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SUPERCONDUCTING PAIRING OF SPIN POLARONS IN THE $t-J$ MODEL

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A quasiparticle spectrum of doped holes and their superconducting pairing in the CuO_2 plane is studied within a spin polaron $t-J$ model on a two-sublattice antiferromagnet. A self-consistent system of equations for hole and magnon matrix Green functions in the noncrossing approximation is solved numerically by the fast Fourier transformation method. We obtain a strong renormalization of the hole spectrum due to spin fluctuations that result in formation of spin polarons described by the coherent part of the spectrum. We also observe a singlet d-wave superconducting pairing for two spin polarons on different sublattices, mediated by spin-fluctuation exchange. A maximal superconducting temperature $T_c \simeq 0.01t$ is obtained around the hole concentration 0.25 for $t = 0.4J$. We argue that the superconducting pairing of spin polarons for the $t-J$ model with strong electron correlations represents the mechanism of high-temperature superconductivity.

1. Introduction

Recently experimental evidences in favor of a d-wave superconducting pairing in high-T_c cuprates [1] have been supported by theoretical studies of models with strong electron correlations [2]. Many unconventional normal state properties of cuprates can be explained only by proper treatment of strong electron correlations on copper sites which could be also important for superconducting pairing. The simplest model allowing for the electron correlations is a two-dimensional Hubbard model with on-site repulsion U and hopping energy t [3]. Recent studies [4] - [7] of the Eliashberg equations for the Hubbard model in the weak coupling limit, $U \leq 4t$, have shown a d-wave pairing mediated by spin fluctuation exchange. In the vicinity of antiferromagnetic instability near half filling a superconducting temperature T_c of order $0.02t$ has been obtained.

In the strong coupling limit, $U \gg t$, the Hubbard model can be reduced to the $t-J$ model [3,8]. Exclusion of doubly occupied states in electronic hopping and their strong coupling with spin fluctuations with an exchange energy $J \simeq 4t^2/U$ does not allow applying mean field type approximations or perturbation theory. Exact numerical studies [2,9,10] for small clusters within the $t-J$ model show a d-wave superconducting instability. However, to elucidate the nature of this pairing, an analytical treatment of the $t-J$ model is needed. For this purpose we can employ a spin polaron model [11,12] obtained from the $t-J$ model in the region of small hole concentrations. A number of studies of this model [11]- [18] predicts that a doped hole dressed by strong antiferromagnetic spin fluctuations can propagate coherently as a quasiparticle – spin polaron, with weight $Z_k \simeq J/t$. Besides a narrow quasiparticle band of order J there is a broad incoherent band at higher energies. It is quite natural to suggest that the same spin fluctuations could mediate a superconducting pairing of the spin polarons. Recently this problem was treated in the framework of the standard BCS formalism [19,20]. A simple model of quasiparticles with numerically evaluated spectrum and effective pairing interaction in the atomic limit [19] and mediated by antiferromagnetic magnon exchange [20] has been used. However, since the pairing spin-fluctuation energy is of the same order as a quasiparticle bandwidth J the weak coupling BCS equation is inadequate to treat the problem. A full self-consistent solution of the Eliashberg equations and spin fluctuation susceptibility is needed to resolve this problem.

In this paper for the first time a consistent solution of the strong coupling spin polaron model at finite temperatures and hole concentrations for normal and superconducting states is presented. A numerical solution of a self-consistent system of equations for hole and magnon Green functions unambiguously proves a singlet d-wave superconducting pairing. The maximum superconducting temperature T_c of order $0.012t$ is obtained around hole concentrations $\delta = 0.25$ for $t = 0.4J$.

Combining the results for the Hubbard model [4]-[7] obtained in the weak coupling limit with the present one for the strong coupling spin polaron model we can argue that the spin-exchange pairing could be the true mechanism for high-temperature superconductivity proposed earlier by several groups within a phenomenological approach (see, e.g., [21] - [23]).

