Dynamics of the Pairing Interaction in the Hubbard and *t*-*J* Models of High-Temperature Superconductors

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The question of whether one should speak of a ''pairing glue'' in the Hubbard and *t*-*J* models is basically a question about the dynamics of the pairing interaction. If the dynamics of the pairing interaction arises from virtual states, whose energies correspond to the Mott gap, and give rise to the exchange coupling *J*, the interaction is instantaneous on the relative time scales of interest. In this case, while one might speak of an ''instantaneous glue,'' this interaction differs from the traditional picture of a retarded pairing interaction. However, as we will show, the dominant contribution to the pairing interaction for both of these models arises from energies reflecting the spectrum seen in the dynamic spin susceptibility. In this case, the basic interaction is retarded, and one speaks of a spin-fluctuation glue which mediates the *d*-wave pairing.

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The question of whether the pairing interaction in the cuprate superconductors should be characterized as arising from a ''pairing glue'' has recently been raised [1]. As we will discuss, this is a question about the dynamics of the pairing interaction, and it will be answered when we know more about the frequency dependence of the cuprate superconducting gap. From the *d*-wave ($\cos k_x - \cos k_y$) momentum dependence of the cuprate gap, we know that the pairing interaction is spatially a short-range, dominantly near-neighbor attraction. However, in spite of pioneering angle-resolved photoemission spectroscopy [2–6], tunneling [7–9], and infrared conductivity [10,11] studies, we do not yet have sufficient information to definitively characterize its dynamics. Thus, while there is a growing consensus that superconductivity in the high T_c cuprates arises from strong short-range Coulomb interactions between electrons rather than the traditional electron-phonon interaction, the precise nature of the pairing interaction remains controversial.

This is the case even among those who agree that the essential physics of the cuprates is contained in the Hubbard and *t*-*J* models. For example, both Anderson's resonating-valence-bond (RVB) theory [12] and the spin-fluctuation exchange theory [13–15] lead to a short-range interaction which forms $d_{x^2-y^2}$ pairs. However, the dynamics of the two interactions differ. In the RVB picture, the superconducting phase is envisioned as arising out of a Mott liquid of singlet pairs. These pairs are bound by a superexchange interaction J which is proportional to t^2/U. Here t is the effective hopping matrix element between adjacent sites, and U is an on site Coulomb interaction. J is determined by the virtual hopping of an electron of a given spin to an adjacent site containing an electron with an opposite spin [16]. Thus, the dynamics of J involves virtual excitations above the Mott gap, which is set by U, and the pairing interaction is essentially instantaneous. In this case, as Anderson has noted [1], one should not speak of a ''pairing glue'' in the same sense that this term is used when referring to a phonon-mediated interaction. In the spin-fluctuation exchange picture, the pairing is viewed as arising from the exchange of particle-hole spin fluctuations whose dynamics reflect the frequency spectrum seen in inelastic magnetic neutron scattering. This spectrum covers an energy range which is small compared with U or the bare bandwidth $8t$. In this case, the pairing interaction is retarded, and, in analogy to the traditional phonon mediated pairing, one says that the spin fluctuations provide the pairing glue. So the question of whether there is a pairing glue offers a way of distinguishing different pairing mechanisms. Here by using numerical techniques we show that the dominant contribution to the pairing interaction is associated with the spectral region characteristic of the spin fluctuations. This suggests that the cuprate dynamic spin susceptibility measured by inelastic neutron scattering should be reflected in the frequency dependence of the *d*-wave gap.

In the superconducting state, the Nambu self-energy $\hat{\Sigma}(k, \omega)$ can be parametrized as

$$\hat{\Sigma}(k, \omega) = [1 - Z(k, \omega)] w \tau_0 + X(k, \omega)\tau_3 + \phi(k, \omega)\tau_1. \quad (1)$$

Here τ_0, τ_1, and τ_3 are the Pauli spin matrices, $Z(k, \omega)$ and $X(k, \omega)$ describe the so-called normal components of the self-energy, and the gap function $\phi(k, \omega)$ describes the anomalous part which contains information on the internal structure of the pairs. The complex gap function $\phi(k, \omega) = \phi_1(k, \omega) + i\phi_2(k, \omega)$ satisfies the Cauchy relation

$$\phi_1(k, \omega) = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{\phi_2(k, \omega')}{\omega' - \omega} d\omega', \quad (2)$$

and, for $\omega = 0$, one has

$$\phi_1(k, 0) = \frac{2}{\pi} \int_0^\infty \frac{\phi_2(k, \omega')}{\omega'} dw'. \quad (3)$$

