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EXCHANGE AND SPIN-FLUCTUATION SUPERCONDUCTING PAIRING IN THE HUBBARD MODEL IN THE STRONG CORRELATION LIMIT

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1 Introduction

Since the discovery of the high temperature superconductivity in cuprates, it has been believed by many researchers that an electronic mechanism could be responsible for the high values of T_c. The accumulated experimental evidence of the singlet $d_{x^2-y^2}$-wave superconducting pairing in high-T_c cuprates strongly supports this idea [1, 2]. At present, various phenomenological models for the spin-fluctuation pairing mechanism are known [2, 3]. Numerical finite cluster calculations also suggest $d_{x^2-y^2}$-wave superconducting instability for models with strong electron correlations [4]. Anderson [5] was the first to stress the importance of the strong electron correlations in copper oxides. He proposed to take them into account in the one-band two-dimensional (2D) Hubbard model [6] in the vicinity of half-filling,

$$H = -t \sum_{\langle ij \rangle \sigma} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow} , \qquad (1)$$

where t is an effective transfer integral for the nearest neighbor sites, $\langle ij \rangle$, U is the repulsive Coulomb single-site energy. A number of attempts to obtain superconducting pairing within the microscopical theory for the Hubbard model have been made.

Several papers considered the Hubbard model (1) in the weak correlation limit, $U \leq W$, where $W = 2zt$ is the bandwidth, $z = 4$, in a 2D model. In the framework of the conserving fluctuation exchange approximation (FLEX), self-consistent systems of equations for the normal and anomalous one-electron Green functions were solved [7]-[10]. In the vicinity of the antiferromagnetic (AFM) instability near half filling, $d_{x^2-y^2}$-wave superconducting pairing with temperature $T_c \simeq 0.02\ t$ was obtained. These direct numerical solutions of the strong coupling Eliashberg-type equations for the Hubbard model in the weak correlation limit unambiguously predict the occurrence of a $d_{x^2-y^2}$-wave pairing mediated by spin fluctuation exchange. Nevertheless, the superconducting solution was found only in a narrow range of U, very close to the AFM instability in the model. Higher order corrections to the effective interactions can also be important [11].

A realistic description of the cuprates is obtained in the strong correlation limit, $U > W$, however. The superconducting pairing due to the kinematic interaction in the Hubbard model (1) in the limit $U \to \infty$ was first proposed by Zaitsev and Ivanov [12]. Similar results were obtained by Plakida and Stasyuk [13] by means of the equation of motion method for the two-time Green functions (GF) [14]. The mean-field approximation (MFA) considered in these papers yielded s-wave pairing, which is irrelevant for strongly correlated systems [15]. Later on, the GF approach to the study of the MFA of the t–J model

[15, 16] resulted in $d_{x^2-y^2}$-wave superconducting pairing due to the exchange interaction J. Self-energy corrections to the $t-J$ model were considered by Izyumov et al. [17] within a diagram technique for the Hubbard operators and by Plakida et al. [18] within a projection technique for the GF. In the latter paper a direct numerical solution of the strong coupling equations in the self-consistent Born approximation demonstrated the occurrence of $d_{x^2-y^2}$-wave pairing mediated by AFM superexchange and spin fluctuations.