2. Polaron model

We will study a spin polaron model on a two sublattice antiferromagnetic (AF) background. Starting from the standard $t-t'-J$ model we introduce for electron operators $\tilde{c}_{i\sigma} = c_{i\sigma}(1-n_{i-\sigma})$ the following representation in terms of hole spinless fermion operators on two sublattices with spin up ($i \in\uparrow$) and spin down ($i \in\downarrow$):

$$\tilde{c}_{i\uparrow} = h_i^+,\ \tilde{c}_{i\downarrow} = h_i^+ S_i^+ \ (i \in\uparrow); \quad \tilde{c}_{i\downarrow} = f_i^+,\ \tilde{c}_{i\uparrow} = f_i^+ S_i^- \ (i \in\downarrow) \tag{2.1}$$

where $S_i^{\pm} = S_i^x \pm S_i^y$ are spin operators on the corresponding sublattices. This representation rigorously excludes doubly occupied states and takes into account strong AF spin correlations in electron hopping.

By employing the linear spin-wave approximation in terms of the 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 write the spin polaron model in the form:

$$H_{t-J} = \sum_{kq}(h_k^+ f_{k-q}[g(k,q)\alpha_q + g(q-k,q)\beta_{-q}^+] + \text{H.c.}) +$$

$$+ \sum_k(\epsilon_k - \mu)(h_k^+ h_k + f_k^+ f_k) + \sum_q \omega_q(\alpha_q^+\alpha_q + \beta_q^+\beta_q). \tag{2.2}$$

Here $g(k,q) = (zt/\sqrt{N/2})(u_q\gamma_{k-q} + v_q\gamma_k)$ is the hole-magnon interaction where $z = 4$ is the number of the nearest neighbours on a square lattice with N sites, $u_k = ((1+\nu_k)/2\nu_k)^{1/2}$, $v_k = -\text{sign}(\gamma_k)\,((1-\nu_k)/2\nu_k)^{1/2}$, $\nu_k = \sqrt{1-\gamma_k^2}$, $\gamma_k = \frac{1}{2}(\cos ak_x + \cos ak_y)$. The next nearest neighbour hopping energy is $\epsilon_k = 4t' \cos ak_x \cos ak_y$. The chemical potential μ should be calculated self-consistently as a function of a hole concentration δ and temperature T from the equation: $\delta = \langle h_i^+ h_i \rangle + \langle f_i^+ f_i \rangle$. The spin-wave energy is $\omega_k = SzJ(1-\delta)^2 \nu_k$. The summation over wave-vectors in (2.2) and below is restricted to $N/2$ points in the AF Brillouin zone.

3. Green functions

To discuss a singlet superconducting pairing within the spin polaron model (2.2), we consider the matrix Green function (GF) for holes on two sublattices defined in (2.1):

$$G_{hh}(k,z) = \langle\langle h_k^+ \mid h_k \rangle\rangle_z = \langle\langle f_k^+ \mid f_k \rangle\rangle_z = -\langle\langle f_k \mid f_k^+ \rangle\rangle_{-z} \qquad (3.1)$$

$$G_{hf}(k,z) = \langle\langle h_k^+ \mid f_{-k}^+ \rangle\rangle_z = -\langle\langle f_{-k}^+ \mid h_k^+ \rangle\rangle_z = \langle\langle f_{-k} \mid h_k \rangle\rangle_z \qquad (3.2)$$

where Zubarev's notation [24] for the anticommutator GF was used with $z = \omega + i\epsilon$.