Based upon this, a useful measure of the frequency dependence of the pairing interaction [17] is

$$I(k, \Omega) = \frac{\frac{2}{\pi} \int_0^\Omega \frac{\phi_2(k,\omega')}{\omega'} d\omega'}{\phi_1(k, 0)}. \quad (4)$$

It gives the fraction of the zero frequency gap function which arises from frequencies below Ω. In order to obtain some insight into $I(k, \Omega)$, we first consider the case of Pb. Here the k dependence of the gap function is negligible, and only the frequency dependence enters. The imaginary part of the gap function $\phi_2(\omega)$, determined from tunneling data [18], is shown as the solid curve in Fig. 1. The dashed curve shows $\alpha^2 F(\omega)$. By using this result for $\phi_2(\omega)$ along with the value of $\phi_1(\omega = 0)$, we have evaluated $I(\Omega)$. As seen in Fig. 1(b), $I(\Omega)$ increases as Ω passes through the characteristic transverse and longitudinal Pb phonon frequencies plus Δ_0. It then exhibits a broad maximum and settles down to a value that exceeds 1. The maximum arises from the change in sign of $\phi_2(\omega)$ which occurs at a frequency 2–3 times the characteristic frequencies of the retarded part of the interaction. The reason that the asymptotic value of $I(\Omega)$ exceeds unity is that the nonretarded screened Coulomb pseudopotential leads to a negative, frequency-independent, contribution $\phi_{\rm NR}$ to the real part of $\phi_1(\omega)$. In this case, the Cauchy relation Eq. (2) becomes

$$\phi_1(\omega = 0) = \frac{2}{\pi} \int_0^\infty \frac{\phi_2(\omega')}{\omega'} d\omega' + \phi_{\rm NR}, \quad (5)$$

and at high frequencies $I(\Omega)$ exceeds 1 by the nonretarded contribution $-\phi_{\rm NR}/\phi_1(0)$.

The models that we will consider have a square two-dimensional lattice with a near-neighbor one-electron hopping t. The Hubbard model has an on site Coulomb interaction U, and its Hamiltonian is

$$H = -t \sum_{\langle ij \rangle s} (c_{is}^\dagger c_{js} + c_{js}^\dagger c_{is}) + U \sum_i n_{i\uparrow} n_{i\downarrow} - \mu \sum_{is} n_{is}, \quad (6)$$

with μ a chemical potential which sets the site filling $\langle n \rangle$. Here c_{is}^+ creates an electron of spin s on site i, and $n_{is} = c_{is}^+ c_{is}$ is the site occupation number operator for spin s. The t-J model is the large U limit of the Hubbard model in which no double site occupancy is allowed and near-neighbor spins are coupled by an exchange interaction J:

$$H = -t \sum_{\langle ij \rangle s} (\tilde{c}_{is}^\dagger \tilde{c}_{js} + \tilde{c}_{js} \tilde{c}_{is}) + J \sum_{\langle ij \rangle} \left(\mathbf{S}_i \cdot \mathbf{S}_j - \frac{1}{4} n_i n_j \right) \quad (7)$$

Here $\mathbf{S}_i = \tilde{c}_{is}^\dagger \boldsymbol{\sigma}_{ss'} \tilde{c}_{is'}$, and $\tilde{c}_{is}^\dagger$ is a projected fermion operator defined as $c_{is}^\dagger (1 - n_{i-s})$.

Exact diagonalization calculations were carried out for the t-J model on a square cluster of $N = 32$ sites. This particular cluster exhibits the full local symmetries of the underlying square lattice and has all of the most symmetric k points in reciprocal space [19]. Here we will consider the 0-, 1-, and 2-hole sectors. One hole doped onto a 32-site cluster corresponds to a doping $x \simeq 0.03$.

