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# Pairing glue in the two-dimensional Hubbard model

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Cluster dynamical mean-field calculations are used to construct the superconducting gap function of the two-dimensional Hubbard model. The frequency dependence of the imaginary part of the gap function indicates that the pairing is dominated by fluctuations at two characteristic frequencies: one at the scale of the hopping matrix element $t$ and one at a much lower scale. The lower-frequency component becomes more important as the doping is reduced into the pseudogap regime. Comparison to information on the spin-fluctuation spectrum of the model suggests that superconductivity arises from exchange of spin fluctuations. The inferred pairing glue function is in remarkable qualitative consistency with the pairing function inferred from optical conductivity data.

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The physical origin and theoretical understanding of the high transition temperature superconductivity observed [1] in layered copper-oxide materials is an important open issue in condensed-matter physics. One key question [2,3] is the extent to which superconductivity in these materials is due to fluctuations whose exchange provides a "pairing glue," binding electrons together into Cooper pairs. In conventional superconductors such as lead or mercury, superconductivity is generally believed to arise from exchange of phonons, i.e., collective fluctuations of ionic positions, whose properties and coupling to electrons are accurately described by the Migdal-Eliashberg theory [4,5]. In these conventional materials, direct evidence for the importance of phonons was obtained from theoretical [6] and experimental [7] studies of the frequency-dependent gap function, $\Delta(\omega)$, defined in more detail below. Within Migdal-Eliashberg theory, $\Delta(\omega)$ has structure at the frequencies of the bosons making the dominant contribution to the superconducting pairing. It also has structure of the opposite sign at higher frequencies associated with the screened Coulomb interaction, which makes a repulsive contribution to the superconductivity [6]. Observation [7] of these structures provided a definitive confirmation of the role of phonons in conventional superconductors.

The superconductivity in the copper-oxide high-$T_c$ materials is believed to arise from electron-electron interactions, with phonons playing a minimal role. One of the central questions is whether the important effect of the interactions is to produce a collective electronic fluctuation (such as a magnon) whose exchange gives rise to superconductivity [8] or whether there is a pairing tendency intrinsic to strongly correlated materials in the vicinity of a Mott state [2]. In situations where strong electron-electron interactions are dominant, there is no *a priori* reason for Migdal-Eliashberg equations to apply, although proximity to a quantum critical point may justify such a treatment in some cases [9,10]. However, it is plausible that even if a Migdal-Eliashberg treatment is not theoretically justified, the frequency dependence of $\Delta$ may provide insight into the origin of superconductivity, with low-frequency structure indicating fluctuation-mediated pairing while structure at high frequencies (for example, on the order of the bare interaction strength) might indicate a pairing tendency intrinsic to a strongly correlated Mott state [2,3,11].

Here we present results of a study of the $\Delta(\omega)$ corresponding to the $d$-wave superconducting state of the two-dimensional Hubbard model, a candidate model [12] for the description of copper-oxide superconductivity. Our results suggest that superconductivity in this model is, in fact, driven by the exchange of spin fluctuations, but reveals features which remain to be understood. Our work is inspired in part by previous works of Poilblanc, Maier, and Scalapino [3,11]; see also the subsequent work of [13,14] and [15]. Except for Ref. [11], these papers did not analyze the gap function, focusing instead on the anomalous part of the self-energy or the anomalous component of the Green function. There are other technical differences as well, which we will mention below, but our work does agree with the main qualitative conclusion, which is that the dominant contribution to the pairing comes from spin fluctuations.

The Hubbard model may be written in a mixed momentum/position representation as

$$H = \sum_{k\sigma} c^{\dagger}_{k\sigma}\,(\varepsilon_k - \mu)\,c_{k\sigma} + U\sum_i n_{i\uparrow}n_{i\downarrow}, \tag{1}$$

where the operator $c^{\dagger}_{k\sigma}$ creates an electron of spin $\sigma = \uparrow, \downarrow$ in momentum state $k$ and $n_{i\sigma}$ is the operator giving the density of spin $\sigma$ electrons on site $i$. We set the lattice constant to unity. In the case of interest here, the momentum index $k$ runs over the Brillouin zone of a two-dimensional square lattice. The chemical potential is $\mu$ and $\varepsilon_k$ is the energy dispersion, which we take to have the simple nearest-neighbor hopping form $\varepsilon_k = -2t\,(\cos k_x + \cos k_y)$. The two-dimensional square lattice Hubbard model is known to exhibit both a "pseudogap" [16] and $d_{x^2-y^2}$ superconductivity [17–20]. Many properties of the superconducting state, including the doping dependence of the superconducting phase diagram [21] and the interplay of the photoemission [21], Raman, and interplane conductivity spectra [22] with the pseudogap, have been shown to be in good qualitative agreement with experiment. However, the physical origin of the superconductivity has remained unclear.