To obtain self–consistent equations for the GF (3.1), (3.2) we employ the self–consistent Born approximation (SCBA) (or the noncrossing diagram approximation) which has been proved to be quite reasonable in calculation of the one–hole spectrum in the normal state (see, e.g. [11]– [18]). In SCBA we get the following equations for the self-energies of the GF (3.1), (3.2)

$$\Sigma_{hh}(k,i\omega_n) = -T \sum_q \sum_m G_{hh}(q,i\omega_m)\lambda_{11}(k,k-q \mid i\omega_n - i\omega_m), \qquad (3.3)$$

$$\Sigma_{hf}(k,i\omega_n) = -T \sum_q \sum_m G_{hf}(q,i\omega_m)\lambda_{12}(k,k-q \mid i\omega_n - i\omega_m). \qquad (3.4)$$

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

$$\lambda_{11}(k,q \mid i\omega_\nu) = g^2(k,q)D(q,-i\omega_\nu) + g^2(q-k,q)D(-q,i\omega_\nu), \qquad (3.5)$$

$$\lambda_{12}(k,q \mid i\omega_\nu) = g(k,q)g(q-k,q)\{D(q,-i\omega_\nu) + D(-q,i\omega_\nu)\}. \qquad (3.6)$$

Here the diagonal magnon GF $D(q,\omega) = \langle\langle \alpha_q \mid \alpha_q^+ \rangle\rangle_\omega$ can be written as

$$D(q,\omega) = \frac{\omega + \omega_q + \Pi_{22}(q,\omega)}{[\omega - \omega_q - \Pi_{11}(q,\omega)][\omega + \omega_q + \Pi_{22}(q,\omega)] + \mid \Pi_{12}(q,\omega) \mid^2}. \qquad (3.7)$$

Within the SCBA the polariazation operators are as follows

$$\Pi_{11}(q,i\omega_\nu) = T \sum_k \sum_m \{g^2(k,q)G_{hh}(k,i\omega_m)G_{hh}(k-q,i\omega_\nu + i\omega_m) - g(k,q)g(q-k,q)G_{hf}(k,i\omega_m)G_{hf}(k-q,i\omega_\nu + i\omega_m)\} \qquad (3.8)$$

$$\Pi_{12}(q,i\omega_\nu) = T \sum_k \sum_m \{g(k,q)g(q-k,q)G_{hh}(k,i\omega_m)G_{hh}(k-q,i\omega_\nu + i\omega_m) - g^2(k,q)G_{hf}(k,i\omega_m)G_{hf}(k-q,i\omega_\nu + i\omega_m)\} \qquad (3.9)$$

where $\Pi_{22}(q,i\omega_\nu) = \Pi_{11}(-q,-i\omega_\nu)$.

4. Numerical Results and Discussion

To calculate superconducting temperature T_c we can study only the linearized system of the Eliashberg equations for the normal GF (3.1)

$$G_{hh}(k, i\omega_n) = \frac{1}{i\omega_n + \epsilon_k - \mu - \Sigma_{hh}(k, i\omega_n)}, \tag{4.1}$$

and for the superconducting gap function (3.4)

$$\phi(k, i\omega_n) = \sum_p \sum_m \lambda_{12}(k, k-p \mid i\omega_n - i\omega_m)\phi(p, i\omega_m)\times$$

$$\times\, G_{hh}(p, i\omega_m) G_{hh}(-p, -i\omega_m). \tag{4.2}$$

At first a self-consistent calculation of the normal GF (4.1) with the self-energy operator (3.3) has been done for a given concentration of holes $\delta = \frac{1}{2} + \frac{2T}{N}\sum_k \sum_{n=0}^{\infty} G(k, i\omega_n)$. Then the gap equation (4.2) has been solved and the leading eigenvalue for the pairing eigenfunctions $\phi(q, i\omega_n)$ of a given symmetry has been obtained. The calculations were performed for the hole concentrations in the range $0.02 \le \delta \le 0.35$ and for the parameters of the spin polaron model (2.2): $J = 0.4$ and $t' = -0.1$ (all energies here and below are measured in units of t).