The gap function $\phi(k, \omega)$ can be extracted by combining Lanczos results for the one-electron Green's function $G(k, \omega)$ and Gorkov's off-diagonal Green's function [17,19]

$$F(k, \omega) = \bar{F}(k, \omega + i\eta) + \bar{F}(k, \omega - i\eta) \quad (8)$$

with

$$\bar{F}(k, z) = \langle \Psi_0(N-2) | \tilde{c}_{-k,-\sigma} \frac{1}{z - H + E_{N-1}} \tilde{c}_{k\sigma} | \Psi_0(N) \rangle. \quad (9)$$

Here the number of electrons in the initial and final ground states differ by 2, and E_{N-1} is defined as $E_{N-1} = [E_0(N) + E_0(N-2)]/2$. For a finite cluster, the diagonal Green's function is defined as

$$G(k, \omega) = \langle \Psi_0(N-2) | \tilde{c}_{k\sigma} \frac{1}{\omega + i\eta - H + E_{N-1}} \times \tilde{c}_{k\sigma}^+ | \Psi_0(N-2) \rangle + \langle \Psi_0(N) | \tilde{c}_{k\sigma}^+ \frac{1}{\omega - i\eta + H - E_{N-1}} \tilde{c}_{k\sigma} | \Psi_0(N) \rangle. \quad (10)$$

With this definition, both $G(k, \omega)$ and $F(k, \omega)$ have the same set of energy poles. By using a continued fraction Lanczos-based method, both $G(k, \omega)$ and $F(k, \omega)$ have been calculated and the gap function $\phi(k, \omega)$ determined from

$$\phi(k, \omega) = -\frac{F(k, \omega)}{G(k, \omega) G(k, -\omega) + F^2(k, \omega)}. \quad (11)$$

Results for $\phi(k, \omega)$ and $I(k, \Omega)$ for $J/t = 0.3$ and $x \sim 3\%$ ($N = 32$), with $k = (0, \pi)$, are plotted in Fig. 2. We believe that finite size effects are responsible for $\phi_2(k, \omega)$ starting

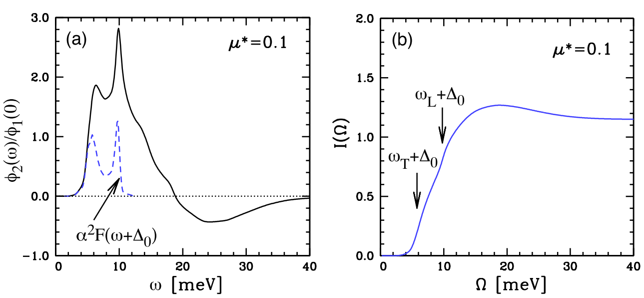

FIG. 1 (color online). (a) The imaginary part of the Pb gap function $\phi_2(\omega)$ versus ω (solid curve). The peaks in $\phi_2(\omega)$ occur at the transverse ω_T and longitudinal ω_L peaks of $\alpha^2 F(\omega)$ (dashed curve) shifted up by the gap Δ_0. (b) The pairing interaction spectral weight $I(\Omega)$ versus Ω for Pb. $I(\Omega)$ increases as Ω passes through $\omega_T + \Delta_0$ and $\omega_L + \Delta_0$ reflecting the transverse and longitudinal phonon contributions to the pairing. At larger values of Ω, $I(\Omega)$ exceeds unity because $\phi_1(0)$ is reduced from the value that it would have just due to the phonons by the presence of the nonretarded screened Coulomb pseudopotential μ^*.

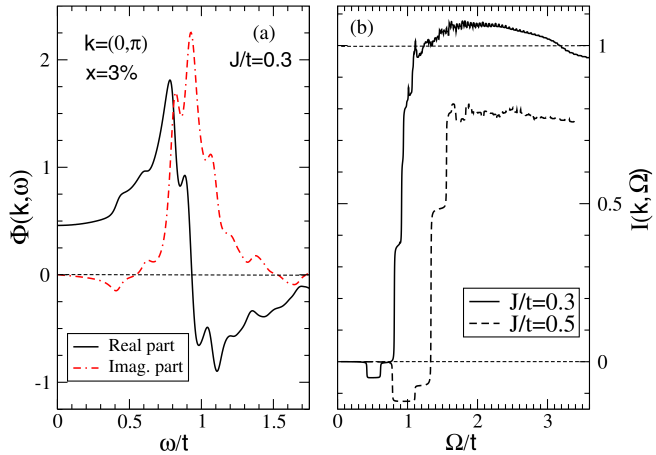

FIG. 2 (color online). (a) The real (solid curve) and imaginary (dashed curve) parts of $\phi_2(k,\omega)$ versus ω/t obtained for a 32-site cluster. Here $k=(0,\pi)$, $J/t=0.3$, and the doping $x\simeq 3\%$. (b) $I(k,\Omega)$ versus Ω/t for $J/t=0.3$ (solid curve) and $J/t=0.5$ (dashed curve) for $k=(0,\pi)$ and $x\simeq 3\%$. Here a broadening $\eta=0.05$ was used for (a) and $\eta=0.005$ for (b).

