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Superconducting pairing of spin polarons in the t-J model

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The pairing of quasiparticles in a CuO_2 plane is studied within a spin-polaron formulation of the t-t'-J model. Our numerical solution of the Eliashberg equations unambiguously shows d-wave pairing between spin polarons on different sublattices mediated by the exchange of spin fluctuations, and a strong doping dependence of the quasiparticle bandwidth. The transition temperature T_c is an increasing function of J/t and crosses a maximum at an optimal doping concentration $\delta_{\rm opt}$. For the t-J model with $J/t=0.4$ we obtain $T_c \simeq 0.013t$ at $\delta_{\rm opt} \simeq 0.2$. [S0163-1829(97)52218-1]

Recent experimental evidence in favor of d-wave superconducting pairing in high-T_c cuprates[1] supports theoretical studies of models with strong electron correlations.[2] The minimal model describing hole motion in a CuO_2 plane is the t-J (Ref. 3) or t-t'-J (Ref. 4) model. Numerical studies[2,5,6] of small t-J clusters suggest a d-wave superconducting instability. Yet to elucidate the nature of this pairing, an analytical treatment of the t-J model is needed. For this purpose we use a spin-polaron formulation for the t-J model[7] deduced in the region of small hole concentrations. A number of studies of this model[7,8] predict that doped holes dressed by strong antiferromagnetic spin fluctuations propagate coherently as quasiparticles (spin polarons[9]) with weight increasing with J/t. It is quite natural to expect that the same spin fluctuations induce superconducting pairing of the spin polarons. Recently a simplified treatment of this problem has been presented in the framework of the standard BCS theory assuming a rigid band model for the quasiparticles and a phenomenological interaction.[10–12] However, since the spin-fluctuation energy is of the same order as the doping dependent quasiparticle bandwidth $\sim J$ a strong coupling approach is necessary.

In this paper we present a consistent solution of the strong coupling spin-polaron model at finite temperatures and hole concentrations for normal and superconducting states. A numerical solution of a self-consistent system of equations for hole and magnon Green functions proves singlet d-wave superconducting pairing. The gap function shows interesting additional structure on top of the simple $\Delta_k = \Delta_0(\cos k_x - \cos k_y)$ which reflects the Fermi-surface geometry. The doping dependence of T_c around $\delta_{\rm opt}$ has the form of an inverted parabola, similar to experiment, and a $T_c^{\rm max} \sim 60$ K. Combining these results with already existing weak coupling studies for the Hubbard model[13,14] we argue that the spin-exchange pairing is the true mechanism for high-temperature superconductivity as proposed earlier by several groups based on more phenomenological approaches.[1,15–17]

We will study a spin-polaron model on a two sublattice antiferromagnetic (AF) background which has been successfully tested in the single hole case[8] as well as for finite hole concentration and temperature.[18] Our main assumption here is, that the spin-polaron approach gives a reasonable description also in the spin liquid regime provided the AF correlation length is sufficiently large compared to the Cooper pair and polaron radius. This is a view that has been stressed before.[10–12] The polaron radius is 2 lattice constants for $J/t=0.4$.[19]

Spinless fermion operators h_i^+ and f_i^+ are introduced for holes on different sublattices, i.e., on the $\uparrow(\downarrow)$ sublattice the constrained electron operators $\tilde{c}_{i\sigma} = c_{i\sigma}(1-n_{i-\sigma})$ of the t-J model are replaced by $\tilde{c}_{i\uparrow} = h_i^+$, $\tilde{c}_{i\downarrow} = h_i^+ S_i^+$ ($\tilde{c}_{i\downarrow} = f_i^+$, $\tilde{c}_{i\uparrow} = f_i^+ S_i^-$), where $S_i^{\pm} = S_i^x \pm S_i^y$ are spin operators. This representation excludes doubly occupied states and takes into account strong AF spin correlations in the electron hopping.