 

The first issue in our study is the definition of $\Delta$. The electron Green function in the superconducting state may be written on the Matsubara axis as

$$\mathbf{G}(k,i\omega_n)^{-1} = \begin{pmatrix} i\omega_n - \varepsilon_k - \Sigma^N(k,i\omega_n) & \Sigma^A(k,i\omega_n) \\ \Sigma^A(k,i\omega_n) & i\omega_n + \varepsilon_k + \Sigma^N(k,-i\omega_n) \end{pmatrix}, \quad (2)$$

where $\Sigma^{N,A}$ are the normal and anomalous components of the electron self-energy, and we have chosen phases so that the anomalous self-energy is real. Equation (2) implies that

$$\det(G^{-1}) = -\left[1 - \frac{\Sigma_o^N(k,i\omega_n)}{i\omega_n}\right] \times \{\omega_n^2 + [\varepsilon^\star(k,i\omega_n)]^2 + \Delta^2(k,i\omega_n)\}, \quad (3)$$

with

$$\Sigma_{o,e}^N = \frac{\Sigma^N(k,i\omega_n) \mp \Sigma^N(k,-i\omega_n)}{2}, \quad (4)$$

$$\varepsilon^\star = \frac{\varepsilon_k + \Sigma_e^N(k,i\omega_n)}{1 - \frac{\Sigma_o^N(k,i\omega_n)}{i\omega_n}}, \quad (5)$$

$$\Delta(k,i\omega_n) = \frac{\Sigma^A(k,i\omega_n)}{1 - \frac{\Sigma_o^N(k,i\omega_n)}{i\omega_n}} \equiv \frac{2i\omega_n F(k,i\omega_n)}{G(k,i\omega_n) - G(k,-i\omega_n)}. \quad (6)$$

After continuation to the real axis $i\omega_n \to \omega - i\delta$, Eq. (6) becomes $\Delta(\omega) = 2\omega F(k,\omega)/[G(k,\omega) - G^*(k,-\omega)]$. This formula was given by [11], except that the complex conjugation of $G(k,-\omega)$ was omitted.

We identify the Fermi surface (renormalized by interactions and possibly changed by superconductivity) as the locus of $k$ points such that $\varepsilon^\star(k,\omega=0) = 0$ so that $\Delta$ is the gap at the Fermi surface. In the Migdal-Eliashberg theory, the $\Delta$ defined in this way has structure at the frequencies of the pairing phonons. We propose that $\Delta$ contains information about pairing more generally.

To calculate $\Delta$, we use the dynamical cluster approximation (DCA) version [23,24] of cluster dynamical mean-field theory [25] along with the continuous-time auxiliary field (CT-AUX) [26] implementation of the continuous-time quantum Monte Carlo algorithm [27,28] and submatrix updates [29]. In the DCA, the Brillouin zone is partitioned into $N$ equal area tiles labeled by central momentum $K$ and the self-energy is approximated as a piecewise continuous function,

$$\Sigma(k,\omega) = \sum_K^N \phi_K(k)\Sigma_K(\omega), \quad (7)$$

with $\phi_K(k) = 1$ if $k$ is in the tile centered on $K$, and 0 otherwise. The self-energies $\Sigma$ are matrices in Nambu space with normal and anomalous components and are obtained from the solution of an auxiliary quantum impurity model. $\Delta$ is constructed as a function of Matsubara frequencies from the self-energies via Eq. (6).

