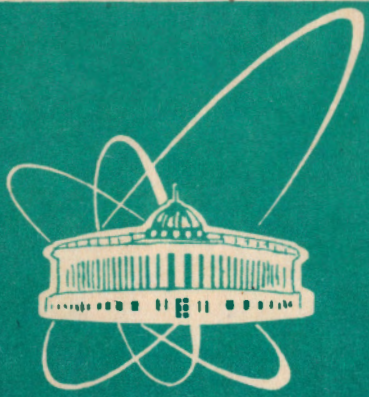

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SUPERCONDUCTING PAIRING IN THE SINGLET BAND OF THE EMERY MODEL

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1 Introduction

In the last years one observes a renewed interest in investigating the electron-phonon coupling mechanism for superconducting pairing in the high-temperature superconductors. There are a lot of experimental evidences for lattice effects in high-temperature superconductors (see e.g. [1]). And also calculations within the local density approximation (LDA) for the electron-phonon coupling constants have been recently performed which demonstrated a strong coupling of electrons with particular phonon modes both for La_2CuO_4-based compounds [2] and for $YBa_2Cu_3O_7$ ones [3].

But in the LDA strong electron correlations on copper sites cannot be properly taken into account which questions the results of these calculations. Intensive antiferromagnetic (AF) spin fluctuations which result directly from the strong electron correlations play an essential role in the explanation of a number of anomalous properties of copper oxides in the normal state. The AF spin fluctuations can also bring about superconducting pairing as it was proposed by several groups (see, e.g. [4, 5, 6]). Therefore, a more rigorous description of electron-phonon coupling in the strongly correlated system with a consistent account for AF spin fluctuations is desirable to investigate the nature of high temperature superconductivity.

The electronic structure and the low-lying charge-spin excitations of the CuO_2-planes are most accurately described within the Emery model [7]. By introducing the Hubbard operators which properly take into account the nonfermionic character of quasiparticles after the exclusion of doubly occupied d-hole states, one can obtain Eliashberg equations where in addition to the electron-phonon coupling the exchange pairing is readily observed [8]. But in the Hubbard I type approximation for the d-band in [8] as well as in the mean field approximation for slave bosons in [9] one cannot properly take

into account the formation of new quasiparticle bands due to the Coulomb and spin correlations. Namely the formation of singlet states plays an essential role in the low-energy electronic properties of the CuO_2 planes [10]. The appearance of singlet quasiparticle states inside the p-d gap was proved by different methods based on exact diagonalization [11], cluster calculations [12, 13], projection technique [14, 15] and other calculations.

In recent papers [16, 17] a simple analytical method was proposed which permits to reduce the two-band Emery model to an effective singlet-triplet model (see also [18]). Applying the equation of motion method for Green functions to this effective problem we found a reasonable description of the electronic structure which includes the singlet band [17]. Using this formalism for the electronic structure we investigate in the present paper the pairing which is induced by both the electron-phonon and the exchange interaction.

In the next Sect.2 we briefly formulate the singlet band model [16]. The resulting electronic structure [17] is shortly explained in Sect.3. The Migdal-Eliashberg equations for the matrix Green functions are derived in Sect.4. The dependence of the superconducting transition temperature T_c on the hole concentration n is calculated in Sect.5. In the Conclusions we summarize the results.

2 Singlet band model

We consider the Emery model in the limit of strong correlations at the copper sites, $U_d \to \infty$. By taking into account only the most important terms it can be written in a simple form:

$$H = \epsilon_d \sum_{i,\sigma} \tilde{d}^+_{i\sigma} \tilde{d}_{i\sigma} + \epsilon_p \sum_{m,\sigma} p^+_{m\sigma} p_{m\sigma} + t \sum_{i,m,\sigma} S_{im} \, (\tilde{d}^+_{i\sigma} p_{m\sigma} + h.c.), \qquad (1)$$

where $\tilde{d}^+_{i\sigma} = d^+_{i\sigma}(1 - n_{i\bar{\sigma}})$ denotes the creation of a hole on a copper site i provided there is no other hole with spin $\bar{\sigma} = -\sigma$. The operator $p^+_{m\sigma}$ creates a hole on an oxygen site m and $S_{im} = \pm 1$ depending on the position of the site m in the unit cell i in agreement with [10]. The hopping $p - d$ integral t and the difference between the hole energy levels for oxygen and copper, $\Delta = \epsilon_p - \epsilon_d$, are the only two parameters in the model (1).