By employing the linear spin-wave theory in terms of Holstein-Primakoff operators, $S_i^+ \simeq a_i$, ($i \in \uparrow$), $S_i^+ \simeq b_i^+$, ($i \in \downarrow$) and performing the Bogoliubov canonical transformation, $a_k = v_k \alpha_k + u_k \beta_{-k}^+$, $b_k = v_k \beta_k + u_k \alpha_{-k}^+$, we obtain the spin polaron model

$$H_{t-J} = \sum_{kq} \{ h_k^+ f_{k-q} [g(k,q)\alpha_q + g(q-k,q)\beta_{-q}^+] + \text{H.c.} \} + \sum_k \epsilon_k (h_k^+ h_k + f_k^+ f_k) + \sum_q \omega_q (\alpha_q^+ \alpha_q + \beta_q^+ \beta_q). \tag{1}$$

Here $g(k,q) = (zt/\sqrt{N/2})(u_q \gamma_{k-q} + v_q \gamma_k)$ is the hole-magnon interaction, $z=4$ is the number of the nearest neighbors on a square lattice with N sites, $u_k = [(1+\nu_k)/2\nu_k]^{1/2}$, $v_k = -\text{sgn}(\gamma_k)[(1-\nu_k)/2\nu_k]^{1/2}$, $\nu_k = \sqrt{1-\gamma_k^2}$, $\gamma_k = \frac{1}{2}(\cos k_x + \cos k_y)$. The next-nearest-neighbor hopping energy is $\epsilon_k = (4t' \cos k_x \cos k_y - \mu)$. The chemical potential μ is calculated self-consistently as a function of hole concentration δ and temperature T from $\delta = \langle h_i^+ h_i \rangle + \langle f_i^+ f_i \rangle$. The spin-wave energy is $\omega_q = SzJ(1-\delta)^2 \nu_q$ where $(1-\delta)^2$ is a mean-field renormalization factor. We neglect here the contact hole-hole interaction which was found to be unimportant for polaron

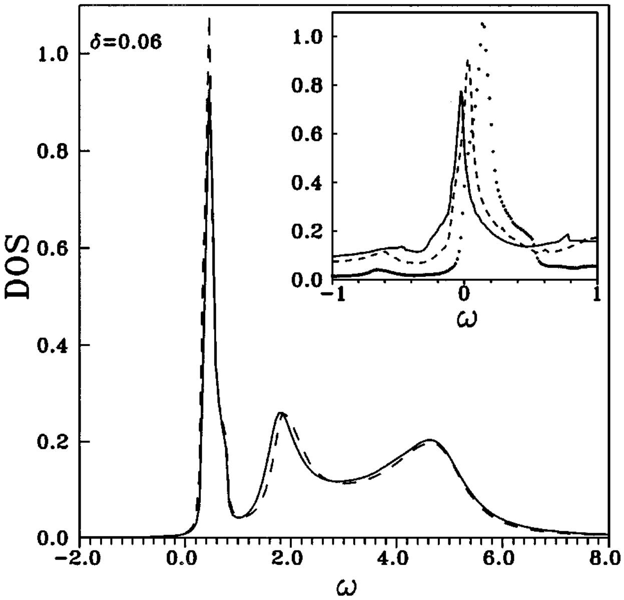

FIG. 1. The density of states (DOS) for the hole concentration $\delta=0.06$ at $T=0.012t$. The solid (dashed) line corresponds to calculations with the full (zero-order) magnon Green function. In the inset DOS is given for $\delta=0.1$, 0.25, 0.35 (from right to left) for the zero-order magnon spectra.

pairing.[11] The summation over wave vectors in Eq. (1) and below is restricted to the AF Brillouin zone.

To discuss superconducting pairing within the spin-polaron model (1), we consider the matrix Green function (GF) for holes on two sublattices $G_{hh}(k,z)=\langle\langle h_k^+|h_k\rangle\rangle_z=\langle\langle f_k^+|f_k\rangle\rangle_z$ and the anomalous GF $G_{hf}(k,z)=\langle\langle h_k^+|f_{-k}^+\rangle\rangle_z=-\langle\langle f_{-k}^+|h_k^+\rangle\rangle_z$, where Zubarev's notation[21] for the anticommutator GF was used with $z=\omega+i\epsilon$. To obtain self-consistent equations for these GF's we employ the self-consistent Born approximation (SCBA) which provided good results for the one-hole spectrum in the normal state.[7,8,20] In SCBA we get for the self energies

$$\Sigma_{hh}(k,i\omega_n)=-T\sum_{q,m} G_{hh}(q,i\omega_m)\lambda^{11}_{k,k-q}(\omega_n-\omega_m), \quad (2)$$

$$\Sigma_{hf}(k,i\omega_n)=-T\sum_{q,m} G_{hf}(q,i\omega_m)\lambda^{12}_{k,k-q}(\omega_n-\omega_m), \quad (3)$$

where the Matsubara frequencies $\omega_n=\pi T(2n+1)$. The interaction functions are

$$\lambda^{11}_{k,q}(\omega_\nu)=g^2(k,q)D(q,-i\omega_\nu)+g^2(q-k,q)D(-q,i\omega_\nu),$$

$$\lambda^{12}_{k,q}(\omega_\nu)=g(k,q)g(q-k,q)\{D(q,-i\omega_\nu)+D(-q,i\omega_\nu)\}.$$

