On the origin of the pseudogap in underdoped cuprates

Th.A. Maier, M. Jarrell, A. Macridin, and F.-C. Zhang

Department of Physics, University of Cincinnati, Cincinnati OH 45221, USA

We investigate the microscopic origin of the pseudogap in the weakly doped 2D Hubbard model using Quantum Monte Carlo within the dynamical cluster approximation. We compare our results with proposed scenarios for the pseudogap. All our numerical evidence is in favor of spin-charge separation as described in the resonating valence bond picture as the cause of the pseudogap behavior. Scenarios of "preformed pairs", the coupling of quasiparticles to antiferromagnetic spin-fluctuations and stripes are inconsistent with our results.

Introduction

The existence of a pseudogap, i.e. a large suppression of low-frequency spectral weight in the normal state of underdoped high-temperature superconductors, is now a commonly accepted experimental fact. A multitude of experiments has probed the magnetic, thermodynamic, transport and optical properties of the underdoped cuprates (for an overview see Refs. [3][4]).

Some of the earliest indications of a pseudogap in the spin-channel were found in NMR-experiments [3], where the spin-susceptibility as measured by the Knight-shift was seen to decrease with decreasing temperature well above the superconducting critical temperature $T_c$. Further indirect evidence of a pseudogap was found in specific heat measurements [4]. In underdoped samples, the electronic contribution starts to decrease with decreasing temperature in the normal state well above $T_c$. In transport measurements the crossover of the linear dependence of the ab-plane resistivity in temperature to a stronger dependence [5] was taken as evidence for the opening of a pseudogap. However, the most direct and reliable measurements of the normal state pseudogap are angle-resolved photoemission experiments [6]. A highly anisotropic ($d_{x^2-y^2}$-like) suppression of low-energy spectral weight persisting far above $T_c$ has been found in underdoped samples. This pseudogap closes at a temperature $T^*$ consistent with the crossover temperatures determined from other measurements.

Theorists have responded with several scenarios [7][8][9][10][11][12][13][14] for the pseudogap. Scenarios, based on the vicinity of the underdoped system to antiferromagnetic ordering, hold the coupling of quasiparticles to antiferromagnetic spin fluctuations responsible for the pseudogap behavior [8]: As a consequence of short-ranged antiferromagnetic correlations, a shadow-band forms and a pseudogap opens up in the density of states.

Motivated by the fact that the pseudogap has the same symmetry as the superconducting gap, "preformed pair" scenarios associate the pseudogap with fluctuations that lead to $d$-wave superconductivity [10]. In these scenarios the transition to the normal state is controlled by the vanishing of the superfluid density and not the closing of the superconducting gap. Due to strong pairing correlations above $T_c$, precursors of the superconducting gap are seen as pseudogap in the low-energy excitations.

Ideas involving spin-charge separation are based on the resonating valence bond (RVB) picture [10]. In these scenarios the pseudogap is due to $d$-wave singlet pairing of spin $1/2$, charge neutral fermions, called spinons. At $T_c$ the holons, i.e. spin 0 charge excitations, become coherent and recombine with spinons to form electron pairs which render the system superconducting.

Further scenarios are based on the existence of a quantum critical point (QCP) close to optimal doping that associate the pseudogap with a broken symmetry (see eg. Ref. [11]). Other approaches that ascribe the formation of the pseudogap to the presence of strong charge fluctuations are motivated by the observation of charge stripes in some cuprate superconductors.

Presently, there is no consensus as to the origin of the pseudogap in the underdoped cuprates so numerical investigations based on model calculations are highly desirable. Early in the history of high-$T_c$ superconductors it was realized that the two-dimensional (2D) Hubbard model in the intermediate coupling regime, i.e. where the Coulomb interaction is of the order of the bandwidth, or closely related models like the t-J-model, should capture the essential low-energy physics of the cuprates [13].

In this report we study the pseudogap behavior of the 2D Hubbard model using the dynamical cluster approximation [14][15][16][17][18][19] (DCA). The DCA is a non-perturbative approach for the thermodynamic limit, which systematically incorporates the effects of nonlocal correlations to local approximations like the dynamical mean field approach (DMFA) [19], by mapping the lattice onto a self-consistently embedded cluster of size $N_c$. We solve the cluster problem using a combination of Quantum Monte Carlo (QMC) and the maximum entropy method to obtain dynamics [20]. Since further insight into the pseudogap phenomenon can be obtained by studying the effects of lattice frustration, we also present results for the 2D Hubbard model with additional next nearest neighbor hopping $t'$. We show that our results for the pseudogap behavior in the 2D Hubbard model support the RVB picture and exclude other mechanisms for the pseudogap.