In the numerical calculations we have used the fast Fourier transformation [25] for a finite mesh of 64×64 **k**-points in the full Brillouin zone ($0 \le k_x, k_y \le 1$), in units of $2\pi/a$, and 200-700 points for Matsubara frequencies with a constant cut $\omega_{max} = 10t$ in the summation over it. Usually 10 – 30 iterations were needed to obtain a solution for the self energy with an accuracy of order 0.001. To calculate the hole spectral function $A(k, \omega) = -\frac{1}{\pi}\mathrm{Im}\,\langle\langle h_k \mid h_k^+\rangle\rangle_{\omega+i\epsilon}$ and the density of states (DOS) $A(\omega) = \frac{1}{N}\sum_k A(k, \omega)$ a Pade approximation was used for analytical continuation from Matsubara points on the imaginary axis.

Calculations of the spin polaron quasiparticle spectrum have been done at finite temperature $T = 0.012$ that is slightly higher then the maximal superconducting temperature discussed below. Computations of the hole spectral functions $A(k, \omega)$ at different **k**-points show that for small hole concentrations $\delta \le 0.10$ there are no much differences for spectral functions calculated with renormalized and unrenormalized magnon energy in the interaction function, equation (3.5). In Fig.1(a) we compare the results of calculations for hole density of states $A(\omega)$ with renormalized (solid line) and unrenormalized (dashed line) magnon spectra for $\delta = 0.06$ that demonstrates a small effect of magnon renormalization.

However, at higher hole concentrations a negative contribution to the magnon spectral density appears at $\omega < 0$ due to excitation of electron-hole pairs. That results in negative values for hole spectral functions in the incoherent part of the spectrum. This negative contribution develops at first for long wavelength magnons as has been pointed out already in [17,18]. Since the main quasiparticle peak at $\mathbf{k} = (\pi/2, \pi/2)$ does not change much in shape with doping the picture of spin polarons as stable quasiparticle seems to be relevant even at large hole concentrations. This robust behaviour of spin polarons with doping can be explained by a small size of the polarons in comparisons with antiferromagnetic correlation length at quite large exchange energy.In Fig. 1(b) we show the density of states in the vicinity of the quasiparticle peak at large hole concentrations $\delta = 0.1, 0.25, 0.35$ (from right to left) calculated with unrenormalized magnon spectra.

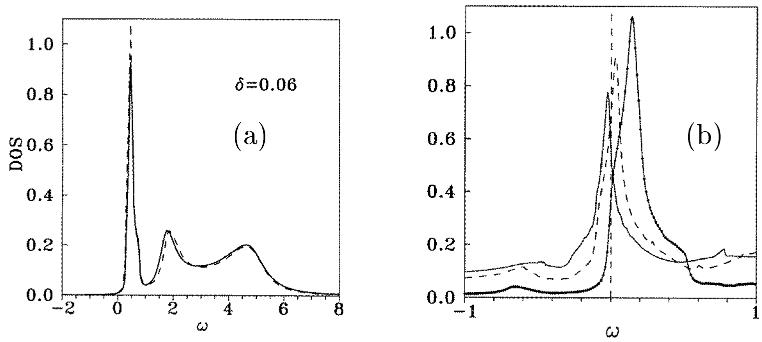

Figure 1. (a) The density of states (DOS) for the hole concentration $\delta = 0.06$. The solid (dashed) line corresponds to calculations with renormalized (unrenormalized) magnon spectra.
(b) DOS for $\delta = 0.1$, 0.25, 0.35 (from right to left) for unrenormalized magnon spectra.

The quasiparticle energy defined as $E(k,0) = \epsilon(k) + \mathrm{Re}\ \Sigma(k,0)$ is shown in Fig.2a for hole concentration $\delta = 0.25$ in the full Brillouin zone. With doping the hole quasiparticle spectrum does not change much in shape but

