Frequency-dependent structure of superconducting gap function in two-dimensional Hubbard model

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Abstract. The frequency dependence of the superconducting gap function represents the dynamics of the electrons forming the Cooper pairs. Bearing the high-temperature superconducting cuprates in mind, we calculate the superconducting gap function in the two-dimensional Hubbard model by means of a cluster extension of the dynamical mean-field theory. We scrutinize the frequency dependence and its change with temperature, doping concentration and interaction strength. The calculated superconducting gap function shows various different behaviors from the anomalous self-energy, owing to a strong frequency dependence of the normal self-energy. The calculated results also suggest that the superconductivity is stronger when the interaction strength is as large as or slightly smaller than the bare band width and is suppressed for larger interactions.

1. Introduction
The Cooper pairing in a superconductor ricochets through the dynamics of quasiparticles. In conventional superconductors, the understanding of the quasiparticle dynamics served to establish the phonon-mediated mechanism of the pairing [1]: A frequency-dependent superconducting gap function, extracted from an experimental tunneling-conductance spectrum through the Migdal-Eliashberg theory [2], conformed to a measured phonon spectrum, giving a firm evidence of the phonon glue.

In cuprate high-temperature superconductors, however, no consensus has been achieved on the pairing mechanism. It is then of great interest to elucidate the quasiparticle dynamics in the cuprates. In particular, in analogy with the conventional superconductors, the frequency dependence of the superconducting gap function may hold a key to unveiling the pairing mechanism. However, because of the $d$-wave momentum dependence of the superconducting gap, it is not easy to extract the gap function from the tunneling data. Moreover, the applicability of the Migdal-Eliashberg theory itself has not been established for the cuprates [3]. These difficulties have prevented the cuprates from in-depth studies of quasiparticle dynamics.

A theoretical development in the past few decades, on the other hand, has made it possible to calculate the superconducting gap function in an unbiased nonperturbative way. In particular, cluster extensions [4, 5, 6] of the dynamical mean-field theory [7, 8] (CDMFT) have been developed and applied to the two-dimensional (2D) Hubbard model, a standard model for the cuprates. These studies have revealed the presence of a sharp low-energy peak in the superconducting gap function or the anomalous self-energy [9, 10, 11, 12, 13, 14]. This is reminiscent of the phonon peak in the conventional strong-coupling superconductors but is
emergent from strong electronic correlation effects in the Hubbard model. A quantitative analysis of this peak’s contribution [9] indeed showed that the peak gives a major contribution to the superconductivity and therefore is at the origin of high critical temperature \( T_c \). In Ref. [13] we revealed that this peak originates from a hybridization of a low-energy electron with a hidden fermionic excitation emergent from the strong correlation effect. We then clarified in detail the changes of the self-energy structure with doping, temperature, and interaction strength [15]. In this paper, we focus on the changes of the superconducting gap function against these parameters, providing a complementary data to the self-energy presented in Ref.[15].

2. Model and method

We study the 2D single-band Hubbard model on a square lattice. The Hamiltonian reads

\[
H = \sum_{k\sigma} \epsilon(k) c_{k\sigma}^\dagger c_{k\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow},
\]

where \( c_{k\sigma} (c_{k\sigma}^\dagger) \) annihilates (creates) an electron with spin \( \sigma \) and momentum \( k = (k_x, k_y) \), \( c_{i\sigma} \) \((c_{i\sigma}^\dagger)\) is its Fourier component at site \( i \), and \( n_{i\sigma} \equiv c_{i\sigma}^\dagger c_{i\sigma} \). Here, \( U \) denotes the onsite Coulomb repulsion and

\[
\epsilon(k) \equiv -2t(\cos k_x + \cos k_y) - 4t' \cos k_x \cos k_y - \mu
\]

is the bare dispersion with \( t \) ( \( t' \) ) being the (next-)nearest-neighbor transfer integral and \( \mu \) being the chemical potential. We take \( t = 1 \) as the unit of energy and \( t' = -0.2 \) throughout the paper. For real cuprates, \( t \) is estimated to be \( \sim 0.3eV \).