The expense of the computation increases rapidly with increasing interaction strength, increasing number of approximants $N$, and decreasing temperature. We present results

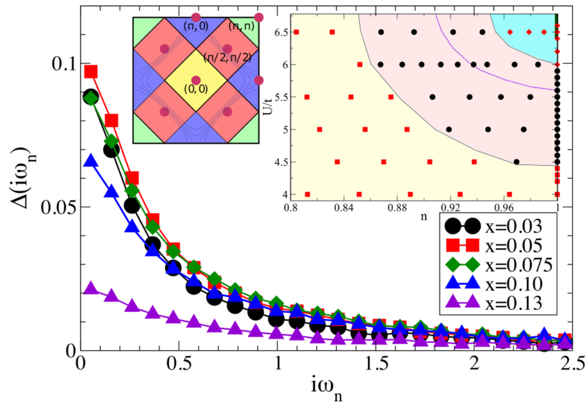


FIG. 1. (Color online) $\Delta(i\omega_n)$ as a function of Matsubara frequency for different dopings at $U = 6t$. Left inset: Momentum-space tiling of the DCA cluster used in this Rapid Communication. Right inset: Phase diagram according to Ref. [30].

for interaction strength $U = 6t$ using $N = 8$ approximants with the standard momentum-space tiling (see left inset to Fig. 1). Previous work [16,21,22] has shown that $N = 8$ is large enough to be representative of the $N \to \infty$ limit, being in particular large enough to represent the difference between zone-diagonal and zone-face electronic properties and therefore large enough to capture the essential physics, including a paramagnetic insulating phase at carrier concentration $n = 1$ per site, a pseudogap regime, and $d_{x^2-y^2}$-symmetry superconductivity existing within a superconducting dome (see phase diagram in right inset of Fig. 1). Comparison of results for various physical quantities including the magnitude of the pseudogap and the density of the pseudogap onset calculated for different cluster sizes suggests quantitative accuracy on the ~25% level [16]. The value $U = 6t$ was chosen to be small enough to permit calculations in the superconducting phase with the precision needed for reliable analytical continuation of self-energies and gap functions, yet large enough to capture the essential physics. However, for $U = 6t$, the superconducting dome is pushed closer to half filling than is the case in actual materials. The eight square tiles are the zone-center and zone-corner momentum sectors $K = (0,0),(\pi,\pi)$, the four symmetry-equivalent zone-diagonal sectors centered on $K = (\pm\pi/2,\pm\pi/2)$, and the two zone-face sectors $K = (\pi,0)$ and $(0,\pi)$. Note that in the $N = 8$ $d$-wave state, symmetry considerations imply that the anomalous self-energy is only nonzero in the sectors centered on $(0,\pi)$ and $(\pi,0)$ and $\Sigma^A_{K=(\pi,0)}(\omega) = -\Sigma^A_{K=(0,\pi)}(\omega) \equiv \Sigma^A(\omega)$. We focus on this sector in what follows, and suppress the explicit momentum arguments.

The CT-AUX method yields results on the imaginary (Matsubara) frequency axis. The main panel of Fig. 1 shows the frequency dependence of the resulting Matsubara-axis gap function for five dopings spanning the superconducting region of the phase diagram. We see that in all cases, the gap function drops rapidly with frequency, becoming indistinguishable from 0 (within our error bars) for Matsubara frequencies greater than about $2.5t$. We also see that the gap function is weakly doping dependent in the middle of the superconducting region, but drops as the edge of the superconducting dome is reached on the high doping side. A similar drop in $\Delta$ occurs on the low doping side of the superconducting dome. The start of this drop may be seen in the $x = 0.03$ data.

We now turn to the behavior of $\Delta$ on the real frequency axis. Viewed as a function of complex variable $z$, $\Delta(z)$ is analytic in the complex plane except for a branch cut along the real frequency axis, $\mathrm{Im}z = 0$. It has a spectral representation

$$\Delta(z) = \int \frac{dx}{\pi} \frac{\mathrm{Im}\Delta(x)}{z - x}. \tag{8}$$

The spectral function $\mathrm{Im}\Delta(x)$ is the object of primary physical interest in the Migdal-Eliashberg-Scalapino-Rowell analysis [6,7]. Direct inversion of Eq. (8) to find $\mathrm{Im}\Delta$ in terms of the computed quantity $\Delta(i\omega_n)$ is a mathematically ill-posed problem, necessitating use of a numerical analytical continuation process [31]. The Matsubara axis $\Delta$ is an even function of frequency, implying that the spectral function $\mathrm{Im}\Delta$ is an odd function of frequency, whereas the standard maximum entropy continuation methodology [31] requires a non-negative spectral function. We therefore rearrange Eq. (8) as