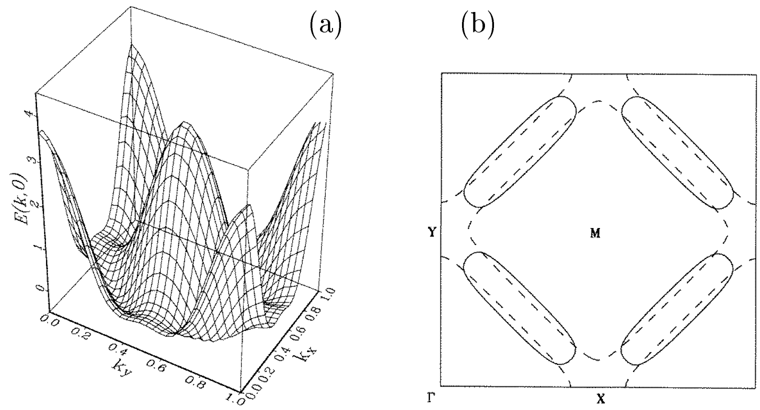

Figure 2. (a) The quasiparticle spectrum $E(\mathbf{k},0) = \epsilon(\mathbf{k}) + \mathrm{Re}\Sigma(\mathbf{k},\omega=0)$.
(b) The Fermi surface (FS) $E(\mathbf{k}_F,0) = 0$ in the full Brillouin zone at $\delta = 0.25$. The dashed line represents FS for $t' = 0$ ($\epsilon(\mathbf{k}) = 0$).

the bandwidth increases substantially. So, the rigid band approximation adopted in [19], [20] seems to be inadequate. In Fig.2b the Fermi surface defined as $E(k_F,0) = 0$ is shown for hole concentration $\delta = 0.25$ by thick line. It has a 4-pocket like form characteristic for $t-J$ model at low hole concentration. However, if we neglect the next-nearest-neighbour hopping, $t' = 0$, we get for the quasiparticle energy: $E(k, 0) = \mathrm{Re}\ \Sigma(k, 0)$ and for the corresponding Fermi surface, $\mathrm{Re}\ \Sigma(k_F, 0) = 0$. In that case we have a large Fermi surface for $\delta = 0.25$ shown in Fig.2b by dashed line. At lower hole concentration a transition from large Fermi surface to a 4-pocket like one occurs quite sharply.

Temperature dependence of the momentum distribution for holes in the spin polaron model was investigated in some details in [16] where it was shown that the Fermi surface washed out at some temperature of the order $T_d \approx 1.5J\delta$. So at quite low temperatures $T \approx 0.01$ considered here the Fermi surface does not change much with temperature. It should be also pointed out that high density of states in the present calculations (see Fig.1) results from a narrowing of a free electron bandwidth due to strong correlations (spin polaron formation) and has nothing to do with the van Hove singularity.

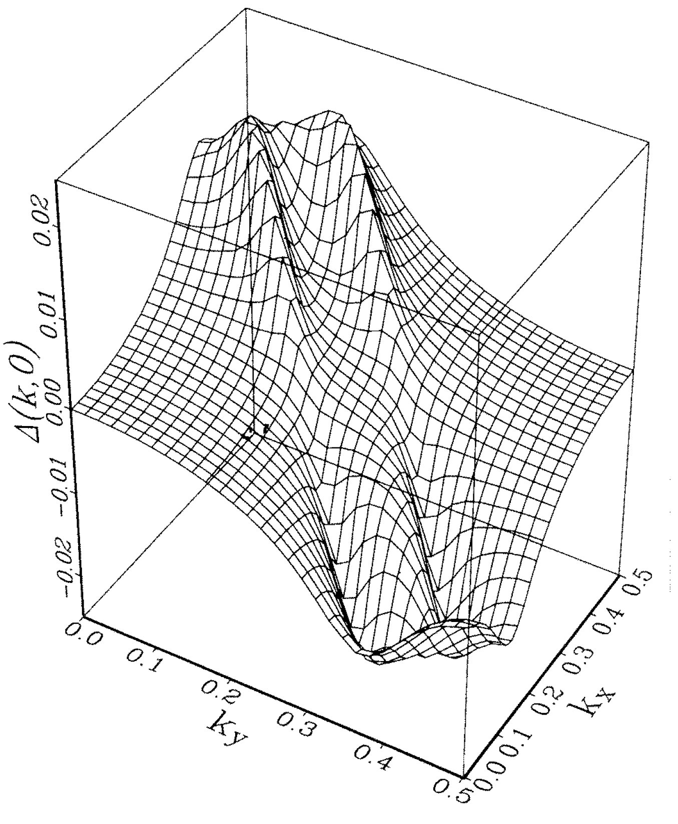

Figure 3. The gap function $\Delta(\mathbf{k}, \omega = 0)$ versus $\mathbf{k}$ (in units of $2\pi/a$).