The diagonal magnon GF $D(q,\omega)=\langle\langle\alpha_q|\alpha_q^+\rangle\rangle_\omega$ in the zero-order approximation is given by $D^0(q,\omega)=(\omega-\omega_q)^{-1}$ with the doping-dependent magnon energy ω_q. The full magnon GF is determined by the matrix equation $\hat{D}^{-1}(q,\omega)=(\hat{D}^0)^{-1}(q,\omega)-\hat{\Pi}(q,\omega)$ where the renormalization of the magnon energy due to particle-hole excitations is

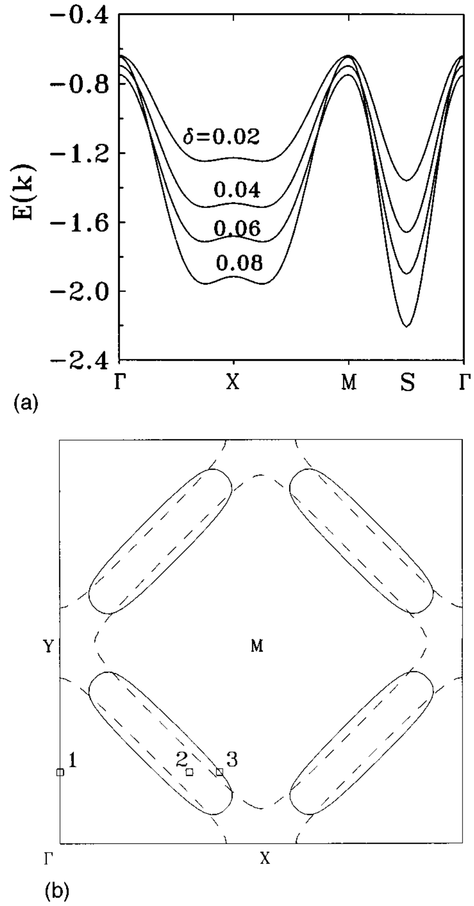

FIG. 2. (a) The quasiparticle spectrum $E(\mathbf{k})$ and (b) the Fermi surface (FS) $E(\mathbf{k}_F)=0$ of the t-t'-J(t-J) model for $\delta=0.25$ is given by the solid (dashed) line ($t'=-0.1$, $J=0.4$).

described by the polarization operator $\hat{\Pi}(q,\omega)$. This is calculated in a one-loop approximation using the fully renormalized hole GF.

The superconducting temperature T_c is calculated from the linearized form of the Eliashberg equation for the gap function

$$\phi(k,i\omega_n)=\sum_p\sum_m \lambda^{12}_{k,k-p}(i\omega_n-i\omega_m)G_{hh}(p,i\omega_m)\times G_{hh}(-p,-i\omega_m)\phi(p,i\omega_m). \quad (4)$$

The first step is a self-consistent calculation of the normal GF $G_{hh}(k,i\omega_n)=[i\omega_n+\epsilon_k-\Sigma_{hh}(k,i\omega_n)]^{-1}$ with the self-energy operator (2) for a given concentration of holes $\delta=\frac{1}{2}+(2T/N)\Sigma_k\Sigma_n G_{hh}(k,i\omega_n)$. The numerical calculations were performed using fast Fourier transformation (FFT) (Ref. 22) for a mesh of 64×64 k points in the full Brillouin zone ($0\leqslant k_x,k_y\leqslant 1$), in units of 2π. In the summation over the Matsubara frequencies we used up to 200–700 points with constant cutoff $\omega_{\max}=10t$. The FFT for the momentum integration is possible due to the particular momentum dependence of $g(k,q)$. Usually 10–30 iterations were needed to obtain a solution for the self energy with an accuracy of order 0.001. Padé approximation was used to calculate the

