Superconductivity and the Pseudogap in the Two-Dimensional Hubbard Model

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Recently developed numerical methods have enabled the explicit construction of the superconducting state of the Hubbard model of strongly correlated electrons in parameter regimes where the model also exhibits a pseudogap and a Mott insulating phase. $d_{x^2-y^2}$ symmetry superconductivity is found to occur in proximity to the Mott insulator, but separated from it by a pseudogapped nonsuperconducting phase. The superconducting transition temperature and order parameter amplitude are found to be maximal at the onset of the normal-state pseudogap. The emergence of superconductivity from the normal state pseudogap leads to a decrease in the excitation gap. All of these features are consistent with the observed behavior of the copper-oxide superconductors.

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Layered perovskite-based copper oxide compounds display three remarkable properties: d-wave superconductivity with unprecedentedly high transition temperatures [1], a nontrivial (''Mott'') insulating state [2], and non-Fermi-liquid physics, most notably a ''pseudogap'' regime in which the density of states is strongly suppressed in some parts of the Brillouin zone but not in others [3]. P. W. Anderson [2] argued that these three classes of phenomena have a common origin as strong-correlation effects understandable in terms of the two-dimensional repulsive Hubbard model, a minimal model of interacting electrons on a lattice with Hamiltonian

$$H = \sum_{p,\sigma} (\epsilon_p - \mu) c^\dagger_{p,\sigma} c_{p,\sigma} + U \sum_i n_{i,\uparrow} n_{i,\downarrow}, \qquad (1)$$

where $\varepsilon_p = -2t(\cos p_x + \cos p_y) + 4t' \cos p_x \cos p_y$ an electron dispersion and $U > 0$ a local interaction which disfavors double occupancy of a site.

In the years since Anderson's paper, the interplay of the pseudogap and superconductivity and the relation of both to the Hubbard model have been of central interest to condensed matter physicists. The existence of d-wave superconductivity in the Hubbard model has been demonstrated by perturbative analytic calculations [4] (later improved by renormalization group methods [5,6]) and by numerics [7,8]. The issue of the pseudogap has been more controversial. It has been variously argued that the pseudogap is a signature of unusual superconducting fluctuations [9–11], of a competing nonsuperconducting phase or regime [3,12], or of physics not contained in the Hubbard model [13]. Theoretical determination of the interplay of the pseudogap and superconductivity in the Hubbard model is important in helping resolve this controversy, and will provide insight into the pseudogap phenomenon and into strongly correlated superconductivity more generally, but this requires access to intermediate or strong couplings for which perturbation theory is inadequate.

The development of cluster dynamical mean field theory [14] has provided important nonperturbative information about the Hubbard model. Dynamical mean field theory approximates the electron self-energy in terms of a finite number of auxiliary functions determined from the solution of an N-site quantum impurity model and becomes exact as N tends to infinity. In this Letter we use dynamical mean field methods to determine the interplay of superconductivity and the pseudogap in the Hubbard model. This is challenging because the theory of the superconducting state involves both normal (N) and anomalous (A) components of the Green's function G and self-energy Σ, leading to a doubling of the size of all matrices involved in the calculation, and hence to at least an eightfold increase in computational burden, which is further increased by the need to reach very low temperatures.

We have constructed the superconducting state and studied its interplay with the pseudogap using clusters of $N = 4, 8, 16$ sites, a size range found in previous work [15] to be large enough to distinguish generic $N \to \infty$ behavior from that specific to particular clusters. Specifics of our methods are given in the Supplemental Material [16]; here we briefly note that a key aspect of our study is the use of recently developed ''submatrix update'' numerical techniques [17–19] which enable access to couplings strong enough to produce a pseudogap at temperatures low enough to construct the superconducting state for cluster size N large enough to reasonably represent the $N \to \infty$ limit. Our key results are that the pseudogap and superconductivity are competing phases and that, remarkably, the onset of superconductivity within the pseudogap phase leads to a decrease in the excitation gap, in sharp contrast

to conventional situations where the onset of superconductivity increases the gap.