Mean-field type approximations of the strong correlation limit $U > W$ of the original Hubbard model (1), within the projection technique for GF, were reported in a number of papers. The use of the Roth method as a decoupling scheme for the calculation of higher order correlation functions resulted in $d_{x^2-y^2}$-wave superconducting symmetry [19]. To escape uncontrollable decoupling, Avella et al. [20] imposed kinematical restrictions to the Hubbard operators (the Pauli principle) to obtain superconducting solutions of the s- and d-type symmetry. Later on, Stanescu et al. [21] showed that the superconducting pairing for conventional electron (hole) pairs in MFA was absent and proposed a pairing mechanism for the composite excitations $\eta_{ij,\sigma} = c_{i\sigma} n_{js}$ (with (i,j) being the nearest neighbors). The use of the Roth decoupling procedure for the calculation of the anomalous correlation function $\langle c_{i\sigma} c_{i-\sigma}\, n_{js} \rangle$ and of the Pauli principle for the calculation of higher order normal correlation functions were found to emerge in high T_c superconductivity in the $d_{x^2-y^2}$-channel for the composite excitations [21]. However, the onset temperature following from these calculations strongly depends on the scheme of approximation, [19, 20] or on the particular solution [21]. In the limit of large U, extremely small T_c values are obtained as a consequence of the fact that the anomalous correlations are induced by pairing at the same lattice site, hence they should disappear in the limit $U \to \infty$. In addition, in the MFA, the self-energy operator caused by kinematic interaction is ignored, while as shown for the $t-J$ model [18], the self-energy of the anomalous GF is also responsible for the nonlocal spin-fluctuation d-wave superconducting pairing.

An open question is whether the one-band Hubbard model (1) is comprehensive enough to include all the essential features of the high temperature superconductors, or a model of increased complexity is needed. As demonstrated previously, [22, 23] an appropriate description of the normal state properties of these systems needs the consideration of a two-band singlet-hole Hubbard model derived from the $p-d$ model [24]. A description of the superconducting properties emerging from this two-band model is possible within an approach based on the GF technique [25].

In the present paper, we report an in-depth exploration of some key features of the two-band singlet-hole Hubbard model [22, 23]. We find that the

exchange interaction in the MFA and the spin-fluctuation electron scattering induced by the kinematical interaction in the second order result in the singlet $d_{x^2-y^2}$-wave pairing of the conventional electron pairs at different lattice sites. To treat rigorously the strong correlations, the Hubbard operator technique within the projection method for the GF [18] is used. The equation for the superconducting gap is numerically solved within the weak coupling approximation and T_c is calculated for several hole concentrations. Our results agree with the recent investigations of the Hubbard model within the dynamical cluster approximation, where the self-energy has been calculated in the non-crossing approximation for the 4-cluster model [26, 27].

The paper is organized as follows. In Sec. 2, the general formalism and the Dyson equation for the matrix GF in Nambu notation are derived for the two-band Hubbard model. In Sec. 3, it is shown that the superconducting pairing is mediated by the exchange interaction in the MFA. The self-energy is calculated in Sec. 4 and the weak coupling approximation limit is considered in Sec. 4.2. Numerical results and their discussion are provided in Sec. 5. Conclusions are presented in Sec. 6.

2 General formalism

For the high-T_c cuprates, the p–d model [24] is more realistic than the original Hubbard model (1). It can be reduced to the asymmetric Hubbard model with the lower Hubbard subband occupied by one-hole Cu d-like states and the upper Hubbard subband occupied by two-hole $p-d$ singlet states [22, 23]

$$\begin{aligned} H &= E_1 \sum_{i,\sigma} X_i^{\sigma\sigma} + E_2 \sum_i X_i^{22} + \sum_{i\neq j,\sigma} \{t_{ij}^{11} X_i^{\sigma 0} X_j^{0\sigma} \\ &+ t_{ij}^{22} X_i^{2\sigma} X_j^{\sigma 2} + 2\sigma t_{ij}^{12} (X_i^{2\bar{\sigma}} X_j^{0\sigma} + \text{H.c.})\} \end{aligned} \tag{2}$$