Formalism

A detailed discussion of the DCA formalism was given in previous publications [14][15][16][17][18][19][20]. The DCA is based on the assumption [21] that the lattice...
self-energy is only weakly momentum dependent and can be approximated by a constant within each of a set of cells centered at a corresponding set of cluster $K$-points. The Green-functions used to calculate the self-energy are coarse-grained or averaged over these cells. This greatly reduces the complexity of the lattice problem to that of a periodic cluster embedded in a host which has to be determined self-consistently. The DCA reduces to the DMFA for a cluster size of one and becomes exact when the cluster size is equal to the system size.

**Results** We present results of DCA calculations for the conventional 2D Hubbard model characterized by an overlap integral $t$ between nearest neighbors and $t'$ between next nearest neighbors and an on-site Coulomb repulsion $U$. We set $t = 0.25$ and choose the magnitude $|t'/t| \leq 0.5$, so that the band-width $W = 8t = 2$, and study the intermediate coupling regime $U = W$. We study the initial corrections to the DMFA by setting the cluster size to $N_c = 4$, the smallest cluster size which allows for d-wave pairing. We have previously shown that this cluster size is large enough to capture the qualitative low-energy physics of the cuprate superconductors $[22, 23]$. Due to numerical restrictions we are currently not able to perform systematic studies with increasing cluster size. The $N_c = 4$ simulations presented in this paper should therefore be interpreted as qualitative extended mean-field results that describe effects on short-length scales (within the cluster).

Our results are summarized in the temperature-doping $(T$-$\delta)$ phase diagram shown in Fig. 1. We find regions of antiferromagnetism, d-wave superconductivity, pseudogap and Fermi-liquid like behaviors. In this report we focus on the pseudogap behavior found at low doping $\delta$. The pseudogap region is characterized by a suppression of spin excitations below a crossover temperature $T^*$, defined via the maximum in the spin-susceptibility (see Fig. 2a for $t' = 0$ and doping $\delta = 0.05$) when accompanied by the formation of a pseudogap in the density of states for temperatures $T < T^*$ (see Fig. 2b). $T^*$ at zero doping is of the order of the magnetic exchange coupling $J = 4t'^2/U = 0.125$. To a very good approximation, $T^*$ is equal to the mean-field Neél temperature. These observations indicate that short-ranged antiferromagnetic correlations are a prerequisite to the pseudogap.

Thus, it is natural to explore the scenario in which the antiferromagnetic short-range order causes the pseudogap. To this end we study the effects of lattice frustration, i.e. of the magnitude of the next nearest neighbor hopping integral $t'$ on the pseudogap. With increasing $|t'|$ the spins on the lattice become frustrated and antiferromagnetic correlations are expected to be suppressed. On the other hand, we expect a possible RVB spin-liquid state to be essentially resistant to, or even be stabilized by finite values of $t'$. In Ref. [7] it was shown that the ground state of the frustrated antiferromagnetic Heisenberg model is almost exactly reproduced by a RVB wave function. In Fig. 2a we plot our results for the antiferromagnetic susceptibility for different values of $t'$. Clearly antiferromagnetic correlations are suppressed as a function of increasing magnitude of $t'$.

On the other hand, the density of states plotted in Fig. 2b remains unchanged near the Fermi surface with increasing magnitude of $t'$. In addition, the temperature $T^*$ where the anomaly in the uniform magnetic susceptibility shown in Fig. 1 occurs, is essentially unaffected by the value of $t'$. Lattice frustration has little effect on the pseudogap. Thus we conclude that short-ranged antiferromagnetic correlations alone cannot be responsible for the evolution of the pseudogap, inconsistent with scenarios based on the coupling of quasiparticles to antiferromagnetic spin-fluctuations $[8]$. Moreover, we infer that these results favor RVB physics over antiferromagnetic short-range order as the origin of the pseudogap.