Our analysis builds on previous dynamical mean field results. In pioneering papers Lichtenstein and Katsnelson [20] and Maier *et al.* [21] showed that the $N = 4$ cluster dynamical mean field approximation yielded $d_{x^2-y^2}$ superconductivity while subsequent studies of Maier and collaborators [7] on clusters with N as large as 26 provided convincing evidence that the superconductivity found in the small cluster calculations is not an artifact, but rather is a property of the infinite cluster size limit, i.e., of the Hubbard model. However, the studies of Ref. [7] were restricted to a modest interaction, $U = 4t$, too small to give a pseudogap, and to relatively high temperatures, so that the superconducting state was not constructed and transition temperature was inferred from studies of the pair susceptibility. Very recently Yang and collaborators [22] analyzed the pairing susceptibility for higher interaction strengths where a pseudogap occurred, but still did not construct the superconducting state.

The pioneering work of Huscroft *et al.* [23] showed the existence of a normal-state pseudogap in the dynamical mean field approximation and many authors (using mainly $N = 4$ approximations) have studied its properties [24–42] and several groups (still within the 4-site approximation) have studied the interplay of superconductivity and the pseudogap [32,43–47]. A key finding of the 4-site work, in contrast to the larger-cluster studies of Ref. [22] is that superconductivity persists all the way to the Mott insulating boundary, leaving open the question whether it is the pseudogap per se, or simply Mott physics, which suppresses the superconductivity.

More recent developments [18] have enabled researchers to access clusters large enough to obtain a reasonable picture of the $N \to \infty$ limit [15,22,48–52]. It has been found [15] that in the dynamical cluster approximation (DCA) clusters of size $N > 4$ the Mott transition is multistaged, with the fully gapped Mott insulating state being separated from the Fermi liquid state by an intermediate phase, in which regions of momentum space near the $(0, \pi)/(\pi, 0)$ point are gapped and regions of momentum space near $(\pm\pi/2, \pm\pi/2)$ are not. By contrast, in most of the $N = 2, 4$ calculations reported to date there is at half filling no intermediate phase separating the insulator and the Fermi liquid [35,36], while if the insulator is destroyed by doping an intermediate phase with a suppressed, but nonzero, density of states is found [35,36,42]. In this Letter we extend the new methodology to examine the properties of the superconducting state at N large enough to properly represent the pseudogap.

The right-hand panel of Fig. 1 shows the phase diagram determined from a comprehensive survey of parameter space for the $N = 8$ dynamical cluster approximation, which previous work [15] shows adequately represents the $N \to \infty$ normal state physics of the model. Studies of selected U and doping values in the computationally much more expensive $N = 16$ site cluster confirm (lower left panel) that the physics found for $N = 8$ is generic. The scan of the phase diagram is conducted at temperature $T = t/40$ but checks of selected interaction and doping values at our lowest accessible temperature $T = t/60$ (see also Ref. [53]) indicate that lower temperatures do not bring significant changes (see Supplemental Material).