To derive the singlet band it is reasonable to simplify this Hamiltonian (1) further. For that we follow mainly [16, 17]. Let us summarize the main steps: Introducing the symmetric combination of oxygen operators $p^{(s)}_{i\sigma}$ in the unit cell i according to [10], we can define the Wannier states $c_{i\sigma}$ by the equation

$$p^{(s)}_{i\sigma} = \frac{1}{2}\sum_m S_{im} p_{m\sigma} = \sum_j \nu_{ij}\ c_{j\sigma}. \tag{2}$$

The overlapping parameters

$$\nu_{jl} = \frac{1}{N}\sum_k \sqrt{1 - \frac{1}{2}(\cos k_x + \cos k_y)}\ e^{ik(j-l)} \tag{3}$$

rapidly decrease with the distance $(j-l)$: $\nu_0 = \nu_{jj} \simeq 0.96$, $\nu_1 = \nu_{j\ j\pm a_{x/y}} \simeq -0.14$, etc. (see [16]). In the following we will take into account ν_0, ν_1 and $\nu_2 = \nu_{j\ j+a_x+a_y} \simeq -0.02$ as it was done in [17]. The lattice constants a_x, a_y are taken to be unity in (3). In terms of the orthogonal Wannier states $c_{i\sigma}$ in (2) we can write the Hamiltonian in the form:

$$\begin{aligned} H &= \sum_{i\sigma}\{\epsilon_d\ \tilde{d}^+_{i\sigma}\tilde{d}_{i\sigma} + \epsilon_p\ c^+_{i\sigma}c_{i\sigma} + V_0\ (\tilde{d}^+_{i\sigma}c_{i\sigma} + h.c.)\} \\ &+ \sum_{i\neq j\sigma} V_{ij}\ \{\tilde{d}^+_{i\sigma}c_{j\sigma} + h.c.\}, \end{aligned} \tag{4}$$

where $V_{ij} = 2t\ \nu_{ij}$ and $V_0 = 2t\ \nu_0$. Since $|V_{ij}| \ll V_0$ one can consider the last term in (4) as a small perturbation to the diagonal part given by the first term in (4).

As was shown in [16, 17], the first part can be diagonalized within one unit cell. For this we introduce the one-hole state

$$|f_\sigma\rangle = \cos\theta_1 \; d_\sigma^+|0\rangle - \sin\theta_1 \; c_\sigma^+|0\rangle \tag{5}$$

and two-hole states – singlet$|\psi\rangle$ and triplets $|\tau_0\rangle$, $|\tau_{2\sigma}\rangle$:

$$|\psi\rangle = \cos\theta_2 \; \frac{1}{\sqrt{2}} \; (d_\uparrow^+ c_\downarrow^+ - d_\downarrow^+ c_\uparrow^+) \; |0\rangle - \sin\theta_2 \; c_\uparrow^+ c_\downarrow^+ \; |0\rangle, \tag{6}$$

$$|\tau_0\rangle = \frac{1}{\sqrt{2}} \; (d_\uparrow^+ c_\downarrow^+ + d_\downarrow^+ c_\uparrow^+) \; |0\rangle, \qquad |\tau_{2\sigma}\rangle = d_\sigma^+ c_\sigma^+ \; |0\rangle, \tag{7}$$

where $\tan 2\theta_1 = 2V_0/\Delta$, $\tan 2\theta_2 = 2\sqrt{2}V_0/\Delta$. The corresponding one-hole E_f and two-hole energies E_ψ and E_τ are given by:

$$\begin{aligned} E_f &= \frac{1}{2}(\epsilon_d + \epsilon_p) - \frac{1}{2}\sqrt{\Delta^2 + 4V_0^2}, \\ E_\psi &= \frac{1}{2}(\epsilon_d + 3\epsilon_p) - \frac{1}{2}\sqrt{\Delta^2 + 8V_0^2}, \\ E_\tau &= \epsilon_d + \epsilon_p. \end{aligned}$$

The singlet states (6) are the lowest among the two-hole states and have to be filled first with doping. By projecting the hopping term in (4) onto the low-energy subspace (5), (6), (7) one derives an effective singlet-triplet model (for details see [16, 17, 18]).

As was shown in [17], the mixing between singlet and triplet bands is rather small and will be neglected in the present paper. We consider only the one-hole states $|f_\sigma\rangle$ (5) and the singlet states $|\psi\rangle$ (6). By introducing the Hubbard operators in this subspace

$$X_i^{\sigma\sigma} = |f_{i\sigma}\rangle\langle f_{i\sigma}|, \quad X_i^{\psi\psi} = |\psi_i\rangle\langle\psi_i|, \quad X_i^{\psi\sigma} = |\psi_i\rangle\langle f_{i\sigma}|, \tag{8}$$

we can write the effective Hamiltonian in first order of V_{ij}:

$$H_t = E_f \sum_i X_i^{\sigma\sigma} + E_\psi \sum_i X_i^{\psi\psi} + \sum_{i \neq j\sigma} t_{ij} (X_i^{\psi\sigma} X_j^{\sigma\psi} + h.c.) \tag{9}$$

with the effective hopping integral [17]

$$t_{ij} = V_{ij} K_{\psi\psi}, \quad \text{where} \quad K_{\psi\psi} = 2A_x^{\psi} A_c^{\psi}$$

and

$$A_x^{\psi} = -\frac{1}{\sqrt{2}} \sin\theta_1 \cos\theta_2, \quad A_c^{\psi} = \sin\theta_1 \sin\theta_2 + \frac{1}{\sqrt{2}} \cos\theta_1 \cos\theta_2.$$

The Hamiltonian (9) becomes active if the number of holes n exceeds the value of one. There is a Hamiltonian similar to (9) which describes the lower copper band (or the upper Hubbard band in the electron picture) [17]. In lowest order of V_{ij} one has no mixing terms in the Hamiltonians which correspond to transitions between both bands, but the copper band influences the singlet band (9) by means of the spectral strength as will be explained later on.