CDMFT [5] maps in a self-consistent way the model (1) onto an effective impurity problem consisting of a small interacting cluster coupling to a dynamical mean field which is a function of Matsubara frequency \( \omega_n = i(2n + 1)\pi T \). Here, \( T \) is the temperature. We solve the effective impurity problem with a finite-temperature version [16] of the exact diagonalization method [17] which is extended to a superconducting state [18, 13]. We use a \( 2 \times 2 \) cluster and eight-site bath which represent the dynamical mean field. After a self-consistent loop converges, we calculate the real-frequency \( (\omega) \) properties, by replacing \( i\omega_n \) with \( \omega + i\eta \), where \( \eta = \eta_0(1 + \omega^2) \) with \( \eta_0 = 0.05 \) is a smearing factor (though in the following equations, we omit the factor \( i\eta \) for simplicity). For more details, we refer the readers to Ref.[15].

A typical output of the CDMFT is the single-particle Green’s function. In the superconducting state, it is written in the Nambu-matrix form as

\[
\hat{G}(k, \omega) = \begin{pmatrix}
G(k, \omega) & F(k, \omega) \\
F(k, \omega)^* & G(k, -\omega)^*
\end{pmatrix},
\]

where \( G ( F) \) is the retarded normal (anomalous) Green’s function. Here we have chosen the \( U(1) \) gauge to make the two anomalous components be the same. The normal and anomalous self-energies, \( \Sigma^{nor} \) and \( \Sigma^{ano} \), are defined by

\[
\begin{pmatrix}
\Sigma^{nor}(k, \omega) & \Sigma^{ano}(k, \omega) \\
\Sigma^{ano}(k, \omega)^* & \Sigma^{nor}(k, -\omega)^*
\end{pmatrix} = \begin{pmatrix}
\omega - \epsilon(k) & 0 \\
0 & \omega + \epsilon(k)
\end{pmatrix} \left[ \hat{G}(k, \omega) \right]^{-1}.
\]

With \( \Sigma^{nor} \) and \( \Sigma^{ano} \) obtained above, the superconducting gap function \( \Delta \) is defined by [19]

\[
\Delta(k, \omega) = \Sigma^{ano}(k, \omega) \left[ 1 - \frac{1}{2\pi \omega} \Sigma^{nor}(k, \omega) - \Sigma^{nor}(k, -\omega)^* \right].
\]

With the \( 2 \times 2 \) cluster, a direct calculation is possible only at four momentum points: \((0,0), (\pi,0), (0,\pi)\) and \((\pi,\pi)\), among which only the \((\pi,0)\) and \((0,\pi)\) points (both of which are equivalent by symmetry except for the sign of the anomalous component) possess the anomalous component in the \( d \)-wave superconducting state. Therefore, we focus only on \( k = k_{AN} \equiv (0, \pi) \) in the following.
3. Results and discussions
We first show in figure 1 the temperature evolution of the anomalous functions, $\Delta$, $\Sigma^{ano}$, and $F$ at the electron density $n \simeq 0.95$. As we see that these anomalous functions vanish at $T = 0.06$ and become finite for $T \leq 0.05$, we find $0.05 < T_c < 0.06$. As $T$ decreases, the amplitudes of $\Delta$, $\Sigma^{ano}$ and $F$ increase, with a peak developing at low energy in their imaginary parts. The scale of $\Delta$ is much smaller than that of $\Sigma^{ano}$ because $\Sigma^{or}$, appearing in the denominator of Eq. (5), is substantial and suppresses $\Delta$, as we discuss in more detail below. It would be interesting to point out here that these low-energy peaks of $\text{Im}\Delta$ and $\text{Im}\Sigma^{ano}$ shift to higher energy with lowering $T$ while the (negative) peak of $\text{Im}F$ shifts to lower energy.

Figure 2 shows the doping evolution of the anomalous functions at $T = 0.01$ in the superconducting state. Note that in the present $2 \times 2$ CDMFT calculation, the optimal doping is located around 10%, i.e., $n \simeq 0.9$ (see figure 2(a) in Ref.[15]). As the doping increases, the peaks of $\text{Im}\Delta$ and $\text{Im}\Sigma^{ano}$ shift to lower energies with decreasing amplitude. Around the peak energy of $\text{Im}\Delta$, $\text{Re}\Delta$ changes its sign and is enhanced at low energy. This lifts the value of the “BCS” (static) gap, defined by

$$\text{Re}\Delta(k, \omega = 0) = \frac{2}{\pi} \int_{0}^{\infty} \frac{\text{Im}\Delta(k, \omega')}{\omega'} d\omega',$$

as was first pointed out in Ref.[9].