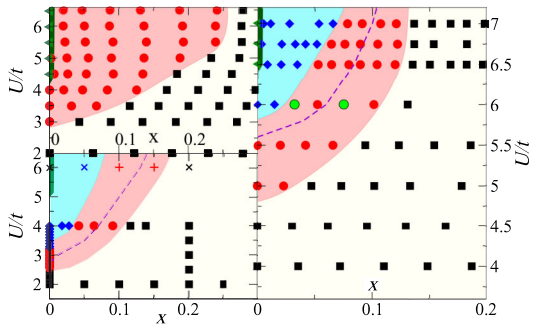

FIG. 1 (color online). Superconducting phase diagram of the two-dimensional Hubbard model in the plane of interaction strength U and carrier concentration x computed using the 8-site (right panel), the 4-site (left upper panel), and 16-site (left lower panel) DCA dynamical mean field approximation at temperature $T = t/40$ with $t'/t = 0$. Dashed line: location of the normal state pseudogap onset. Circles and shading (red online) indicate the superconducting region; squares (black online) and no shading the nonsuperconducting Fermi liquid; diamonds and lighter shading (blue online) the nonsuperconducting pseudogap region; triangles and heavy solid line (dark green online) the Mott insulating region at $n = 1$ and $U > U_c$. Open circles (light green online) denote the points analyzed in Fig. 2. "Cross" and "plus" symbols in the lower left panel denote points determined by Yang *et al.* [22] to be nonsuperconducting and superconducting, respectively.

$d_{x^2-y^2}$-symmetry superconductivity, with a typical transition temperature $\sim t/40 \approx 100$ K (using a $t \approx 0.3$ eV representative of the CuO_2 superconductors) occurs in a band of interaction strength and density, vanishing if interaction or doping is tuned too far away from the insulating state but separated from the Mott insulator by a region of pseudogapped but nonsuperconducting states. This result, previously inferred from extrapolation of the pairing susceptibility [22] at high temperature, is here confirmed. The onset of the normal state pseudogap (dashed line) corresponds to the maximum in the superconducting order parameter (see Supplemental Material [16]) and to the maximum in transition temperature (see below). The inset of Fig. 2, Supplemental Material [16], shows that the superconducting region remains separated from the pseudogap even as $T \to 0$.

The upper left panel shows that the situation is different in the $N = 4$ approximation. In this case, superconductivity extends all the way to the boundary of the Mott phase, as has previously been found [45–47,54]. We believe that the difference arises because in the 8- and 16-site cluster approximations the pseudogap leads at $T = 0$ to a complete suppression of the density of states in the momentum region $(0, \pi)$ important for superconductivity; in the 4-site approximations the pseudogap produces a density of states

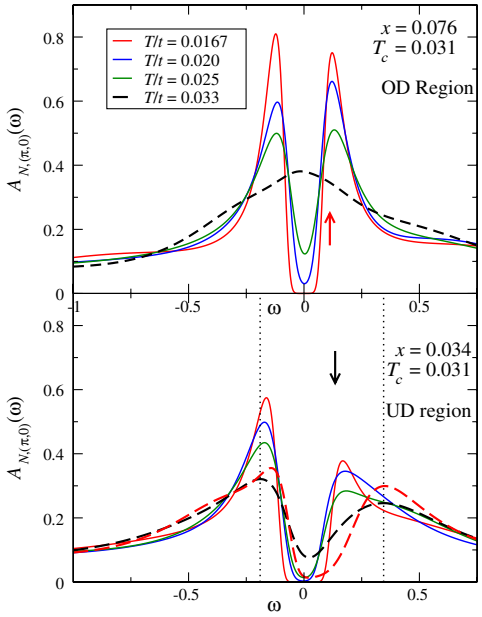

FIG. 2 (color online). Analytically continued spectral function computed at $U = 6t$ for the antinodal sector showing temperature evolution of gap structure for a typical optimally doped or overdoped state ($x = 0.076$, upper panel) and underdoped pseudogap state ($x = 0.034$, lower panel). Solid lines: superconducting spectral function. Heavy dashed lines: normal state spectral function, obtained for $T = t/30$. Light dashed line (lower panel): normal state density of states at $T = t/60$ obtained by suppressing superconductivity. Arrows mark spectral function maxima used to determine superconducting gap size Δ. Dotted lines: pseudogap energy at $T = t/30$ obtained from the maximum in the spectral function.

which is suppressed relative to the Fermi liquid, but is still nonvanishing in the regions important for superconductivity (see, e.g., Fig. 3 of Ref. [36] or Fig. 2 of Ref. [47]). Variational Monte Carlo studies [55–62] also do not find an intermediate nonsuperconducting phase; the difference may have to do with the ability of the variational wave functions to represent the physics of the pseudogap but this issue demands further research.