where $X_i^{nm} = |in\rangle\langle im|$ are the Hubbard operators for the four states $n, m = |0\rangle, |\sigma\rangle, |2\rangle = |\uparrow\downarrow\rangle$, $\sigma = \pm 1/2$, $\bar{\sigma} = -\sigma$. The energy parameters are given by $E_1 = \epsilon_d - \mu$ and $E_2 = 2E_1 + \Delta$ respectively, where ϵ_d is a reference (renormalized) energy of the d-hole, μ is the chemical potential, and $\Delta = \epsilon_p - \epsilon_d$ is the renormalized charge transfer energy (see [22]). Here and in what follows, the superscript 2 and 1 refers to the singlet and one-hole subbands, respectively. The hopping integrals can be written as $t_{ij}^{\alpha\beta} = K_{\alpha\beta} V_{ij}$, $V_{ij} = 2t\nu_{ij}$, where t is the $p-d$ hybridization parameter and ν_{ij} are the overlapping parameters for the Wannier oxygen states. For the nearest and second neighbors they are equal to: $\nu_1 = \nu_{j\ j\pm a_{x/y}} \simeq -0.14$, $\nu_2 = \nu_{j\ j\pm a_x \pm a_y} \simeq -0.02$. The coefficients $K_{\alpha\beta}$ depend on the dimensionless parameter t/Δ and for the realistic value $\Delta = 2t$ we have for the singlet subbands $t_{eff} \simeq K_{22} 2\nu_1 t \simeq 0.14t$. Hence the

ratio of the charge-transfer gap to the bandwidth $W = 8t_{eff}$, $\Delta/W \simeq 2$, so that the Hubbard model (2) corresponds to the strong correlation limit.

The Hubbard operators entering (2) obey the completeness relation

$$X_i^{00} + X_i^{\sigma\sigma} + X_i^{\bar{\sigma}\bar{\sigma}} + X_i^{22} = 1, \tag{3}$$

which rigorously preserves the constraint of no double occupancy at each lattice site i.

To discuss the superconducting pairing within the model Hamiltonian (2), we define the two-band four-component Nambu operators $\hat{X}_{i\sigma}^{\dagger}$ and $\hat{X}_{i\sigma}$, where

$$\hat{X}_{i\sigma}^{\dagger} = (X_i^{2\sigma} \; X_i^{\bar{\sigma}0} \; X_i^{\bar{\sigma}2} \; X_i^{0\sigma}) \tag{4}$$

and $\hat{X}_{i\sigma}$ is obtained from (4) by Hermitian conjugation. The pairing correlations of these operators are described within the GF approach. The two-time anticommutator retarded GF associated to the site (i, j) is a 4×4 matrix

$$\tilde{G}_{ij\sigma}(t-t') = -i\theta(t-t')\langle\{\hat{X}_{i\sigma}(t), \hat{X}_{j\sigma}^{\dagger}(t')\}\rangle = \langle\langle \hat{X}_{i\sigma}(t) \,|\, \hat{X}_{j\sigma}^{\dagger}(t')\rangle\rangle, \tag{5}$$

where Zubarev's notation [14] was used. The $(\mathbf{q}, \omega)$ Fourier-representation of the GF is defined by the equation

$$\tilde{G}_{ij\sigma}(t-t') = \frac{1}{2\pi}\int_{-\infty}^{+\infty} \mathrm{d}\omega \; \mathrm{e}^{-i\omega(t-t')} \, \frac{1}{N}\sum_{\mathbf{q}} \mathrm{e}^{i\mathbf{q}\cdot(\mathbf{i}-\mathbf{j})} \, \tilde{G}_{\mathbf{q}\sigma}(\omega), \tag{6}$$

To get the QP spectrum of the system, we use the equation of motion method. Differentiation with respect to t of the GF (5) and use of the Fourier transform (6) result in the following equation [25]

$$\omega\tilde{G}_{ij\sigma}(\omega) = \delta_{ij}\tilde{\chi} + \langle\langle \hat{Z}_{i\sigma} \,|\, \hat{X}_{j\sigma}^{\dagger}\rangle\rangle_{\omega}, \tag{7}$$

where $\hat{Z}_{i\sigma} = [\hat{X}_{i\sigma}, H]$ and

$$\tilde{\chi} = \langle\{\hat{X}_{i\sigma}, \hat{X}_{i\sigma}^{\dagger}\}\rangle = \begin{pmatrix} \chi_2 & 0 & 0 & \chi_3 \\ 0 & \chi_1 & \chi_3 & 0 \\ 0 & \chi_3^* & \chi_2 & 0 \\ \chi_3^* & 0 & 0 & \chi_1 \end{pmatrix}.$$