The second order of V_{ij} gives rise to the exchange interaction:

$$H_{ex} = \frac{1}{2} \sum_{i \neq j} J_{ij} (X_i^{\sigma\bar{\sigma}} X_j^{\bar{\sigma}\sigma} - X_i^{\sigma\sigma} X_j^{\bar{\sigma}\bar{\sigma}}), \tag{10}$$

with the exchange integral $J_{ij} = 2a(V_{ij})^2/\Delta$ and where the constant a is given in [16]. For $\Delta = 2t$ one gets the following estimations for the nearest neighbour hopping and exchange interactions: $t_{ij} \simeq 2t\nu_1 K_{\psi\psi} \simeq 0.16\Delta$ and $J_{ij} \simeq 0.05\Delta$ [16]. However, in our present numerical calculations, we will choose the exchange integral J_{ij} as a parameter independent of the given values for the Emery model, whereas we will calculate the hopping integrals t_{ij} from Δ and t always. That is due to our crude mean-field-like approximation for the exchange induced pairing which would bring about too large, unreasonable, values of T_c.

The effective problem (9,10) looks like the well-known $t-J$ model [10]. However, our procedure allows the determination of the effective hopping t_{ij} and exchange integrals J_{ij} from the parameters of the Emery model in

a much better way than it was originally proposed [10]. Furthermore, we included next nearest neighbour hopping. But the most serious difference concerns the inclusion of the lower copper band which allows to take into account the spectral weight transfer [21] in a first approximation. That influences the results at least qualitatively.

It should be pointed out that the Hubbard operators (8) describe composite singlet quasiparticles for a strongly correlated system ($U_d \to \infty$) which cannot be obtained in the simple one-particle approximation usually used in the LDA approach.

To consider the electron-phonon coupling we introduce a model interaction in the form

$$H_{ep} = \sum_{ij} Q_i g(i-j) X_j^{pp}, \tag{11}$$

where the local normal coordinate $Q_j = \frac{1}{\sqrt{N}} \sum_q Q_q \exp(iqj)$ describes lattice vibrations of a particular symmetry. For simplicity we consider only one branch of phonon spectra described by the Hamiltonian:

$$H_{ph} = \frac{1}{2} \sum_q (P_q^2 + \omega_q^2 Q_q^2). \tag{12}$$

where ω_q is a phonon frequency of the normal mode. The electron-phonon interaction for singlets $g(i-j)$ depends on the deformation potentials for the energy levels for d- and p-holes in the crystal field. Electron-phonon coupling due to the modulation of the hopping integral t_{ij} in (9) is omitted here since it seems to be much smaller in ionic cuprates in comparison with crystal field modulation effects due to lattice vibrations (see e.g. [19]).

3 Electronic structure

To discuss the superconducting pairing within the model (9)-(12) we consider the equation of motion method for the matrix Green function

$$\hat{G}_{ii',\sigma}(t-t') = \ll \Psi_{i\sigma}(t) | \Psi^{+}_{i'\sigma}(t') \gg, \tag{13}$$

in terms of the Nambu operators:

$$\Psi_{i\sigma} = \begin{pmatrix} X_i^{\sigma\psi} \\ X_i^{\psi\bar{\sigma}} \end{pmatrix}, \qquad \Psi^{+}_{i\sigma} = \left(X_i^{\psi\sigma} \; X_i^{\bar{\sigma}\psi} \right), \tag{14}$$

where Zubarev's notation for the anticommutator Green function (13) was used [20].

Since the exchange interaction $J_{ij} \propto |V_{ij}|^2$ is much smaller than the hopping term $t_{ij} \propto V_{ij}$ we can consider the exchange interaction and the electron-phonon coupling (11) as a small perturbation to the singlet quasiparticle band energy given by the hopping Hamiltonian (9). Furthermore, we are interested in the electronic structure of the paramagnetic state for not too small doping values. Therefore, we calculate the electronic structure by means of H_t (9) only. For that we introduce the zero order Green function $\hat{G}^0$. According to [17] we can derive the following equation of motion which describes the quasiparticle band structure without any pairing effects:

$$(\omega\tau_0 - \epsilon_\psi \tau_3)\, \hat{G}^0_{ii',\sigma}(\omega) = \delta_{ii'} \hat{\chi}_\psi + \sum_j \hat{\Omega}^{\sigma}_{ij} \hat{G}^0_{ji',\sigma}(\omega), \tag{15}$$

where $\epsilon_\psi = E_\psi - E_f$ and

$$\hat{\chi}_\psi = \tau_0\, \chi_\psi, \qquad \chi_\psi = \langle X_i^{\sigma\sigma} + X_i^{\psi\psi} \rangle. \tag{16}$$