In the present paper we consider only the linearized Eliashberg equation (4.2) for the pairing energy $\phi(k, i\omega_n)$ to study the symmetry of the superconducting order parameter and to evaluate the superconducting temperature T_c. Looking for even functions of wave-vector $\mathbf{k}$ that are realized in the singlet pairing we obtained only d-type symmetry for the gap function. In Fig.3 we show $\mathbf{k}$-dependence of the gap function $\Delta(\mathbf{k}, \omega = 0)$,

$\Delta(\mathbf{k},\omega) = \phi(\mathbf{k},\omega)/Z(\mathbf{k},\omega)$, in the quarter of the full Brillouin zone for $\delta = 0.25$ and $T/T_c \approx 0.8$. It has the typical d-wave symmetry with two ridges resulted from sharp changes of the interaction function at the Fermi surface. In Fig. 4 frequency dependence of Re $\Delta(\mathbf{k},\omega)$ (a) and

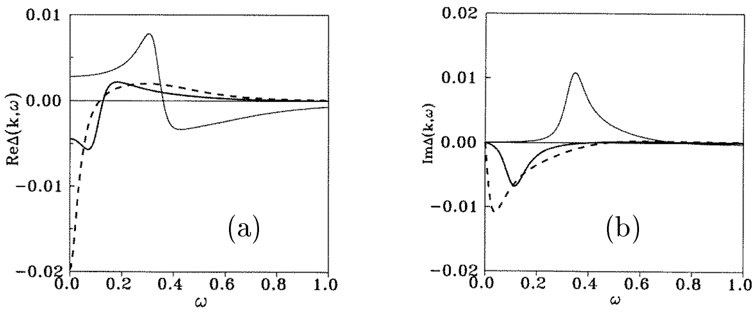

Figure 4. (a) Re $\Delta(\mathbf{k},\omega)$ and
(b) Im $\Delta(\mathbf{k},\omega)$ versus ω for a set of (k_x, k_y) points: inside FS (0, 0.19) – thin line; at (0.19, 0.19) - straight line: $\Delta = 0$; at AF Brillouin zone boundary (0.31, 0.19) – thick line, and near FS (0.38, 0.19)– dashed line. ($\delta = 0.25$ and $T/T_c \approx 0.8$.)

Im $\Delta(\mathbf{k},\omega)$(b) is shown for a set of (k_x, k_y) points: inside the Fermi surface (0, 0.19) – thin line, at AF Brillouin zone boundary (0.31, 0.19) – thick line, and near Fermi surface (0.38, 0.19)– dashed line. The gap function changes sign after crossing the $k_x = k_y = 0.19$ point where it is equal to zero (cp. Fig. 3). It is interesting that the characteristic for the pairing theory cut off energy of order $J \simeq 0.4$ away from the Fermi surface (see the thick and thin lines) becomes much smaller near the Fermi surface (see the dashed line). Therefore we have really a strong coupling limit for spin polaron pairing where all quasiparticles are paired contrary to the weak coupling in conventional superconductors. Quite large values of Im $\Delta(k,\omega)$ near the Fermi surface, shown in Fig. 4(b), also differ from the results for conventional superconductors.