$$\Delta(i\omega_n) = \Delta(i\omega_n = 0) + i\omega_n \int \frac{dx}{\pi} \frac{\frac{\mathrm{Im}\Delta(x)}{x}}{i\omega_n - x} \tag{9}$$

and continue $\frac{\Delta(i\omega_n) - \Delta(i\omega_n = 0)}{i\omega_n}$ by standard methods. We obtain $\Delta(i\omega_n = 0)$ by fitting $\Delta(i\omega_{n=1,2,3})$ at the lowest three Matsubara frequencies to a parabola.

A potentially serious difficulty is that there is no guarantee that $\mathrm{Im}\Delta/\omega$ (or, equivalently, $\mathrm{Im}\Sigma^A/\omega$) is of definite sign. For example, in the usual Migdal-Eliashberg theory, the Coulomb pseudopotential leads to a sign change at frequencies somewhat above the phonon frequencies, reflecting the repulsive (depairing) contribution of the Coulomb repulsion in conventional metals [6]. Reference [11] presented exact-diagonalization results for the t-J model consistent with a non-negative $\Sigma^A(\omega)/\omega$ (note that the time-ordered F is displayed in that paper) and the $\Sigma^A$ presented in Ref. [15] is non-negative. The results presented in Ref. [3], on the other hand, are consistent with a weakly negative $\Sigma^A$ at higher frequencies, while Ref. [14] displays a $\mathrm{Im}\Sigma^A(\omega)/\omega$ with large-amplitude high-frequency oscillations. A recent solution of the Eliashberg equations for a model involving two competing spin fluctuations also displayed a sign change in the gap function as frequency was increased above a characteristic frequency [32].

We have investigated the sign of $\mathrm{Im}\Delta(\omega)/\omega$ in two ways. First, we cross-checked our results by use of a Padé continuation method [33] that makes no assumption about the sign of $\mathrm{Im}\Delta(\omega)/\omega$. This method consistently found a positive-definite $\mathrm{Im}\Delta(\omega)/\omega$ with no evidence for any sign change. Second, we considered the particle-hole symmetric ($n = 1$) situation. In this case, the self-energy for the $(\pi,0)$ sector is also particle-hole symmetric and obeys the condition $\Sigma^N(z) = -\Sigma^{N,*}(-z)$, so that the impurity model Green function [in the $K = (0,\pi)$ sector] and the self-energy matrix are diagonalized at all frequencies by the Majorana combinations $c^\dagger_{k\sigma} \pm c_{-k,-\sigma}$. In this $\pm$ basis, we have

$$\Sigma^{\pm}(z) = \Sigma^N(z) \pm \Sigma^A(z). \tag{10}$$

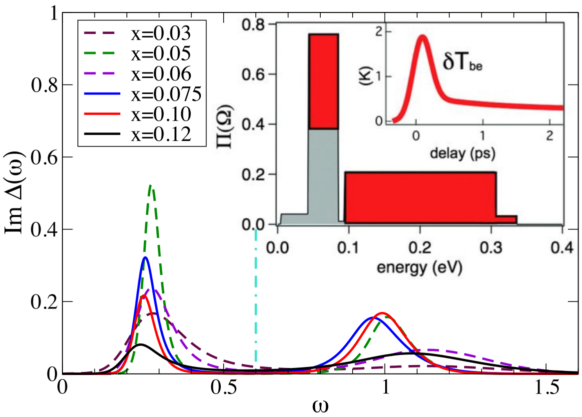


FIG. 2. (Color online) Main panel: Imaginary part of real frequency gap function computed for different dopings. Dashed curves label dopings within the pseudogap regime and solid curves label dopings outside the pseudogap regime. The vertical dashed line indicates the frequency cutoff chosen in the inset of Fig. 3. Inset: Experimental data reproduced from Ref. [34].