Here we assumed a paramagnetic ground state which implies that χ_ψ in (16) does not depend on the spin and τ_0 and τ_3 in (15) are the Pauli matrices. The

frequency matrix $\hat{\Omega}_{ij}^{\sigma}$ is defined by the projection of the equation of motion for the zero-order Green function onto the subspace of singlet quasiparticles (see [17], [22]):

$$\chi_\psi(\Omega_{ij}^{\sigma})_{11} = \delta_{ij}\sum_l t_{il}\langle X_i^{\psi\bar{\sigma}} X_l^{\bar{\sigma}\psi}\rangle + \\ +(1-\delta_{ij})\, t_{ij}\, \Big(\langle (X_i^{\sigma\sigma}+X_i^{\psi\psi})(X_j^{\sigma\sigma}+X_i^{\psi\psi})\rangle \;+\; \langle X_i^{\sigma\bar{\sigma}} X_j^{\bar{\sigma}\sigma}\rangle\Big). \quad (17)$$

The other diagonal element is given by complex conjugation

$$(\Omega_{ij}^{\sigma})_{22} = -(\Omega_{ij}^{\bar{\sigma}})_{11}^{+}$$

and the off-diagonal elements are zero. Using the Hubbard I type approximation as in [17]:

$$\langle X_i^{\sigma\bar{\sigma}} X_j^{\bar{\sigma}\sigma}\rangle \simeq 0, \quad \langle (X_i^{\sigma\sigma}+X_i^{\psi\psi})(X_j^{\sigma\sigma}+X_i^{\psi\psi})\rangle \simeq \chi_\psi^2$$

and neglecting the energy shift $\propto \delta_{ij}$ in (17) we find for the frequency matrix after Fourier transformation $(\Omega_{ij}^{\sigma})_{11} \rightarrow \Omega(k)$:

$$\Omega(k) = \chi_\psi \sum_j^{l\neq j} t_{lj}\; e^{ik(j-l)}. \quad (18)$$

The quasiparticle strength χ_ψ and the chemical potential μ depend on the doping. To calculate that we take into account the lower copper band which has a spectral strength of $\chi = \langle X_i^{\sigma\sigma}\rangle$ [17]. For a partly filled singlet band, where the filling $S_\psi = N_k/N$ is given from the number of occupied k-values N_k, we find from the definition (16) of the quasiparticle strength:

$$\chi_\psi = \chi + \chi_\psi S_\psi. \quad (19)$$

The total number of holes has a contribution from the copper band and from the singlet band (see also [17])

$$n = 2\chi + \chi_\psi C_{\psi\psi} S_\psi. \quad (20)$$

where

$$C_{\psi\psi} = 2(A_x^{\psi})^2 + 2(A_z^{\psi})^2$$

and where the spectral strength of the copper band decreases with doping according to $\chi = 1 - n/2$ [17]. The solution of eqs. (19) and (20) determines χ_ψ in the form

$$\chi_\psi = \frac{0.5}{1 - S_\psi(1 - C_{\psi\psi}/4)}.$$

One can see that the spectral strength of the singlet band χ_ψ increases with the doping in rough agreement with recent cluster calculations [21].

The simplification in comparison to our former calculation of the electronic structure [17] consists mainly in the neglection of the singlet-triplet coupling. However, that has only a minor influence on the results as can be seen in Fig.1. There, we present the density of states defined by:

$$N(\epsilon) = \frac{1}{N}\sum_k \delta(\epsilon - \epsilon_k), \quad \epsilon_k = \epsilon_c + \Omega(k) - \mu \tag{21}$$

at the chemical potential μ and compare it with the full solution. This definition differs from the imaginary part of the Green function by the quasiparticle weight χ_ψ. We plotted the density of states without the reduction factor χ_ψ since that quantity determines T_c as will become clear later on. The peak in the density of states corresponds to the half filled singlet band and occurs at roughly $n \simeq 1.24$. Please note that it would occur at a higher value of $n \simeq 1.33$ if we neglected the spectral weight transfer from the lower copper band. The decrease of the effective density of states for higher doping values is due to the increase of χ_ψ and correspondingly the increase of the bandwidth.

