we denote as $|(12)(34) + (41)(23)|$ with $\langle ab\rangle$ representing a singlet bond between sites $a$ and $b$. The upper panel of fig. 4 shows the probability that this state is represented in the thermal ensemble corresponding to mean density $n = 1$ for different interaction strengths $U$; the transition at $U \approx 4.2t$ manifests itself as a dramatic change (within our accuracy, the jump associated with a first-order transition). We have performed CDMFT calculations to verify that the same state and same physics control the transition studied in refs. [19,21].

The plaquette singlet state has strong intersite correlations of both $d$-wave and antiferromagnetic nature. It is natural to expect these correlations to open a gap in the electronic spectrum. To investigate this possibility we computed the DCA momentum averages of the lattice Green function using density $n = 1$, and antiferromagnetic and singlet pairing gaps of magnitude $\Delta = 1.3t$ to obtain mean-field estimates of the impurity model spectral functions. The dotted and dash-dotted lines in fig. 2 show the antiferromagnetic results. (Use of a $d$-wave pairing gap would yield very similar results, except that instead of a clean gap at 0 one finds a “soft” gap with a linearly vanishing density of states). The evident similarity to the calculations reinforces the argument that it is the local correlations which are responsible for the gapped behavior.

We finally consider the effect of doping. The model we study is particle-hole symmetric. For definiteness we present results for electron doping. In a Fermi liquid, the imaginary part of the real-axis self-energy is $\text{Im}\Sigma(p, \omega \rightarrow 0) \propto \omega^2$. The spectral representation $\Sigma(\omega_n) = \int \frac{d\omega}{\pi} \text{Im}\Sigma(p, x)/(i\omega_n - x)$ then implies that at small $\omega_n$, $\text{Im}\Sigma(p, \omega_n) \propto \omega_n$. We find that in the $S = (0, 0)$ and $D = (\pi, \pi)$ momentum sectors, this relation is obeyed at all dopings. The behavior in the $P = (0, \pi)$, $(\pi, 0)$-sector is different, as is shown in fig. 5. The dashed line shows the self-energy for the half-filled model. The $\omega^{-1}_n$ divergence, arising from the insulating gap, is evident. For large enough doping ($x \gtrsim 0.15$) the expected Fermi-liquid behavior is observed (and indeed for $x > 0.2$ the self-energy is essentially the same in all sectors); however for smaller dopings, up to $x \approx 0.15$, $\text{Im}\Sigma_P$ does not extrapolate to 0 as $\omega_n \rightarrow 0$, indicating a non–Fermi-liquid behavior in this momentum sector.

To explore further the non–Fermi-liquid behavior we present in fig. 6 the density of states in the $P = (0, \pi)$, $(\pi, 0)$-sector, obtained by analytical continuation of our quantum Monte Carlo data. A comparison to fig. 2 shows that as the chemical potential is increased the Fermi level moves into the upper of the two bands. In addition, for the lower dopings a small “pseudogap” (suppression of density of states) appears near the Fermi level while for $x = 0.15$ the value of the spectral function...
and then for $x/ \gtrsim 0.15$ in the $P$-sector, signalling the restoration of the Fermi-liquid behavior. The results may be interpreted as “Fermi arcs” or as hole pockets bounded by the edges of the $D = (\pi, \pi)$-sector: the momentum resolution of the 4-site DCA is insufficient to distinguish the two. As the doping is further increased the “Fermi arc” regions rapidly grow and the pseudogap fills in, leading to a restoration of a conventional Fermi surface for $x > 0.15$.

The lower panel of fig. 4 shows that this non–Fermi-liquid behavior can be related to the prominence of the plaquette singlet and the plaquette triplet states. The contribution of the plaquette triplet state peaks at $x \approx 0.15$, while the contribution of the 6-electron singlet state remains small, indicating a prominent role for antiferromagnetic (rather than $d$-wave singlet) correlations at this doping. However, the increasing prominence of the 6-electron singlet state as doping is increased strongly suggests that the larger doping Fermi-liquid–like state will be susceptible to a pairing instability. Similar results were found in CDQMC calculations by Kyung and collaborators [7], who attributed them to antiferromagnetic correlations, by Zhang and Imada [19] and by Haule and Kotliar [24].

In summary, we have shown that the insulating behavior (at doping $x = 0$) and non–Fermi-liquid behavior (at doping $0 < x < 0.15$) found at relatively small $U$ in cluster dynamical mean-field calculations [7,17–19,21,25] may be understood as a consequence of a potential-energy–driven transition to a state with definite, strong spatial correlations, mainly of the plaquette singlet type. Doping this state leads to a low-energy pseudogap for momenta in the $P = (0, \pi), (\pi, 0)$-sector. Superconducting correlations (marked by the prominence of the 6-electron states) do not become important until beyond the critical concentration at which Fermi-liquid behavior is restored. Our results are consistent with the finding of Park et al. [21] that the $U$-driven transition is first order (although unlike those authors we have not performed a detailed study of the coexistence region). We interpret the transition as being driven by Slater (spatial ordering) physics, whereas Park et al. interpret their results as arising from a strong coupling, Mott phenomenon. Moukouri and Jarrel [25] argue that Slater physics is not important because in a 2d model with Heisenberg symmetry long-range order does not set in until $T = 0$. We believe, however, that the results for double occupancy shown in fig. 3 and the dominance of particular states in the sector statistics plot, fig. 4, provide strong evidence that the physics is indeed dominated by local order, consistent with Slater-type physics. The importance of spatial correlations for the spectral function and non–Fermi-liquid behavior was previously stressed by Jarrell and co-workers [18] and Zhang and Imada [19]. We also suggest that the short-range order is responsible for the features noted by Chakraborty and co-workers in the optical conductivity and spectral function [20]. Calculations in progress will extend the results presented here to larger clusters.
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