out negatively and that the corresponding negative dip in $I(k,\Omega)$ is an artifact. These negative values are almost undetectable in earlier calculations on ladders for which it is known that finite size effects are much smaller [17]. For $J/t=0.3$, the rapid increase in $I(k,\Omega)$ as Ω/t exceeds ~ 0.75 reflects the dynamic contributions of the spin fluctuations, and the broad maximum arises from the negative swing in $\phi_2(k,\omega)$ which occurs when ω exceeds several times their spectral range. This is similar to the behavior seen in Pb when ω exceeds the spectral range of $\alpha^2F(\omega)$. At higher frequencies in Fig. 2(b), $I(\Omega)$ is seen to decrease below 1. This high frequency behavior in which $I(\Omega)$ drops below 1 is more clearly seen for $J/t=0.5$, as shown by the dashed curve in Fig. 2(b). The fact that at high frequency $I[k=(0,\pi),\Omega]$ lays below 1 means that there is a nonretarded (instantaneous) contribution to the d-wave pairing interaction. In contrast to the case of the traditional low temperature superconductors, here the nonretarded contribution increases the pairing, corresponding to a positive value of $\phi_{\rm NR}(k)/\phi(k,0)$. Furthermore, its relative contribution increases as J/t increases.

For the Hubbard model, one can explore the full dynamic range including the upper Hubbard band so that the Cauchy relation does not have an additional constant term $\phi_{\rm NR}$. To calculate $\phi(k,\omega)$ for the Hubbard model, we have used a dynamic cluster approximation (DCA) [20,21]. The general idea of the DCA is to approximate the effects of correlations in the bulk lattice with those on a finite size cluster with N_c sites and periodic boundary conditions. The DCA maps the bulk ($L\times L$, with $L\to\infty$) lattice problem onto an effective periodic cluster embedded in a self-consistent dynamic mean field that is designed to represent the remaining degrees of freedom. The hybridization of the cluster to the host accounts for fluctuations arising from coupling between the cluster and the rest of the system. Here we have used a noncrossing approximation (NCA) [21,22] to determine $\phi(k_A,\omega)$ for a 4-site 2×2 cluster at a wave vector $k_A=(0,\pi)$. This cluster allows for a gap with d-wave symmetry and is such that within the noncrossing approximation dynamic results can be obtained on the real frequency axis. Similar calculations were performed for the t-J model in Ref. [23].

In mean-field theories such as the DCA, the mean field generates a constant real term $\phi_{\rm MF}(k_A)$. In the infinite cluster size limit, the DCA recovers the exact result, and the mean-field contribution $\phi_{\rm MF}(k_A)$ vanishes. For a finite cluster size, we therefore view this contribution as an artifact and subtract it off of $\phi_1(k_A,\omega)$ before performing the analysis based on the Cauchy relation. $\phi_{\rm MF}(k_A)$ was determined from $\lim_{\omega\to\infty}\phi_1(k_A,\omega)$. The expression for $I(\Omega)$ becomes

$$I(k_A,\Omega)=\frac{\frac{2}{\pi}\int_0^\Omega\frac{\phi_2(k_A,\omega')}{\omega'}d\omega'}{\frac{2}{\pi}\int_0^\infty\frac{\phi_2(k_A,\omega')}{\omega'}d\omega'}=\frac{\frac{2}{\pi}\int_0^\Omega\frac{\phi_2(k_A,\omega')}{\omega'}d\omega'}{\phi_1(k_A,0)-\phi_{\rm MF}(k_A)}. \tag{12}$$

Results showing $I(k_A,\Omega)$ versus Ω for a filling $\langle n\rangle=0.8$ and various values of U/t are plotted in Fig. 3(a). The d-wave projection of the dynamic spin susceptibility

$$\chi''_d(\Omega)=\frac{\langle(\cos k'_x-\cos k'_y)\chi''(k-k',\Omega)(\cos k_x-\cos k_y)\rangle}{\langle(\cos k_x-\cos k_y)^2\rangle} \tag{13}$$