Assuming that the system is in the paramagnetic state, we get for the diagonal terms $\chi_2 = \langle X_i^{22} + X_i^{\sigma\sigma}\rangle = \langle X_i^{22} + X_i^{\bar{\sigma}\bar{\sigma}}\rangle$ and $\chi_1 = \langle X_i^{00} + X_i^{\bar{\sigma}\bar{\sigma}}\rangle = \langle X_i^{00} + X_i^{\sigma\sigma}\rangle$. In view of (3), they fulfill the relationship $\chi_2 = 1 - \chi_1 = n/2$, where n denotes the hole concentration. The correlation function $\chi_3 = \langle X_i^{02}\rangle$ provides a measure to the statistical average of the singlet destruction at the i-th site.

Using the definitions of the Fermi annihilation operators: $c_{i\sigma} = X_i^{0\sigma} + 2\sigma X_i^{\bar{\sigma}2}$ and the identities for the Hubbard operators, $X_i^{0\sigma}X_i^{0\bar{\sigma}} = 0$, $X_i^{\sigma 2}X_i^{\bar{\sigma}2} = 0$, $X_i^{0\downarrow}X_i^{\downarrow 2} = X_i^{02}$, we get

$$X_i^{02} = X_i^{0\downarrow}X_i^{\downarrow 2} = c_{i\downarrow}c_{i\uparrow}, \tag{8}$$

hence $\langle X_i^{02}\rangle$ describes the pairing at the i-th lattice site in two subband. It vanishes for the $d_{x^2-y^2}$-wave symmetry:

$$\chi_3 = \left\langle X_i^{02}\right\rangle = 0. \tag{9}$$

The chemical potential μ is calculated from the equation for the average number of holes,

$$n = \langle N_i\rangle = \sum_{\sigma}\langle X_i^{\sigma\sigma}\rangle + 2\langle X_i^{22}\rangle\ . \tag{10}$$

Using the projection technique described by Plakida, [28] the operator $\hat{Z}_{i\sigma}$ which enters the last term of Eq. (7) is split into two parts:

$$\hat{Z}_{i\sigma} = [\hat{X}_{i\sigma}, H] = \sum_{l}\tilde{E}_{il\sigma}\hat{X}_{l\sigma} + \hat{Z}_{i\sigma}^{(ir)}. \tag{11}$$

Here, the linear combination of the operators $\hat{X}_{l\sigma}$ includes the effect of time averaged forces (the mean-field solution). The irreducible part, $\hat{Z}_{i\sigma}^{(ir)}$, originates in the inelastic quasi-particle scattering. It is defined by the orthogonality condition to the one-particle operators, $\langle\{\hat{Z}_{i\sigma}^{(ir)}, \hat{X}_{j\sigma}^{\dagger}\}\rangle = 0$. From this definition we get the frequency matrix:

$$\tilde{E}_{ij\sigma} = \tilde{\mathcal{A}}_{ij\sigma}\tilde{\chi}^{-1}, \quad \tilde{\mathcal{A}}_{ij\sigma} = \langle\{[\hat{X}_{i\sigma}, H], \hat{X}_{j\sigma}^{\dagger}\}\rangle. \tag{12}$$

If the finite lifetime effects due to $\hat{Z}_{i\sigma}^{(ir)}$ in (11) are neglected and the expression (12) of the frequency matrix is used, then Eq. (7) provides the zero-order GF within the generalized MFA. In the $(\mathbf{q},\omega)$-representation, its expression is given by

$$\tilde{G}_{\sigma}^{0}(\mathbf{q},\omega) = \left(\omega\tilde{\tau}_0 - \tilde{\mathcal{A}}_{\sigma}(\mathbf{q})\tilde{\chi}^{-1}\right)^{-1}\tilde{\chi}\ , \tag{13}$$

where $\tilde{\tau}_0$ is the 4×4 unity matrix.