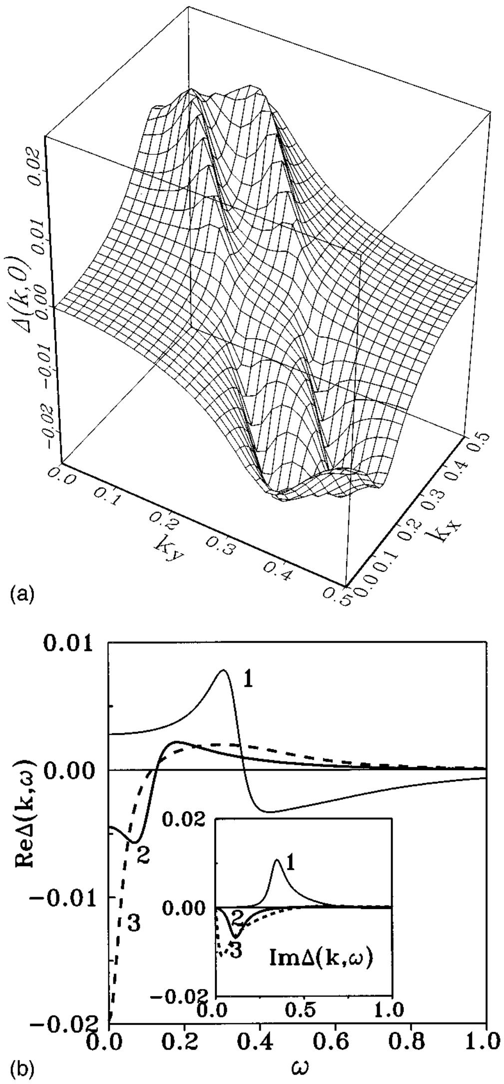

FIG. 3. (a) The gap function $\Delta(\mathbf{k},\omega=0)$ versus $\mathbf{k}$ (in units of $2\pi/a$) and (b) Re $\Delta(\mathbf{k},\omega)$ $[\mathrm{Im}\Delta(\mathbf{k},\omega)$ in the inset$]$ versus ω for a set of (k_x,k_y) points shown in Fig. 2(b) for t-t'-J model ($\delta=0.25$ and $T/T_c\approx 0.8$).

hole spectral function $A(k,\omega)=-(1/\pi)\ \mathrm{Im}\ \langle\langle h_k|h_k^+\rangle\rangle_{\omega+i\epsilon}$ and the density of states (DOS) $A(\omega)$ on the real frequency axis.

In Fig. 1 results for $A(\omega)$ of the t-t'-J model are shown for various doping concentrations. The peak in the DOS of width $\Delta W\leqslant J$ near the chemical potential $\mu=0$ results from the shallow quasiparticle dispersion $E(k)$ along the AF-zone boundary [Fig. 2(a)]. We find that the shape of the quasiparticle dispersion even at $\delta\sim 0.25$ is still similar to the shape of the dispersion in the single hole case. Yet a rigid band description fails since the scale ΔW and the total quasiparticle bandwidth W grow significantly with δ. The peak of the DOS coincides with μ at the transition from hole to electron-like Fermi surfaces (FS). This occurs at a concentration which depends on t'. In Fig. 2(b) the FS at $\delta=0.25$ is shown for the two models studied in this paper, the t-J and the t-t'-J model with $t'=-0.1t$. Our unit of energy is $t=1$ ($t\sim 0.4$ eV for CuO_2 planes) and $J/t=0.4$. We note that numerical studies of the t-J model suggest that the change of FS topology may occur at a lower doping concentration.[23]

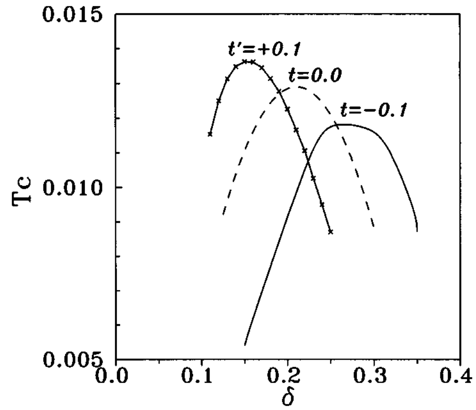

FIG. 4. The superconducting temperature T_c versus hole concentration δ for $J=0.4$ and $t'/t=-0.1,0,+0.1$.

The particle-hole renormalization of the magnon propagator D leads to an instability at small q indicating the disappearance of AF long-range order. In Fig. 1 we compare the DOS $A(\omega)$ at $\delta=0.06$ calculated with D and D_0, which is not ill behaved. The small-q instability has only small effects on $A(k,\omega)$ and $A(\omega)$ since in the small-q regime the spin-charge coupling is small. Therefore we performed our calculations at higher δ with D_0.