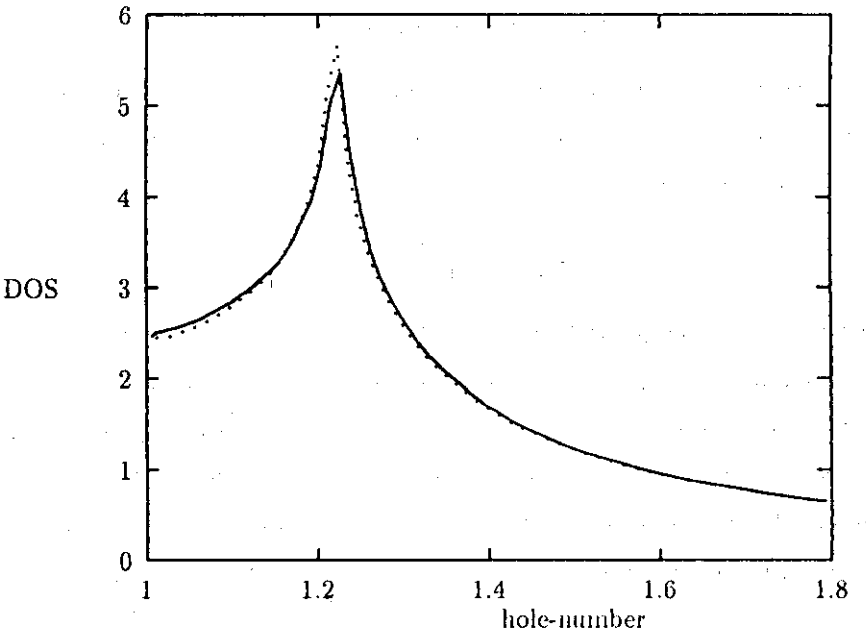

Fig.1: The density of states at the Fermi level for the full singlet-triplet model (full line) and neglecting the singlet-triplet coupling (dashed line)

4 Eliashberg equations

We consider two sources of superconducting pairing, namely the exchange interaction H_{ex} (10) and the electron-phonon coupling H_{ep} (11). Let us first take into account the pairing due to H_{ex} and employ the projection technique as described in [22]. We introduce a pairing matrix A_{ij}^{σ} defined by the equation

$$\chi_{\psi} A_{ij}^{\sigma} = \langle\{[\Psi_{i\sigma}, H_{ex}], \Psi_{j\sigma}^{+}\}\rangle,$$

where $\{\ldots,\ldots\}$ means the anticommutator. Taking into account the commutation relations for the Hubbard operators one gets for the nondiagonal matrix elements

$$\begin{aligned} \chi_\psi(A^\sigma_{ij})_{12} &= J_{ij}\ (\langle X^{\sigma\psi}_i X^{\bar\sigma\psi}_j\rangle + \langle X^{\sigma\psi}_j X^{\bar\sigma\psi}_i\rangle), \\ (A^\sigma_{ij})_{21} &= (A^\sigma_{ij})^+_{12}. \end{aligned} \tag{22}$$

The anomalous correlation functions $< X^{\sigma\psi}_i X^{\bar\sigma\psi}_j >$ can be calculated self-consistently from the Green function $\ll X^{\sigma\psi}_i | X^{\bar\sigma\psi}_j \gg$. It should be noted that we disregard here the so called kinematic pairing [23] due to H_t in agreement with recent results [24] which showed that it is purely an effect of the mean field solution and disappears by the inclusion of higher order terms.

Now we can write down the equation for the full Green function (13) in the form

$$\begin{aligned} (\omega\tau_0 - \epsilon_\psi\tau_3)\,\hat G_{ii',\sigma}(\omega) = \delta_{ii'}\hat\chi_\psi + \sum_j (\hat\Omega^\sigma_{ij} + \hat A^\sigma_{ij})\ \hat G_{ji',\sigma}(\omega) + \\ + \sum_j g(i-j)\ \tau_3\ \ll \Psi_{i\sigma}Q_j | \Psi^+_{i'\sigma}\gg_\omega . \end{aligned} \tag{23}$$

To obtain an equation for the last term in (23) proportional to the electron-phonon coupling (11) we consider the equation for the Green function $\ll \Psi_{i\sigma}Q_j|\Psi^+_{i'\sigma}(t')\gg$ by differentiating it over the second time t'. By adopting the same approximations for the t_{ij}- and the J_{ij}-terms as in eq. (23) we obtain the full Green function in (23) in the form:

$$\hat G_{ij,\sigma}(\omega)^{-1} = \frac{1}{\chi_\psi}\ \{(\omega\tau_0 - \epsilon_\psi\tau_3)\delta_{ij} - \hat\Omega^\sigma_{ij} - A^\sigma_{ij} - \chi_\psi\hat\Sigma^{ph}_{ij}(\omega)\}, \tag{24}$$

where the self-energy operator for electron-phonon coupling is given by (compare [8]):

$$\chi^2_\psi\ \hat\Sigma^{ph}_{ij}(\omega) = \sum_{ll'} g(i-l)\ \tau_3\ \ll \Psi_{i\sigma}Q_l | \Psi^+_{j\sigma}Q_{l'}\gg_\omega\ \tau_3\ g(j-l'). \tag{25}$$

In the Migdal approximation we can neglect vertex renormalization for the electron-phonon interaction and obtain the following equation for the self-energy operator in momentum-representation:

$$\chi_\psi^2\ \hat{\Sigma}^{ph}(q,\omega) = \frac{1}{N}\sum_k \int_{-\infty}^{\infty} d\nu\ K_{ph}(q-k\mid\omega,\nu)\ \tau_3\ [\frac{1}{\pi}\ \mathrm{Im}G_\sigma(k,\nu)]\ \tau_3, \quad (26)$$

where the electron-phonon interaction kernel is given by:

$$K_{ph}(q\mid\omega,\nu) = \int_{-\infty}^{\infty} \frac{dz}{z+\nu-\omega}\ \frac{1}{2}\ (\tanh\frac{\nu}{2T} + \coth\frac{z}{2T})\ \alpha^2F(q,z). \quad (27)$$

In the harmonic approximation (12) we get for the Eliashberg function:

$$\alpha^2F(q,z) = |g(q)|^2\ [-\frac{1}{\pi}\mathrm{Im} \ll Q_q|Q_{-q} \gg] = |g(q)|^2\ \frac{z}{|z|}\ \delta(z^2-\omega_q^2),$$

where $g(q)$ is the Fourier transform of the electron-phonon interaction $g(i-j)$.