Differentiation of the many-particle GF (7) with respect to the second time t' and use of the same projection procedure as in (11) result in the Dyson equation for the GF (5). In the $(\mathbf{q},\omega)$-representation, the Dyson equation is

$$\left(\tilde{G}_{\sigma}(\mathbf{q},\omega)\right)^{-1} = \left(\tilde{G}_{\sigma}^{0}(\mathbf{q},\omega)\right)^{-1} - \tilde{\Sigma}_{\sigma}(\mathbf{q},\omega). \tag{14}$$

The self energy operator $\tilde{\Sigma}_{\sigma}(\mathbf{q},\omega)$ is defined by

$$\tilde{T}_{\sigma}(\mathbf{q},\omega) = \tilde{\Sigma}_{\sigma}(\mathbf{q},\omega) + \tilde{\Sigma}_{\sigma}(\mathbf{q},\omega)\tilde{G}_{\sigma}^{0}(\mathbf{q},\omega)\tilde{T}_{\sigma}(\mathbf{q},\omega), \tag{15}$$

where $\tilde{T}_\sigma(\mathbf{q},\omega) = \tilde{\chi}^{-1}\langle\langle \hat{Z}_\sigma^{(ir)} \,|\, \hat{Z}_\sigma^{(ir)\dagger}\rangle\rangle_{\mathbf{q},\omega}\tilde{\chi}^{-1}$ denotes the scattering matrix. From Eq. (15) it follows that the self-energy operator is given by the *proper* part of the scattering matrix that has no parts connected by the single-particle zero-order GF (13):

$$\tilde{\Sigma}_\sigma(\mathbf{q},\omega) = \tilde{\chi}^{-1}\langle\langle \hat{Z}_\sigma^{(ir)} \,|\, \hat{Z}_\sigma^{(ir)\dagger}\rangle\rangle_{\mathbf{q},\omega}^{(prop)}\,\tilde{\chi}^{-1}. \tag{16}$$

The equations (13), (14), and (16) provide an exact representation for the GF (5). Its calculation, however, requires the use of some approximations for the many-particle GF in the self-energy matrix (16) which describes the finite lifetime effects (inelastic scattering of electrons on spin and charge fluctuations).

3 Mean-field approximation

3.1 The frequency matrix

In the MFA, the calculation of the frequency matrix and of the zero-order GF (13) requires the knowledge of the quantity $\tilde{\mathcal{A}}_{ij\sigma}$, Eq. (12). This needs the equations of motion of the Hubbard operators:

$$\begin{aligned} Z_i^{\sigma 2} &= [X_i^{\sigma 2}, H] = (E_1+\Delta)X_i^{\sigma 2} + \sum_{l\neq i,\sigma'}\left(t_{il}^{22}B_{i\sigma\sigma'}^{22}X_l^{\sigma' 2} - 2\sigma t_{il}^{21}B_{i\sigma\sigma'}^{21}X_l^{0\bar{\sigma}'}\right) \\ &- \sum_{l\neq i} X_i^{02}\left(t_{il}^{11}X_l^{\sigma 0} + 2\sigma t_{il}^{21}X_l^{2\bar{\sigma}}\right), \end{aligned} \tag{17}$$

$$\begin{aligned} Z_i^{0\bar{\sigma}} &= [X_i^{0\bar{\sigma}}, H] = E_1 X_i^{0\bar{\sigma}} + \sum_{l\neq i,\sigma'}\left(t_{il}^{11}B_{i\sigma\sigma'}^{11}X_l^{0\bar{\sigma}'} - 2\sigma t_{il}^{12}B_{i\sigma\sigma'}^{12}X_l^{\sigma' 2}\right) \\ &- \sum_{l\neq i} X_i^{02}\left(t_{il}^{22}X_l^{2\bar{\sigma}} + 2\sigma t_{il}^{12}X_l^{\sigma 0}\right), \end{aligned} \tag{18}$$

and $Z_i^{2\bar{\sigma}} = -\left(Z_i^{\bar{\sigma}2}\right)^\dagger$, $Z_i^{\sigma 0} = -\left(Z_i^{0\sigma}\right)^\dagger$. Here, $B_{i\sigma\sigma'}^{\alpha\beta}$ are Bose-like operators describing the number (charge) and spin fluctuations:

$$B_{i\sigma\sigma'}^{22} = (X_i^{22} + X_i^{\sigma\sigma})\delta_{\sigma'\sigma} + X_i^{\sigma\bar{\sigma}}\delta_{\sigma'\bar{\sigma}} = (\frac{1}{2}N_i + S_i^z)\delta_{\sigma'\sigma} + S_i^\sigma\delta_{\sigma'\bar{\sigma}}, \tag{19}$$

$$B_{i\sigma\sigma'}^{21} = (\frac{1}{2}N_i + S_i^z)\delta_{\sigma'\sigma} - S_i^\sigma\delta_{\sigma'\bar{\sigma}}, \tag{20}$$

$$B_{i\sigma\sigma'}^{11} = \delta_{\sigma'\sigma} - B_{i\sigma\sigma'}^{21}, \quad B_{i\sigma\sigma'}^{12} = \delta_{\sigma'\sigma} - B_{i\sigma\sigma'}^{22}, \tag{21}$$

where use was made of the completeness relation (3), the number operator N_i, Eq. (10), and the spin operators $S_i^z = \sum_\sigma \sigma X_i^{\sigma\sigma}$, $S_i^\sigma = X_i^{\sigma\bar{\sigma}}$. With these

prerequisites, the calculation of the matrix (12) is straightforward,

$$\tilde{\mathcal{A}}_{ij\sigma} = \begin{pmatrix} \hat{\omega}_{ij\sigma} & \hat{\Delta}_{ij\sigma} \\ (\hat{\Delta}^{*}_{ij\sigma})^{(\mathrm{T})} & -\hat{\omega}^{(\mathrm{T})}_{ij\bar{\sigma}} \end{pmatrix}, \tag{22}$$

where $\hat{\omega}_{ij\sigma}$ and $\hat{\Delta}_{ij\sigma}$ are 2×2 matrices, while the superscript (T) denotes the operation of transposition. We have,

$$\begin{aligned} \hat{\omega}_{ij\sigma} &= \delta_{ij} \begin{pmatrix} (E_1 + \Delta)\chi_2 + a^{22}_{\sigma} & a^{21}_{\sigma} \\ (a^{21}_{\sigma})^{*} & E_1\chi_1 + a^{22}_{\sigma} \end{pmatrix} \\ &+ (1 - \delta_{ij})V_{ij} \begin{pmatrix} K^{22}_{ij\sigma} & K^{21}_{ij\sigma} \\ (K^{21}_{ij\sigma})^{*} & K^{11}_{ij\sigma} \end{pmatrix}, \end{aligned} \tag{23}$$

$$\hat{\Delta}_{ij\sigma} = \delta_{ij} \begin{pmatrix} b^{22}_{\sigma} & b^{21}_{\sigma} \\ -b^{21}_{\bar{\sigma}} & b^{11}_{\sigma} \end{pmatrix} + (1 - \delta_{ij})V_{ij} \begin{pmatrix} L^{22}_{ij\sigma} & L^{21}_{ij\sigma} \\ -L^{21}_{ij\bar{\sigma}} & L^{11}_{ij\sigma} \end{pmatrix}. \tag{24}$$

In Eq. (23), the quantities $a^{\alpha\beta}_{\sigma}$ determine energy shifts:

$$a^{22}_{\sigma} = \sum_{m \neq i} V_{im} \left(K_{22} \langle X^{2\bar{\sigma}}_i X^{\bar{\sigma}2}_m \rangle - K_{11} \langle X^{\sigma 0}_m X^{0\sigma}_i \rangle \right), \tag{25}$$

$$\begin{aligned} a^{21}_{\sigma} &= -\sum_{m \neq i} V_{im} \left(K_{22} \langle X^{\sigma 0}_i X^{\bar{\sigma}2}_m \rangle + K_{11} \langle X^{\bar{\sigma}2}_i X^{\sigma 0}_m \rangle \right) \\ &- 2\sigma \sum_{m \neq i} V_{im} K_{12} \left(\langle X^{\sigma 0}_i X^{0\sigma}_m \rangle - \langle X^{2\bar{\sigma}}_m X^{\bar{\sigma}2}_i \rangle \right), \end{aligned} \tag{26}$$