Because the Greens function and $\Sigma$ are diagonal in the $\pm$ basis, the associated spectral functions are positive definite, and standard maximum entropy methods may be used. We have constructed $\mathrm{Im}\Delta$ in the $\pm$ basis for a range of $U$ at $n = 1$, finding results in agreement with direct continuations of $\Delta$ obtained on the assumption that the spectral function associated with $\Sigma^A$ is non-negative. We also constructed $\Delta$ from the continuation of Eq. (6), again finding a non-negative $\mathrm{Im}[\Delta(\omega)]/\omega$ in close agreement with the direct continuation [although sign changes can occur if the complex conjugation mentioned below Eq. (6) is omitted]. We do not find large negative excursions such as that shown in the range $0.5t \lesssim \omega \lesssim t$ in Ref. [11].

Figure 2 shows our principal results: the imaginary part of the gap function of the Hubbard model, computed for different dopings in the superconducting regime of the phase diagram. The support for the spectral function is concentrated in two regions: a peak at the very low frequency $0.25t \lesssim 0.1$ eV (with the usual identification $t \sim 0.3$ eV for cuprates) and a higher peak at a frequency $\sim t$. This two-peak structure is robustly found in continuations of all of our superconducting state data and, although the method is subject to non-negligible systematic uncertainties especially at higher frequencies, the crucial aspects of the results can be inferred directly from the Matsubara-axis data.

The first important qualitative result is that $\mathrm{Im}\Delta$ has negligible support at frequencies higher than those shown in Fig. 2. This result is confirmed by the rapid decrease of $\Delta$ with increasing Matsubara frequency displayed in Fig. 1. If $\mathrm{Im}\Delta$ had significant support at higher frequencies, $\Delta(i\omega_n)$ would not decrease so rapidly to zero. In particular, Ref. [3] reported results of a study of the $N = 4$ approximation, using a non-crossing approximation (NCA) impurity solver, that about 20% of the pairing came from much higher frequencies, of the order of $U$. If this were the case, $\Delta(i\omega_n \approx 2t)$ would be about 20% of its value at $\omega_n = \pi T$. Our Matsubara-axis data clearly rule out this possibility, and a previous analysis of the $N = 4$ approximation by [13] (cf. Fig. 5) also found that $\mathrm{Im}\Sigma^A$ goes rapidly to 0 for frequencies above $\sim 1.5t$. The difference may arise from the use of the NCA solver in Ref. [3]. We conclude that in the Hubbard model, pairing comes from frequencies at most of order $\sim t$, well below the energy of the upper Hubbard band.

We now turn to the detailed frequency dependence. The existence of a very low-frequency peak ($\omega \sim 0.25t \sim 75$ meV) in Im$\Delta$ is a surprising feature of our results. We believe that it is not an artifact of the maximum entropy analytical continuation method used here, which is generally found to yield reliable results for the lowest-frequency features. We have confirmed the results by performing Padé continuations (not shown), which reproduce the position and spectral weight of the low-frequency peak. The existence of significant spectral weight at higher frequencies is also directly implied by the Matsubara-axis data: analysis (not shown) of the data in Fig. 1 reveals that $\Delta(i\omega_n)$ decays more slowly than $\omega_n^{-2}$ for $\omega_n \lesssim t$, contradicting the hypothesis that the $\omega \approx 0.25t$ feature is the only structure in Im$\Delta$. Our experience is that for higher-frequency features, maximum entropy analytical continuation provides reasonable estimates for spectral weights in given frequency regimes, but is not necessarily reliable for the precise position and shape of spectral features. Thus, we believe that while the existence of a low-frequency peak and a higher-frequency structure in Im$\Delta$ as well as their relative weights is clearly established, the structure of two sharp peaks indicated by the analytical continuation is not yet proven. Further, the discretization of momentum space inherent in the DCA may also affect the frequency dependence. We may speculate that the true $N \to \infty$ limit of the model would exhibit a sharp onset at the low frequency followed by a gradual decay over the range $\omega \sim t$. Larger clusters, not accessible with present resources, or other methods would be needed to establish whether this actually occurs.