In order to quantify the contribution from the low-energy peak in $\text{Im}\Delta$ to the static part of the gap, we define the following function,

$$I(k, \Omega) = \frac{2}{\pi \text{Re}\Delta(k, \omega = 0)} \int_{0}^{\Omega} \frac{\text{Im}\Delta(k, \omega')}{\omega'} d\omega',$$

Figure 1. (Color online). Anomalous functions for various temperatures at $U = 8$ and $n \simeq 0.95$. $t = 1$ is the unit of energy. (a), (b), (c) Imaginary parts of $\Delta$, $\Sigma^{ano}$, and $F$, respectively. (d), (e), (f) The corresponding real parts. Note that the real (imaginary) part is (anti)symmetric with respect to $\omega = 0$ and we have shown only the positive-energy side.
Figure 2. (Color online). Anomalous functions for various electron densities at \( T = 0.01 \) and \( U = 8 \). \( t = 1 \) is the unit of energy.

Figure 3. (Color online). (a) \( \text{Im}\Delta(k_{AN}, \omega)/\omega \) at various dopings for \( T = 0.01 \) and \( U = 8 \). \( t = 1 \) is the unit of energy. (b) \( I(k_{AN}, \Omega) \) [defined by Eq. (7)] corresponding to the data in panel (a). (c) \( \text{Im}\Delta, \text{Im}\Sigma^{ano}, \) and \( 1 - \text{Re}[\frac{1}{2\omega}\{\Sigma^{\text{nor}}(k, \omega) - \Sigma^{\text{nor}}(k, -\omega)^*\}] \) [i.e., the real part of the denominator of Eq. (5)] at \( k = k_{AN} \) for \( T = 0.01 \), \( U = 8 \) and \( n = 0.965 \). The blue dot denotes the zero of \( 1 - \text{Re}[\frac{1}{2\omega}\{\Sigma^{\text{nor}}(k, \omega) - \Sigma^{\text{nor}}(k, -\omega)^*\}] \), which gives the peak of \( \text{Im}\Delta \).

in a way similar to that used in Ref.[9] for \( \Sigma^{ano} \). Figure 3(a) plots the integrand of Eq. (7) as a function of \( \omega \) at \( k = k_{AN} \). It shows a low-energy peak for all the dopings studied here. As the doping increases, the peak shifts to a lower energy with decreasing the intensity. Figure 3(b) shows that \( I(k_{AN}, \Omega) \) increases rapidly at around the peak energy. For example, for \( n = 0.965 \),
the low-energy peak in figure 3(a) is located below $\omega \simeq 1$. Then, looking at figure 3(b), we find that $I(k_{AN}, \Omega = 1)$ exceeds 1: A small negative part of $\text{Im}\Delta/\omega$ above $\omega \simeq 1$ remedies the overshoot eventually. For $n = 0.932$ and 0.883, too, $I(k_{AN}, \Omega = 1)$ reaches $\sim 0.8$, manifesting the significant contribution from the low-energy peak. For $n = 0.837$, higher-energy structures also gives a substantial contribution [11] while the low-energy peak still has a major contribution $[I(k_{AN}, \Omega = 0.3) \simeq 0.5]$.

According to the change of the self-energies, the peak of $\text{Im}F$ also shifts to lower energy with doping while the height of the (negative) peak shows a nonmonotonic behavior [figure 2(c)]: It seems to be maximized around the optimal doping. On the other hand, the width of the peak decreases monotonically with doping. As a consequence, $[\text{Re}F(k_{AN}, \omega = 0)]$ increases monotonically with doping while the low-energy area of $\text{Re}F < 0$ becomes narrower. Furthermore, above the energy of that structure, there remains a substantial area of $\text{Re}F > 0$ even at the lowest density $n = 0.837$. These nontrivial behaviors give the domelike doping dependence of the superconducting order parameter [figure 2(a) in Ref. [15]], which corresponds to an $\omega$ integral of $F$.