Figure 2 presents the frequency and temperature dependence of the density of states. The upper panel shows spectra representative of dopings higher than, or interactions weaker than, the values which maximize T_c, so that superconductivity emerges from a relatively conventional normal state. The spectra are consistent with expectations from standard theory [63]: the onset of superconductivity is associated with a suppression of density of states at low frequency and with the formation of density of states ("coherence") peaks. We define the superconducting gap Δ as half of the peak to peak distance. The area in the coherence peaks comes mainly from the states removed at $|\omega| < \Delta$. The gap amplitude develops very rapidly with temperature: only at the temperature closest to T_c is the peak to peak splitting appreciably different from its value at the lowest T.

The situation is quite different when superconductivity emerges from the pseudogap regime. Representative spectra are shown in the lower panel of Fig. 2. The normal state pseudogap is visible at $T > T_c$ as a suppression of the density of states at low frequencies with a broad gap structure at higher frequencies. The $T < T_c$ normal state density of states (obtained by suppressing superconductivity) displays essentially the same behavior. The development of superconductivity is characterized by the formation of coherence peaks at energies *below* the pseudogap, i.e., by a *decrease* in gap magnitude as the superconducting state is entered. This behavior is consistent with recent experimental reports [64] that in underdoped cuprates the emergence of superconductivity out of the pseudogap regime is associated with the formation of new states at energies lower than the pseudogap energy and that the superconducting gap is tied to the pseudogap. Furthermore, most (typically more than 50%) of the spectral weight in the coherence peak is drawn from frequencies greater than Δ.

Figure 3 presents the superconducting transition temperature determined as described in the Supplemental Material [16], as well as the gap values obtained as described above. Similar to the anomalous expectation value (inset, Fig. 1), the transition temperature has a dome-like behavior, with the highest transition temperature occurring near the onset of the normal state pseudogap (insets of Fig. 3), whereas the gap monotonically increases from high to low doping or low to high interaction. We find $2\Delta/T_c \sim 7.5$–8 in the region outside the pseudogap and becoming rapidly larger within the pseudogap regime as the endpoint of the superconducting regime is approached, consistent with dynamical mean field calculations based on 4-site clusters [32,43–47]. In interpreting the numerical value of the gap it is important to note that the DCA procedure, which averages over an entire momentum

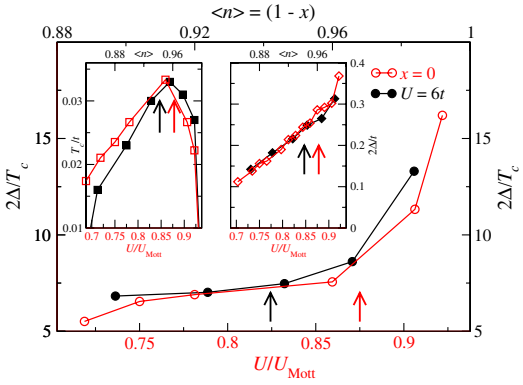

FIG. 3 (color online). Gap to transition temperature ratio $2\Delta/T_c$ (main panel) computed using the 8-site DCA approximation both by varying U at $x = 0$ (open symbols, lower axis, red color, $U_{\mathrm{Mott}} = 6.4t$) and by varying x for $U = 6t$ (filled symbols, upper axis, black). Gap defined as peak to peak distance in analytically continued spectral function. Left inset, squares: doping and interaction dependence of transition temperature for same parameters, showing superconducting dome. Right inset, diamonds: doping and interaction dependence of gap $2\Delta/t$. Arrows: onset of normal state pseudogap.