Now we can write down the Eliashberg equation for the quasiparticle weight $Z(q,\omega)$ and the gap function $\Delta(q,\omega) = \Phi(q,\omega)/Z(q,\omega)$ by introducing the usual notation for the self-energy operator:

$$\chi_\psi\hat{\Sigma}^{ph}(q,\omega) = \omega(1-Z(q,\omega))\tau_0 + \delta E_q(\omega)\tau_3 + \phi(q,\omega)\tau_1. \quad (28)$$

The full gap function is equal to $\Phi(q,\omega) = A(q)+\phi(q,\omega)$, where the Fourier transform of the matrix (22) defines the spin-exchange contribution to the gap function $(A^\sigma(q))_{12} = 2\sigma A(q)$, $2\sigma = \pm 1$.

The ansatz (28) solves the set of equations (24) and (26). Neglecting, as usual, the quasiparticle energy shift δE_q, we can write down the equation for the gap function $\Phi(q,\omega)$ in the form:

$$\begin{aligned}\Phi(q,\omega) &= \frac{1}{N}\sum_k \int_{-\infty}^{\infty} d\nu\{J(q-k)\tanh\frac{\nu}{2T} + K_{ph}(q-k\mid\omega,\nu)\} * \\ &* [-\frac{1}{\pi}\ \mathrm{Im}\ \frac{\Phi(k,\nu)}{\nu^2Z^2(k,\nu) - \epsilon_k^2 - \Phi^2(k,\nu)}]. \end{aligned} \quad (29)$$

where the quasiparticle energy ϵ_k was given in (18). Reserving the full solution of the Eliashberg equations for a further study we will adopt in the following the weak coupling approximation $Z(q,\omega) = 1$ where the electron-phonon kernel will be approximated by:

$$K_{ph}(q \mid \omega,\nu) = \frac{1}{2}U(q)\,\tanh\frac{\nu}{2T}\,\Theta(\omega_0 - |\omega|)\,\Theta(\omega_0 - |\nu|). \qquad (30)$$

The linearized equation for the gap $\Phi(q,\omega) \simeq \Delta(q,\omega)$ takes the form:

$$\Delta(q,\omega) = \frac{1}{N}\sum_k \{U(q-k)\Theta(\omega_0 - |\omega|)\Theta(\omega_0 - |\epsilon_k|) + \qquad (31)$$

$$+2J(q-k)\}\,\frac{\Delta(k,\epsilon_k)}{2\epsilon_k}\,\tanh\frac{\epsilon_k}{2T_c}.$$

To calculate numerically the superconducting transition temperature T_c from this equation we should consider some model interactions for the electron-phonon coupling $U(q)$.

5 Numerical determination of T_c

Let us consider the following model for the electron-phonon interaction in eq. (31):

$$U(q) = U_0 + U_1(\cos q_x + \cos q_y). \qquad (32)$$

Since $U(q) \simeq |g(q)|^2/\omega_q^2 \geq 0$ one has $|2U_1| \leq U_0$. That restricts the possibility of anisotropic pairing caused by the electron-phonon coupling. As was already mentioned, in the numerical calculations, we will take the coupling constant U_s of the exchange interaction

$$2J(q) = U_s(\cos q_x + \cos q_y) \qquad (33)$$

as a parameter.

Now, we derive the gap equations for different symmetries dealing with both pairing mechanisms in parallel. The gap function in eq. (31) will be decomposed into the isotropic $\Delta_0(\omega)$, extended s-wave $\Delta_s(\omega)$ and d-wave $\Delta_d(\omega)$ gap functions according to

$$\Delta(q,\omega) = \sum_i \alpha_i(q)\Delta_i(\omega), \tag{34}$$

with

$$\alpha_0 = 1, \quad \alpha_{s/d}(q) = \cos q_x \pm \cos q_y. \tag{35}$$

To obtain the equations for the gap function $\Delta_i(\omega)$ one should multiply eq. (31) by the corresponding function (35) and integrate over q. As a result, the gap equations for different symmetries decouple:

$$\Delta_0(\omega) = U_0\Theta(\omega_0 - |\omega|)\frac{1}{N}\sum_k \Delta_0(\epsilon_k)\Theta(\omega_0 - |\epsilon_k|)\frac{1}{2\epsilon_k}\tanh\frac{\epsilon_k}{2T_c} \tag{36}$$

$$\Delta_{s/d}(\omega) =$$

$$= U_1\Theta(\omega_0 - |\omega|)\frac{1}{N}\sum_k \Delta_{s/d}(\epsilon_k)\Theta(\omega_0 - |\epsilon_k|)\frac{\alpha_{s/d}(k)^2}{2}\frac{1}{2\epsilon_k}\tanh\frac{\epsilon_k}{2T_c} +$$

$$+ U_s\Theta(\omega_s - |\omega|)\frac{1}{N}\sum_k \Delta_{s/d}(\epsilon_k)\Theta(\omega_s - |\epsilon_k|)\frac{\alpha_{s/d}(k)^2}{2}\frac{1}{2\epsilon_k}\tanh\frac{\epsilon_k}{2T_c}. \tag{37}$$