Another interesting observation in figures 1 and 2 is that the peak of $\text{Im}\Delta$ is always located at an energy higher than that of $\text{Im}\Sigma^{\text{ano}}$. This is different from conventional superconductors, where $\Delta \propto \Sigma^{\text{ano}}$ holds so that their peak positions coincide. According to Eq. (5), the difference between $\Delta$ and $\Sigma^{\text{ano}}$ is ascribed to the denominator on the right hand side of the equation. In conventional superconductors, the frequency dependence of $\Sigma^{\text{nor}}$ is so weak that this denominator is well approximated by an $\omega$-independent renormalization factor at low frequencies. On the other hand, in the superconducting state of the 2D Hubbard model, $\Sigma^{\text{nor}}$ has a strong frequency dependence; in Eq. (5) it eliminates the peak of $\text{Im}\Sigma^{\text{ano}}$ in the numerator and creates another peak at a higher energy. In fact, as we showed in Ref. [13, 15], $\text{Im}\Sigma^{\text{nor}}$ shows peaks at the same energy as $\text{Im}\Sigma^{\text{ano}}$, cancelling the peak of $\text{Im}\Sigma^{\text{ano}}$. The peak of $\text{Im}\Delta$ is then generated by the zero of $1 - \text{Re}\frac{1}{\omega}[\Sigma^{\text{nor}}(k, \omega) - \Sigma^{\text{nor}}(k, -\omega)^*]$, i.e., the real part of the denominator in Eq. (5). Figure 3(c) demonstrates this: At the energy where $\text{Im}\Delta$ shows a peak, the equation, $1 - \text{Re}\frac{1}{\omega}[\Sigma^{\text{nor}}(k, \omega) - \Sigma^{\text{nor}}(k, -\omega)^*] = 0$, is satisfied while the peak of $\text{Im}\Sigma^{\text{ano}}$ is located at a lower energy.

The strongly frequency-dependent structure of $\Sigma^{\text{nor}}$ is produced by an underlying self-energy pole, which generates the pseudogap above $T_\text{c}$ [20, 21, 22, 23, 24, 25, 26, 27, 28, 29]. The self-energy pole can emerge purely from the strong electronic correlation effect in the proximity to the Mott insulator, without breaking any symmetry. This self-energy pole can be interpreted as a fermionic excitation (hidden fermion) coupling to the electron. Then, by considering a Cooper pairing of these hidden fermions, we can explain at least qualitatively all the above nontrivial relations between $\Delta$, $\Sigma^{\text{ano}}$ and $\Sigma^{\text{nor}}$ [13, 15].

Figure 4 compares the anomalous functions at several values of $U$. From $U = 6$ to 8, we see that the amplitude of $\Sigma^{\text{ano}}$ increases. Nevertheless, $\Delta$ does not change significantly, which should again be attributed to the increase of $\Sigma^{\text{nor}}$. From $U = 8$ to 12, however, $\Delta$ shrinks in accordance with the suppression of $\Sigma^{\text{ano}}$. In contrast to these behaviors, $\text{Im}F$ shows a strongest peak at $U = 6$, where $|\text{Re}F(k_{AN}, \omega = 0)|$ is also largest, and shrinks monotonically as $U$ increases. This is qualitatively the same as the behavior of the order parameter; $\langle \epsilon_{i\uparrow}\epsilon_{j\downarrow} \rangle = 0.025$ ($U = 6$), 0.019 ($U = 8$), and 0.014 ($U = 12$), where $i$ and $j$ denote the nearest neighboring sites. Thus, the anomalous functions behave differently from each other while they all indicate the strongest superconductivity for $U = 6 - 8$ and a suppression of it for $U = 12$.

4. Conclusion
We have calculated the frequency dependence of the anomalous functions, $\Delta$, $\Sigma^{\text{ano}}$ and $F$, in the superconducting state of the 2D Hubbard model, with systematically changing the temperature, electron density and interaction strength. In particular, we have focused on the behavior of the
Figure 4. (Color online). Anomalous functions at several values of $U$ for $k = k_{AN}$, $T = 0.01$ and $n = 0.95$. $t = 1$ is the unit of energy.

low-energy peak seen in $\text{Im}\Delta$, which is at the origin of high $T_c$. We have shown that this peak is located at the zero of $1 - \text{Re}\sum_{\text{nor}}(k, \omega) - \sum_{\text{nor}}(k, -\omega^*)$ rather than the peak position of $\text{Im}\Sigma_{\text{ano}}$, unlike the conventional strong-coupling superconductors. This highlights a crucial role of frequency-dependent $\Sigma_{\text{nor}}$, which also manifests itself in the $U$ dependence of $\Delta$. This latter result suggests that $U = 6 - 8$ is an optimal interaction strength for superconductivity. The different behaviors between $\Delta$ and $\Sigma_{\text{ano}}$, owing to the significant contribution from $\Sigma_{\text{nor}}$, suggest that a special care (as indicated in Ref. [13, 15]) is needed to extract the superconducting gap function, as well as the self-energy, from the experimental data on cuprates.

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