Recent experimental evidence in favor of a $d$-wave superconducting pairing in high-$T_c$ cuprates supports theoretical studies of models with strong electron correlations. The minimal model describing hole motion in CuO$_2$ plane is the $t$-$J$ model or $t$-$t'$-$J$ model. Numerical studies 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 deduced in the region of small hole concentrations. A number of studies of this model predict that doped holes dressed by strong antiferromagnetic spin fluctuations propagate coherently as quasiparticles (spin polarons) with weight $Z_k \simeq J/t$. It is quite natural to expect that the same spin fluctuations induce superconducting pairing of the spin polarons. Recently this problem has been treated in the framework of the standard BCS formalism assuming a rigid band model for the quasiparticles. However, since the spin-fluctuation energy is of the same order as a quasiparticle bandwidth $\sim J$ a strong coupling approach is necessary.

In this paper we present the first 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 $\delta_{opt}$ has the form of an inverted parabola, similar to experiment, and a $T_c^{max} \sim 60K$. Combining these results with already existing weak coupling studies for the Hubbard model 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.

We will study a spin polaron model on a two sublattice antiferromagnetic (AF) background which has been successfully tested in the single hole case. Spinless fermion operators $h^+_i$ and $f^+_i$ are introduced for holes on different sublattices, i.e. on the $\uparrow$-sublattice the constrained electron operators $c_{i\sigma} = c_{i\sigma}(1 - n_{i\sigma})$ of the $t$-$J$ model are replaced by $\tilde{c}_{i\uparrow} = h^+_i$, $\tilde{c}_{i\downarrow} = h^+_i S^+_i$ ($\tilde{c}_{i\uparrow} = f^+_i$, $\tilde{c}_{i\downarrow} = f^+_i S^+_i$), where $S^+_i = S^+_i \pm S^+_i$ 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 approximation in terms of the Holstein-Primakoff operators: $S^+_i = a_i$, $(i \in \uparrow)$, $S^+_i = b_i^+$, $(i \in \downarrow)$ and performing the Bogoliubov canonical transformation: $a_k = \nu_k \alpha_k + u_k \beta^+_k$, $b_k = \nu_k \beta_k + u_k \alpha^+_k$, we obtain the spin polaron model:

$$H_{t-J} = \sum_{kq}(h^+_k f_{k-q}[g(k,q)\alpha_q + g(q-k,q)\beta^+_q] + h.c.)$$
$$+ \sum_k \epsilon_k(h^+_k h_k + f^+_k f_k) + \sum_q \omega_q(\alpha^+_q \alpha_q + \beta^+_q \beta_q).$$

(1)

Here $g(k,q) = (z/\sqrt{N/2})(u_q \gamma_{k-q} + v_q \gamma_k)$ is the hole-magnon interaction, $z = 4$ is the number of the nearest neighbors on a square lattice with $N$ sites, $u_k = ((1 + \nu_k)/2\nu_k)^{1/2}$, $v_k = -\text{sign}(\gamma_k)((1 - \nu_k)/2\nu_k)^{1/2}$, $\nu_k = \sqrt{1 - \gamma_k^2}$, $\gamma_k = \sqrt{\cos k_x + \cos k_y}$. The next nearest neighbor hopping energy is $\epsilon_k = (4t' \cos k_x \cos k_y - \mu)$. The chemical potential $\mu$ should be calculated self-consistently as a function of a hole concentration $\delta$ and temperature $T$ from the equation: $\delta = \langle h^+_k h_k \rangle + \langle f^+_k f_k \rangle$. The spin-wave energy is $\omega_q = S^2 \delta (1 - \delta)^2 \nu_q$ where $(1 - \delta)^2$ is the mean field renormalization factor. We neglect here the contact hole-hole interaction which is unimportant in the polaron pairing. The summation over wavevectors in (1) and below is restricted to $N/2$ points in the AF Brillouin zone.

To discuss singlet superconducting pairing within the
spin polaron model \( \square \), we consider the matrix Green function (GF) for holes on two sublattices \( G_{hh}(k, z) = \langle h_k^+ | h_k \rangle_z = \langle f_k^+ | f_k \rangle_z \) and the anomalous GF \( G_{hf}(k, z) = \langle h_k^+ | f_{k}^+ \rangle_z = -\langle f_{-k}^+ | h_k^+ \rangle_z \), where Zubarev’s notation \([17]\) 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 \([7,8,16]\). In SCBA we get for the self-energies

\[
\Sigma_{hh}(k, i\omega_n) = -T \sum_{q,m} G_{hh}(q, i\omega_m) \lambda_{k,k-q}^{11}(\omega_n - \omega_m), \tag{2}
\]

\[
\Sigma_{hf}(k, i\omega_n) = -T \sum_{q,m} G_{hf}(q, i\omega_m) \lambda_{k,k-q}^{12}(\omega_n - \omega_m). \tag{3}
\]

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

\[
\lambda_{k,q}^{11}(\omega_n) = g^2(q, k) D(q, -i\omega_n) + g^2(q - k, q) D(-q, i\omega_n),
\]

\[
\lambda_{k,q}^{12}(\omega_n) = g(q, k) g(q - k, q) \{ D(q, -i\omega_n) + D(-q, i\omega_n) \}.
\]