In the "preformed pairs" scenarios the pseudogap is ascribed to fluctuations that lead to superconductivity at a lower temperature $T_c$. In this case we would expect a corresponding signature in the d-wave pair-field susceptibility, i.e. an enhancement due to pairing correlations in the pseudogap region. In the left panel of Fig. 3 we compare the inverse d-wave pair-field susceptibility $P^{-1}_d$ of the clean system $(x = 0)$ as a function of reduced temperature $T - T_c$ for different dopings $\delta$ in the pseudogap $\delta = 0.025, 0.05$ and overdoped $\delta = 0.20$ regions. Here we are interested in temperatures below $T^*$ indicated by the arrow for $\delta = 0.05$. As the doping increases from the pseudogap to the overdoped region, $P^{-1}_d$ decreases at fixed reduced temperature indicating that pairing correlations in the overdoped region are even more pronounced than in the pseudogap region. Our result in the inset of Fig. 3 for the local cluster $[9]$ equal-time d-wave pair-
Among other scenarios for the pseudogap include the idea of QCP, stripes, and spin-charge separation. In most scenarios, the QCP exists at the zero temperature terminus of $T^*$ versus doping. However, near this point, we find no evidence for a QCP in our simulations; i.e. none of the many susceptibilities that we measure are enhanced as we approach this point. We do not see any signatures of stripes in the charge susceptibility (not shown). However, stripes might be important for larger clusters.

As already discussed, the results for the frustrated system are consistent with a RVB, i.e. spin-charge separated state. In order to address the question of spin-charge separation unambiguously, we would have to calculate the lattice dynamic spin- and charge- structure factors for a range of momenta and extract the spin and charge dispersions. However, these calculations, although formally possible, are presently numerically too expensive to perform. Nevertheless, we believe that we can gain insight into this question by studying the behavior of the corresponding quantities calculated on the cluster only\cite{26}. Preliminary results (not shown here) for the dynamic cluster spin- and charge susceptibilities at low doping are consistent with spin-charge separation: The spin-susceptibility, dominated by fluctuations at $Q = (\pi, \pi)$, becomes suppressed at low frequencies with decreasing temperature well above $T_c$. In the charge-susceptibility, which is strongest at $q = (0, 0)$, weight builds at low frequencies as the temperature is lowered and no sign of a pseudogap is seen.

The results shown in Fig. 4 for the static uniform lattice spin- (circles) and charge-susceptibilities (squares) versus temperature at underdoping ($\delta = 0.05$, left) and overdoping ($\delta = 0.30$, right) support this picture. As already discussed, the spin-susceptibility $\chi_s$ in the underdoped system shows an anomaly at a temperature $T^*$ below which spin-excitations are suppressed. The charge-susceptibility $\chi_c$ in the underdoped system however displays qualitatively different behavior: When the spin degrees of freedom become suppressed at $T \lesssim T^*$, $\chi_c$ starts to rise with decreasing temperature. This clearly indicates that coherence in the charge channel starts to set in with decreasing temperature whereas the spin excitations become suppressed. These results are consistent with recent angle-resolved photoemission experiments \cite{27} where superconducting order in the underdoped system was found to be accompanied by an emerging quasiparticle coherence as seen in the spectra.

Thus, our results for the underdoped region can be interpreted within an RVB, spin-charge separated picture, where the development of the pseudogap originates in the pairing of the spin degrees of freedom and supercondu-
tivity is driven by coherence of the charge excitations. In the overdoped region (right panel in Fig. 4) our results show that the system becomes more conventional, i.e. spin and charge excitations behave in a similar way.

![Figure 4](image-url)

**FIG. 4:** Temperature dependence of the uniform spin and charge susceptibility in the underdoped (left) and overdoped (right) regime when \( U = W = 2, t' = 0 \) and \( N_c = 4 \).

**Summary** We have investigated the microscopic origin of the pseudogap in DCA simulations of the underdoped 2D Hubbard model. We find that short-ranged correlations alone, although necessary for the pseudogap to emerge, is not sufficient to describe its origins. Similarly, although stripe fluctuations may emerge for larger clusters, no indications were found in our calculations, and therefore stripes are not the origin of the pseudogap. Likewise, we find no indication for strong pairing fluctuations for temperatures \( T_c < T < T^* \), in disagreement with pre-formed pairing scenarios. Finally, although we cannot exclude a quantum critical point at finite doping as an origin, we find no evidence for it. Instead, all of our numerical evidence points to spin-charge separation as described by Anderson’s RVB theory as the microscopic origin of the pseudogap. In particular, in the pseudogap region, spin degrees of freedom are suppressed while charge excitations become more coherent with decreasing temperature. At overdoping where no pseudogap is found, spin and charge behave qualitatively similar.

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