We introduced, as an additional parameter, the cut-off spin-fluctuation energy ω_s in (37) which is of the order of the singlet bandwidth. Eq. (37) can be easily solved by a step-wise gap function:

$$\Delta_{s/d}(\omega) = \Delta_{ph}\Theta(\omega_0 - \omega) + \Delta_{sf}\Theta(\omega - \omega_0)\Theta(\omega_s - \omega), \quad \omega > 0. \tag{38}$$

To determine T_c of the isotropic s-wave pairing one obtains a BCS-like equation:

$$\frac{1}{U_0} = \frac{1}{N}\sum_k \Theta(\omega_0 - |\epsilon_k|)\frac{1}{2\epsilon_k}\tanh\frac{\epsilon_k}{2T_c}. \tag{39}$$

Obviously, the isotropic pairing is caused by the electron-phonon coupling only. The exchange interaction drops out, due to its special q-dependence (33). For the extended s-wave or d-wave pairing eq. (37) takes the form:

$$K_{s/d}(\omega_s) = \frac{1}{U_s}\left\{1 - U_s K_{s/d}(\omega_0)\frac{U_1 K_{s/d}(\omega_0)}{1 - U_1 K_{s/d}(\omega_0)}\right\}, \tag{40}$$

where

$$K_{s/d}(\omega_j) = \frac{1}{N}\sum_k \Theta(\omega_j - |\epsilon_k|)\frac{\alpha_{s/d}(k)^2}{2}\frac{1}{2\epsilon_k}\tanh\frac{\epsilon_k}{2T_c}. \tag{41}$$

Since the density of states has a very strong energy dependence

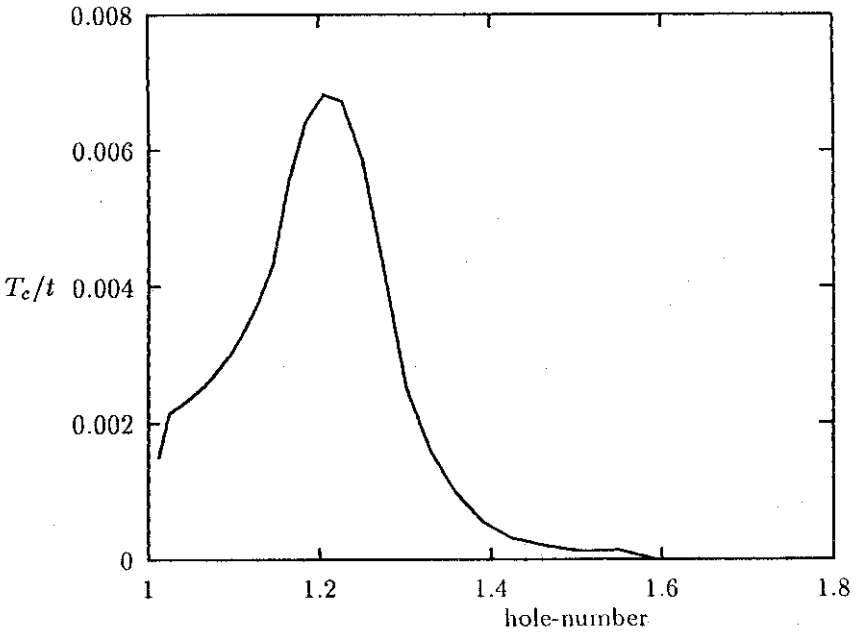

Fig.2: $T_c(n)$ dependence for the isotropic s-wave pairing

and cannot be approximated by its value at the Fermi energy, eqs. (39,40) have to be solved numerically. The results of the calculations are shown in Fig.2 for the isotropic s-wave pairing and in Fig.3 for the extended s- and

d-wave pairing. In the calculations we take the following parameters:

$$U_0 = 0.2, \quad U_1 = 0., \pm 0.1, \quad U_s = 0.2$$

$$\omega_0 = 0.035, \quad \omega_s = 0.2, \quad \Delta = 2.$$

All the energies are given in units of t.