The diagonal magnon GF \( D(q, \omega) = \langle (\alpha_q | \alpha_q^+) \rangle_\omega \) in the zero order approximation is given by \( D^0(q, \omega) = (\omega - \omega_n)^{-1} \) with the doping dependent magnon energy \( \omega_q \). 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 described by the polarization operator \( \hat{\Pi}(q, \omega) \). This is calculated in 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

\[
\phi(k, i\omega_n) = \sum_p \sum_m \lambda_{k,p}^{12}(i\omega_n - i\omega_m) G_{hh}(p, i\omega_m) \times G_{hh}(-p, -i\omega_m) \phi(p, i\omega_m). \tag{4}
\]

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 \( \delta = \frac{1}{2} + \frac{2T}{N} \sum_k \sum_n G_{hh}(k, i\omega_n) \).

The numerical calculations were performed using fast Fourier transformation (FFT) \([18]\) for a mesh of 64\times64 k-points in the full Brillouin zone \((0 \leq k_x, k_y \leq 1)\), in units of \( 2\pi \). In the summation over the Matsubara frequencies we used up to 200-700 points with constant cut-off \( \omega_{max} = 10t \). The FFT for the momentum integration is possible due to the particular momentum dependence of \( g(k, \omega) \). 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 hole spectral function \( A(k, \omega) = -\frac{1}{\pi} \text{Im} \langle (h_k | h_k^+) \rangle_{\omega + i\epsilon} \) 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 \( \Delta W \leq J \) 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 \( \Delta W \) and the total quasiparticle bandwidth \( W \) grow significantly with \( \delta \). The peak of the DOS coincides with \( \mu \) at the crossover from hole to electron like Fermi surfaces (FS). This occurs at a characteristic 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 \( t = 1 \) (in reality \( t \sim 0.4eV \) for \( \text{CuO}_2 \) planes) and \( J/t = 0.4 \). The crossover from hole-to-electron-like FS is consistent with the variation of the Hall constant in \( \text{La}_x\text{Sr}_{2-x}\text{CuO}_4 \).
FIG. 2. (a) The quasiparticle spectrum $E(k)$ and (b) the Fermi surface (FS) $E(k_F) = 0$ of the $t-t' - J (t-J)$ model for $\delta = 0.25$ is given by the solid (dashed) line.

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 $\delta$ with $D_0$. Our main assumption here is, that the spin polaron approach gives a reliable description also in the spin liquid regime provided the AF correlation length is sufficiently large compared to the Cooper pair and polaron radius. The latter quantity is 2 lattice constants for $J/t = 0.4$.

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 $Z(k, i\omega_n) = (1 - Im \Sigma(k, i\omega_n)/\omega_n)^{-1}$. 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.2b: (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 $J \approx 0.4$ 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.

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

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 $t' = -0.11$ and $t' = 0$. These results are quite different from the monotonic increasing $T_c$ obtained within the weak coupling limit of the
BCS equation in [10] and the maximum of $T_c$ found in
[8] near half filling. In our case the maximum of $T_c$ at
$\delta \simeq 0.25$ (or at $\delta \simeq 0.20$ for $t' = 0$) results from the Fermi
level crossing of the peak in the density of states which
coincides with the change of the FS topology.

We have also studied the dependence of $T_c$ on the
exchange energy for $J \leq 4$. $T_c$ increases with $J$ and sat-
urates at $T_c \simeq 0.025t$ for $J \simeq 3$. However, we have not
obtained a large drop of $T_c$ for $J > 3$ observed in small
cluster calculations near phase separation [5], which is
beyond the scope of our study.

In summary, we have solved numerically Eliashberg
equations for the strong coupling spin-polaron model.
We have calculated the quasiparticle spectrum of spin
polarons in the normal state and shown that they un-
dergo superconducting $d$-wave pairing mediated by spin
fluctuations. The high values of superconducting temper-
ature 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.
A key difference from the van Hove scenario, however, is
that the quasiparticle density of states has a width given
by the interaction energy $J$ which is similar to the pairing
energy. 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 explana-
tion for some of anomalous properties of cuprate super-
conductors observed in tunneling experiments (v-shape
gap and large imaginary part), infrared absorption (no
visible gap or gapless superconductivity), ARPES (a line
of gap nodes along ($\pi, \pi$) direction [20]), etc. Our cal-
culations are based on a two sublattice representation,
which is suggested to provide a reasonable description of
spin polaron quasiparticles and their pairing even in the
spin liquid regime, i.e. for hole concentrations where the
AF correlation length is sufficiently large.

An important difference between the phenomenologi-
cal spin-fluctuation theory and our approach is that pair-
ing is dominated in the former by $q \sim (\pi, \pi)$ scattering
and energy transfers $\Delta E < 50$ mev, whereas in our cal-
culations high-energy spin-fluctuations with $q$ near the
AF-zone boundary are most important. Higher energy
neutron scattering data in this momentum and energy
range is however not yet available.

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\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{fig4}
\caption{The superconducting temperature $T_c$ versus hole
concentration $\delta$ for $J = 0.4$, $t' = -0.1t$ (solid line) and $t' = 0$
(dashed line).}
\end{figure}

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