By examining the temperature dependence of the highest eigenvalue in the equation (4.2) at different hole concentrations we can find the temperature when it passes through unity for decreasing T. At this temperature the normal state becomes unstable due to singlet pairing of quasiparticle — spin polarons on different sublattices. In Fig. 5 the dependence of superconducting temperature on hole concentrations is shown for $t' = -0.1$ (solid line) and $t' = 0$ (dashed line). We cannot solve our equation at lower temperatures then $T = 0.004$ and therefore has no results for T_c for $\delta < 0.1$. The maximum of T_c at $\delta \simeq 0.25$ (or at $\delta \simeq 0.20$ for $t' = 0$) is explained by crossing the maximum of the density of hole states by the Fermi level (see Fig. 2(b)). This results are quite different with the monotone increasing of T_c obtained within the weak coupling limit from the BCS equation in [20] and maximum of T_c observed in [10] near half filling, $\delta = 0$, for small clusters.

We also investigate T_c-dependence on the exchange energy for $J \leq 4$. T_c increases with J but saturates at $T_c \simeq 0.025$ 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 [9]. But the latter fenomenon is beyond the scope of our theoretical approach.

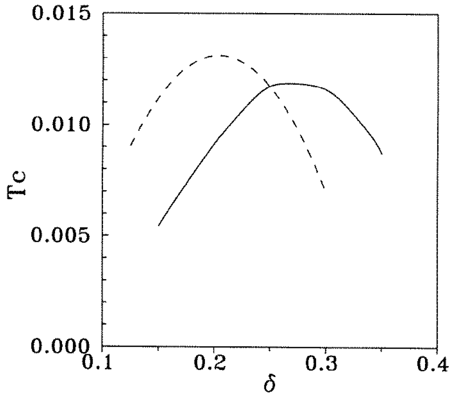

Figure 5. The superconducting temperature T_c versus hole concentration δ for $J = 0.4$, $t' = -0.1t$ (solid line) and $t' = 0$ (dashed line).

In conclusion, we have solved numerically Eliashberg equations (4.1), (4.2) for the strong coupling spin-polaron model (2.2). We have calculated the quasiparticle spectrum of spin polarons in the normal state and their superconducting pairing mediated by spin fluctuations. Unconventional behaviour obtained for the d-wave gap function (a sharp change with energy and large damping near the Fermi surface) suggests an explanation for some of anomalous properties of cuprate superconductors observed in tunnelling experiments (v-shape gap and large imaginary part), infrared absorption (no visible gap or gapless superconductivity), ARPES (a line of gap nodes around (π, π) directions [26]), etc.

Our calculations are based on the two sublattice representation, equation (2.1), which can be proved rigorously for AF background at low hole concentration. However, we believe that spin polarons dressed by AF spin fluctuations are the relevant quasiparticles even in the region of large hole concentrations provided the AF correlation length is much larger then the polaron size, of order of several lattice spacing. So we argue that spin polaron pairing mediated by spin fluctuations could represent the mechanism for high-temperature superconductivity in copper oxides.

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НАДПРОВІДНЕ СПАРЮВАННЯ СПІНОВИХ ПОЛЯРОНІВ У $t-J$ МОДЕЛІ

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В рамках спін-поляронної $t-J$ моделі на двохпідгратковому антиферомагнетику вивчається квазічастинковий спектр домішкових дірок та їх надпровідне спарювання в площині CuO_2. Самоузгоджена система рівнянь для діркових і магнонних матричних функцій Гріна у неперетинаючому наближенні розв'язується чисельно з допомогою алгоритму швидкого перетворення Фур'є. Ми отримуємо сильне перенормування діркового спектру внаслідок спінових флуктуацій, що приводить до формування спінових поляронів, які описуються когерентною частиною спектру. Ми також спостерігаємо синглетне d-хвильове надпровідне спарювання спінових поляронів на різних підгратках, опосередковане обміном спіновими флуктуаціями. Найвища температура надпровідності $T_c \simeq 0.01t$ отримується в околі концентрації дірок 0.25 для $t=0.4J$. Ми наводимо аргументи на користь того, що надпровідне спарювання спінових поляронів у $t-J$ моделі з сильними електричними кореляціями представляє механізм високотемпературної надпровідності.