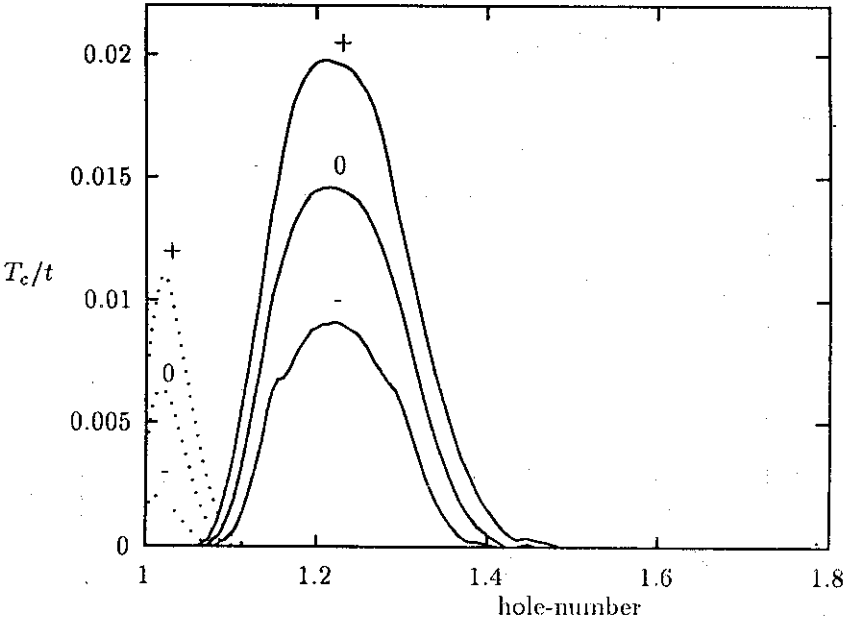

Fig.3: $T_c(n)$ dependence for d-wave pairing (full line) and extended s-wave pairing (dashed line) for different values of U_1 (± 0.1 and 0)

Let us first discuss the dependence of T_c on the number of holes n for the isotropic s-wave pairing. The peak in the density of states at $n \simeq 1.24$ (see Fig.1) gives rise to a more rounded peak for T_c (Fig.2) at a slightly smaller doping value $n \simeq 1.2$. The anisotropic part of the electron-phonon coupling (for $U_1 > 0$) gives a solution of (40) for d-wave or extended s-wave pairing even in the absence of the exchange interaction ($U_s = 0$). However,

that solution is not stable since it has a lower T_c than the isotropic case. That is due to the restriction $U_1 < U_0/2$. We can conclude that the pure electron-phonon coupling prefers isotropic s-wave pairing.

We can realize d-wave or extended s-wave pairing by the exchange interaction. That is shown in Fig.3. The suppression of extended s-wave pairing near to the half filled singlet band can be explained by the factor $\alpha_s(k)$ which is zero at the Fermi level for half filling. Depending on the sign of U_1 the anisotropic part of the electron-phonon coupling enhances or suppresses T_c.

6 Conclusion

In the present paper we study the superconducting pairing in the Emery model (1) for the CuO_2 plane when the Fermi level moves through the singlet band. We consider both the electron-phonon and the exchange mechanisms of pairing. To describe the electronic structure, including the strong correlation effects, we followed our former work [16, 17] and derived an effective $t-J$-like model. The zero order Green function, describing the electronic structure, was obtained by the equation of motion method following [17]. The lower copper band influences the singlet band by means of the spectral weight transfer.

We derived the Migdal-Eliashberg equations for the matrix Green function in terms of Hubbard operators which correspond to singlet quasiparticles. It is interesting to point out that the electronic quasiparticle weight χ_ψ (16) for the singlet Green function drops out from the gap equation (31). Therefore, T_c will be determined by the density of states defined as in (21) which is enhanced due to the bandwidth narrowing caused by the strong correlations. This brings about high values of $T_c \simeq 0.01t$ even for

weak electron-phonon ($U_0 \simeq 0.2t$) and spin-exchange ($U_s \simeq 0.2t$) coupling ($t \simeq 1.5eV$ for the p-d model).

The main task of the present work was the determination of the doping dependence of T_c for different symmetries of the gap function. The peak for the $T_c(n)$ dependence at $n \simeq 1.2$ both for the isotropic s-wave and d-wave pairing (see Figs. 2,3) resembles the universal $T_c(n)$ dependence of the copper oxides. The $T_c(n)$ curve for the extended s-wave pairing has its maximum at a much smaller density of holes, $n \simeq 1.05$ (see Fig.3) and seems to be incompatible with the experimental results. The isotropic and the anisotropic pairings are caused by different mechanisms: Electron-phonon coupling prefers isotropic s-wave pairing, whereas the exchange interaction seems to give rise to d-wave pairing which can be influenced by the anisotropic part of the electron-phonon interaction. Therefore, an experimental verification of the gap symmetry would give some hints for the (yet unknown) underlying pairing mechanism.

One should be aware that our approximation for the electronic structure cannot be the final answer. It surely does not correctly describe details of the order of the exchange energy J. So our approach does not distinguish between the coherent and the incoherent parts of the spectra which is known to be very important at least in the extremely small doping region [25]. Our results become more reliable for larger doping values $n > 1.2$. However, our curves show a quite reasonable overall shape of the $T_c(n)$ dependence. That gives us the hope that a refined electronic structure calculation does not change the main features of our present picture.

The next open question of this paper concerns the absolute values of T_c. Here, we consider only the weak coupling approximation (30) for the electron-phonon kernel (27) in the Eliashberg equation. As it is well known, the weak coupling approximation overestimates the value of T_c. The mean-

field-type approximation (22) for the spin-exchange coupling also greatly overestimates T_c. The effects of strong coupling and pair breaking effects due to spin-fluctuation scattering which should suppress T_c will be discussed elsewhere.

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