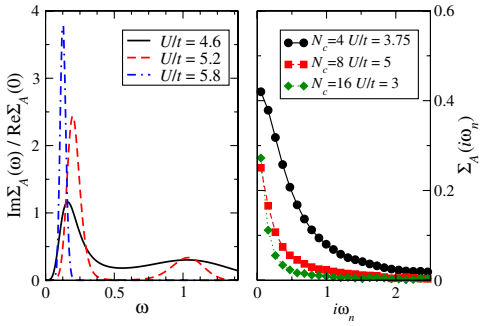

FIG. 4 (color online). Left panel: Imaginary part of self-energy calculated for particle-hole symmetric Hubbard model at $n = 1$, $T = t/60$ and indicated interaction strengths by directly continuing the Matsubara axis self-energy. Right panel: comparison of frequency dependence of anomalous self-energy for 4-, 8-, and 16-site cluster approximations computed at $n = 1$, $T = t/60$, and U values indicated.

sector, places the peak at a somewhat higher energy than the true minimum excitation energy. This difference does not affect the trends of primary interest here.

Further insight into the superconductivity may be obtained from the imaginary part of the real-axis anomalous self-energy obtained by maximum entropy analytical continuation as described in the Supplemental Material [16] and shown in the left panel of Fig. 4. In standard phonon-mediated superconductivity $\mathrm{Im}\Sigma_A$ is peaked at frequencies associated with the phonons [65]. At the weaker coupling $U = 4.6$ $\mathrm{Im}\Sigma_A$ is spread over a range of frequencies up to somewhat larger than $\omega = t$, possibly consistent with a spin fluctuation origin of superconductivity but as the coupling is increased the weight shifts dramatically to lower frequencies, and for the strongest couplings essentially all of the weight is concentrated in a very low frequency peak. This strong coupling behavior is highly unusual, and requires further analysis. We also remark that our 8- and 16-site cluster calculations do not show evidence for the contribution from higher frequency ($\omega \sim U$) scales reported by Ref. [44] (see also [66]). This conclusion is not dependent on analytical continuation: a contribution along the lines of that reported in Ref. [44] would lead to a Matsubara-axis anomalous self-energy which at $\omega \sim 2t$ would be $\sim$20% of its zero frequency value. As can be seen from the right-hand panel of Fig. 4 while in the 4-site cluster the Matsubara axis anomalous Σ function may be different from zero for $\omega \sim 2t$, for the larger clusters it clearly has decayed to zero for $\omega \gtrsim 2t$.

In summary, we have constructed the superconducting phase and analyzed its competition with the pseudogap. We find, robustly over a range of cluster sizes, interaction strengths, and carrier concentrations, that in the Hubbard model the superconducting and pseudogap phases compete. The competition is manifested by the presence of a pseudogapped but nonsuperconducting phase close to the Mott insulator and by a dramatic change in the density of states, in particular a decrease of the gap size when superconductivity emerges from the pseudogap state. In addition, we find that when superconductivity and the pseudogap coexist, the superconductivity is anomalous, with the imaginary part of the self-energies characterized by a sharp large amplitude pole at an energy near zero.

Our results open up important new directions for research. For the two-dimensional Hubbard model fermion sign and matrix size issues restrict us in practice to $N_c \lesssim 16$ and interaction $U \lesssim 7$. These values are large enough to enable access to the doped Mott phase while accessing large enough cluster sizes to obtain reasonable insight into the infinite cluster size limit. Even given these constraints, understanding the anomalous frequency dependence of the anomalous self-energy at strong coupling and further investigation of the interplay between the pseudogap and the superconducting gap, and investigation of two-particle (e.g., Raman) spectra are feasible. In particular the striking similarity between the physical behaviors of the doping-driven and interaction-driven transitions shown in Fig. 3 suggests that the computationally simpler particle-hole symmetric case will provide valuable generally valid information. Going beyond the particle-hole symmetric case, investigations of the effect of second neighbor coupling are important to determine the factors optimizing T_c. Also, a significant difference between our calculations and experiment is that we find a larger anomalous Green function on the electron doped side. Inclusion of long-ranged antiferromagnetism and also extension of our results to the "three-band" copper oxide models is needed to understand these issues further.

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