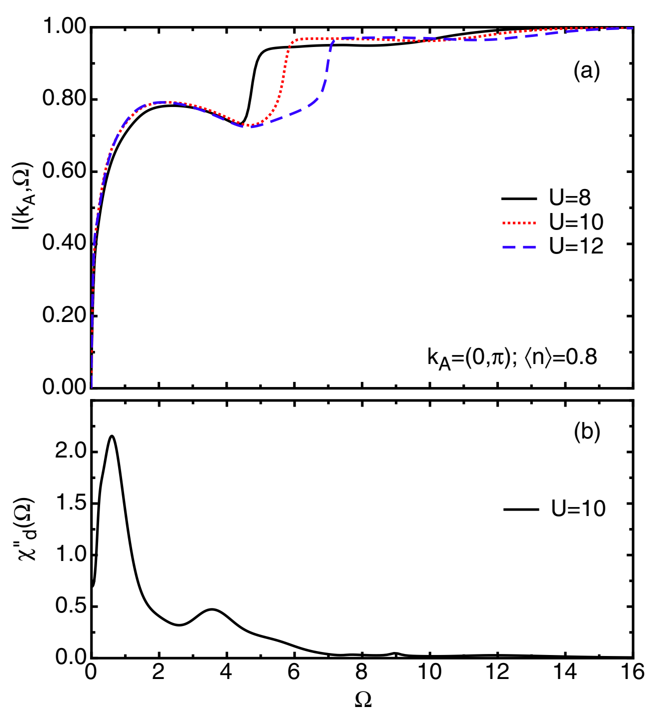

FIG. 3 (color online). (a) $I(k_A,\Omega)$ versus Ω/t for the 2×2 DCA-NCA Hubbard calculation for $T/T_c\simeq 0.95$, $\langle n\rangle=0.8$, and $U/t=8$, 10, and 12. Here $k_A=(0,\pi)$. (b) The d-wave projected $\chi''_d(\Omega)$ versus Ω/t for the same parameters.

was calculated for $U/t = 10$, and $\chi''_d(\Omega)$ is shown in Fig. 3(b). These calculations are for a reduced temperature $T/T_c \simeq 0.95$, so the shift due to the magnitude of the gap at the antinode $\Delta(k_A)$ is negligible.

At low frequencies, $I(k_A, \Omega)$ is seen to increase over the spectral range associated with the spin-fluctuation response seen in $\chi''_d(\omega)$. As Ω exceeds this range, $I(k_A, \Omega)$ passes through a weak maximum and dips down slightly, similarly to the t-J results shown in Fig. 2(b). Then, on a higher energy scale, $I(k_A, \Omega)$ goes to 1. One sees that, as U/t increases, the region over which $I(k_A, \Omega)$ remains below 1 extends to higher energies. For the t-J model this energy was pushed to infinity, but for the Hubbard model the high frequency contribution that takes $I(k_A, \Omega)$ to 1 is associated with the upper Hubbard band.

These numerical results show that the d-wave pairing interaction in the t-J and Hubbard models contain both retarded and nonretarded contributions [24]. The retarded contribution occurs on an energy scale which is small compared to the bare bandwidth $8t$ and the on site Coulomb interaction U. For the Hubbard model, the "nonretarded" contribution occurs on an energy scale set by the Mott gap and is related to excited states involving the upper Hubbard band. For the t-J model, this energy scale is pushed to infinity, and the exchange contribution is instantaneous.

A simple phenomenological form for the d-wave pairing interaction, consistent with these observations, is

$$V_d(k, \omega, k', \omega') = \tfrac{3}{2}\bar{U}^2 \chi(k - k', \omega - \omega') - \bar{J}(\cos k_x - \cos k_y)(\cos k'_x - \cos k'_y). \quad (14)$$

Here $\chi(q, \omega)$ is the dynamic spin susceptibility, and $\bar{U}$ and $\bar{J}$ are effective coupling constants. The retarded contribution to the pairing comes from the first term, and the nonretarded contribution from the second, exchange, term. Unlike the traditional low T_c case where the nonretarded screened Coulomb interaction suppresses the gap, here the nonretarded exchange term enhances the d-wave gap.

The question regarding whether there is a pairing glue is then a question of whether the dominant contribution to $\phi_1(k_A, \omega = 0)$ comes from the integral of $\phi_2(k_A, \omega)/\omega$ [25]. From the results presented here, we conclude that both the t-J and Hubbard models have spin-fluctuation pairing glue. For the cuprate materials, the relative weight of the retarded and nonretarded contributions to the pairing interaction remains an open question. Thus, the continuing experimental search for a pairing glue in the cuprates is important and will play an essential role in determining the origin of the high T_c pairing interaction.

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