The momentum dependence of the gap function $\Delta(k,\omega=0)$, $\Delta(k,\omega)=\phi(k,\omega)/Z(k,\omega)$, is shown in Fig. 3(a) for $\delta=0.25$ and $T/T_c\approx 0.8$. Here $Z(k,\omega)$ is an analytical continuation of the Eliashberg function $Z(k,i\omega_n)=[1-\mathrm{Im}\Sigma(k,i\omega_n)/\omega_n]^{-1}$. The gap function has the typical d-wave symmetry with two ridges resulting from sharp changes of the interaction function at the FS. In Fig. 3(b) the frequency dependence of Re$\Delta($ k$,\omega)$ is shown for a set of (k_x,k_y) points marked in Fig. 2(b): (1) inside the FS, (0, 0.19), (2) at the AF-zone boundary, (0.31, 0.19), (3) near the FS, (0.38, 0.19). The gap function changes sign after crossing the $k_x=k_y=0.19$ point where it is equal to zero. It is interesting that the characteristic energy cutoff for the pairing theory, which is of order $J\simeq 0.4$ away from the FS (curve 1), becomes much smaller near the FS (curves 2 and 3). The sharp change of the real part and the quite large values of Im $\Delta(k,\omega)$ near the FS differ from the results for conventional superconductors. Since the Fermi energy E_F is of the order of the exchange energy J *all quasiparticles* contribute to the pairing state contrary to the weak coupling case in conventional superconductors.

The transition temperature T_c is determined as the temperature where the highest eigenvalue of the linearized Eliashberg equation becomes unity. In all cases the symmetry of the corresponding eigenfunction $\phi(k,\omega)$ is $d_{x^2-y^2}$. In Fig. 4 the dependence of T_c on hole concentration is shown for $t'/t=-0.1,0,+0.1$. These results are quite different from the monotonic increasing T_c obtained within the weak coupling limit of the BCS equation in Ref. 11 and the maximum of T_c found in Ref. 6 near half filling. In our case the maximum of T_c at $\delta\simeq 0.20$ for $t'=0$ results from the Fermi-level crossing of the peak in the density of states which reflects the change of the FS topology.

We have also studied the dependence of T_c on the exchange energy for $J\leqslant 4$. T_c increases with J and saturates at $T_c\simeq 0.025t$ for $J\simeq 3$. Phase separation[5] at large J is outside the scope of our study.

To compare with other theoretical work, we would like to note the striking similarity of the Fermi-surface related structures in the gap function (Fig. 3) and of T_c compared with the results of Dahm *et al.*,[14] who used a completely different weak coupling approach for the Hubbard model.

An important difference between the phenomenological spin-fluctuation theory and our approach is that pairing is dominated in the former by $q\sim(\pi,\pi)$ scattering and energy transfers $\Delta E<50$ meV, whereas in our calculations high-energy spin fluctuations with q near the AF-zone boundary are most important. Our coupling function actually vanishes for $q\rightarrow 0$ and $q\rightarrow(\pi,\pi)$, which is the correct behavior as discussed by Schrieffer.[24] Contrary to the spin-fluctuation theory, vertex corrections are of minor importance in the spin-polaron framework.

In summary, we have solved numerically Eliashberg equations for the strong coupling spin-polaron model. The model itself has no adjustable parameters apart from t,t' and J defining the Hamiltonian. We have analyzed the doping dependence of the quasiparticle spectrum of spin polarons in the normal state and shown that they undergo superconducting d-wave pairing mediated by spin fluctuations. The high values of superconducting temperature and its doping dependence $T_c(\delta)$ is explained by a large peak in the density of states of the spin-polaron quasiparticles in the vicinity of the chemical potential. Thereby we have confirmed the robustness of Dagotto's result, which he obtained for a contact interaction and subsequent BCS treatment. We note a key difference from the standard von Hove scenario: here the high density of states arises as a many-body effect, with the important consequence that the width of the peak in the density of states and the frequency of the exchanged boson are related, and both of the order J. That this is a particularly favorable circumstance for high T_c has already been stressed by Horsch and Rietschel.[25] Furthermore we have found unconventional behavior for the d-wave gap function (a sharp change with energy and large damping near the FS) which suggests an explanation for some of anomalous properties of cuprate superconductors observed in tunneling experiments (v-shape gap and large imaginary part), infrared absorption (no visible gap or gapless superconductivity), angle-resolved photoemission spectroscopy [a line of gap nodes along (π,π) direction].[26]

Note added in proof. A recent inelastic neutron scattering experiment by P. Bourges *et al.* (unpublished) shows evidence for the spin-wave nature of the high-energy spin-excitation spectrum in underdoped $YBa_2Cu_3O_{6.5}$ (T_c=52 K).

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