The fact that Im $\Delta$ is non-negligible only at frequencies $\omega \lesssim t \approx 0.3$ eV, which are low compared to the intrinsic scales of the model such as bandwidth, suggests that the superconductivity arises from exchange of a relatively low-frequency collective electronic excitation. We observe that in the Hubbard model at these interaction scales, the basic spin-fluctuation energy (zone-boundary magnon frequency) $\omega_{\mathrm{SF}}$ is of the order of $t$. This may be seen from Fig. 1 of Ref. [35] (note that the two-magnon peak in the Raman scattering occurs at about the same energy as the maximum of the single-magnon energy); see also Fig. 3 of Ref. [3]. This suggests, in agreement with the results of Refs. [3,11,14,15], that the pairing is spin-fluctuation driven.

The sharp low-frequency peak is remarkable. The inset of Fig. 3, which compares $\int_0^{0.6t} \mathrm{Im}\Delta(\omega)d\omega$ to $\int_0^{2.0t} \mathrm{Im}\Delta(\omega)d\omega$, shows that the relative importance of the low-frequency feature increases slowly as doping is decreased into the pseudogap regime, while the peak position is seen to be approximately the same for all dopings. Note that published results for Im$\Sigma^A$ reveal a low-frequency peak which dramatically changes strength and position as doping is decreased [14,15]; we believe that this is an expression of normal-state physics not directly related to pairing and that the pairing is more accurately represented by $\Delta$. We also note that Fig. 1 shows that the gap value $\approx \lim_{\omega\to 0} \Delta(i\omega_n)$ varies substantially with doping. We therefore believe that although for intermediate dopings

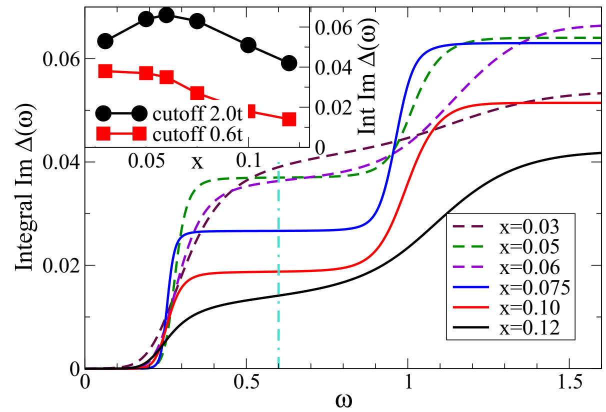


FIG. 3. (Color online) Main panel: Partial integral of Im$\Delta(\omega)$ for the dopings of Fig. 1 up to $\Omega = 1.6t$. Vertical dashed line: Cutoff frequency used in inset. Inset: Integral over the entire frequency range and over the range of the low-frequency pole, as a function of doping.

the peak energy is approximately three times the gap value, the peak feature is not simply an above-gap excitation, but corresponds to a physically significant fluctuation, related in some way to the pseudogap. In remarkable recent experiments [34,36], optical measurements were used to infer a pairing glue spectrum consisting of a sharp peak centered at $\omega \approx 0.07$ eV and a broad continuum extending up to $\approx 0.3$ eV, in striking agreement with the numerical results presented here. Further investigation of the physics of this structure is an important open problem.

It is interesting to speculate on the relation of the structure shown in Fig. 3 to the doping dependence of the transition temperature shown in Fig. 1 of Ref. [22]. The transition temperature is maximal at approximately the pseudogap boundary ($x \approx 0.06$ for the parameters used here); the decrease in $T_c$ as doping is further decreased would then be interpreted as arising from loss of intensity in the higher-frequency $\omega \sim t$ structure in $\Delta$, i.e., to a weakening of the higher-frequency part of the pairing glue.

In conclusion, we have revealed insights into the superconducting state of the two-dimensional Hubbard model. A definition of the gap function valid beyond the Migdal-Eliashberg approximation was introduced, and structure in this gap function was found to indicate that superconductivity arises from exchange of relatively low-frequency collective electronic fluctuations, presumably of magnetic origin. However, the gap function exhibits an unanticipated very low-frequency ($\sim 0.25t$) feature of unknown origin. Understanding the physics of this feature is an important open question. We also remark that neither the Matsubara-axis nor the continued data provide evidence for the power-law scaling of $\Delta$ predicted by quantum critical theories of strongly correlated superconductivity [10].

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