while the quantities $K^{\alpha\beta}_{ij\sigma}$ define renormalized hopping parameters,

$$K^{22}_{ij\sigma} = K_{22}\chi^{cs}_{ij} - K_{11}\langle X^{02}_i X^{20}_j \rangle, \tag{27}$$

$$K^{11}_{ij\sigma} = K_{11}(\chi^{cs}_{ij} + 1 - n) - K_{22}\langle X^{02}_i X^{20}_j \rangle, \tag{28}$$

$$K^{21}_{ij\sigma} = 2\sigma K_{12}(\chi^{cs}_{ij} - \frac{1}{2}n - \langle X^{02}_i X^{20}_j \rangle), \tag{29}$$

where χ^{cs}_{ij} stands for the static charge and spin correlation functions

$$\chi^{cs}_{ij} = \frac{1}{4}\langle N_i N_j \rangle + \langle \mathbf{S}_i \mathbf{S}_j \rangle. \tag{30}$$

In Eq. (24), the site independent correlation functions are given by

$$\begin{aligned} b^{22}_{\sigma} &= \sum_{m \neq i} V_{im} \{ K_{22} (\langle X^{\bar{\sigma}2}_i X^{\sigma 2}_m \rangle - \langle X^{\sigma 2}_i X^{\bar{\sigma}2}_m \rangle) \\ &- 2\sigma K_{12} (\langle X^{\sigma 2}_i X^{0\sigma}_m \rangle + \langle X^{\bar{\sigma}2}_i X^{0\bar{\sigma}}_m \rangle) \}, \end{aligned} \tag{31}$$

$$b_\sigma^{11} = -\sum_{m\neq i} V_{im}\{K_{11}(\langle X_i^{0\sigma}X_m^{0\bar{\sigma}}\rangle - \langle X_i^{0\bar{\sigma}}X_m^{0\sigma}\rangle)$$
$$- 2\sigma K_{12}(\langle X_i^{0\sigma}X_m^{\sigma 2}\rangle + \langle X_i^{0\bar{\sigma}}X_m^{\bar{\sigma}2}\rangle)\}, \quad (32)$$
$$b_\sigma^{21} = \sum_{m\neq i} V_{im}\{K_{22}(\langle X_i^{0\sigma}X_m^{\sigma 2}\rangle + \langle X_i^{0\bar{\sigma}}X_m^{\bar{\sigma}2}\rangle)$$
$$- 2\sigma K_{12}(\langle X_i^{0\sigma}X_m^{0\bar{\sigma}}\rangle - \langle X_i^{0\bar{\sigma}}X_m^{0\sigma}\rangle)\}. \quad (33)$$

The site-dependent anomalous correlation functions are convenient to write as follows

$$L_{ij\sigma}^{22} = -2\sigma K_{21}\langle X_i^{02}N_j\rangle, \quad (34)$$
$$L_{ij\sigma}^{11} = -2\sigma K_{21}\langle (2-N_j)X_i^{02}\rangle, \quad (35)$$
$$L_{ij\sigma}^{21} = \frac{1}{2}(K_{22}\langle X_i^{02}N_j\rangle - K_{11}\langle (2-N_j)X_i^{02}\rangle). \quad (36)$$

According to Eq. (8), the anomalous correlation functions describe the pairing at one lattice site but in different subbands: $\langle X_i^{02}N_j\rangle = \langle X_i^{0\downarrow}X_i^{\downarrow 2}N_j\rangle = \langle c_{i\downarrow}c_{i\uparrow}N_j\rangle$.

3.2 Anomalous Correlation Functions

Let us consider anomalous part $\hat{\Delta}_{ij\sigma}$, Eq. (24), of the frequency matrix. Concerning the site independent anomalous correlation functions in Eqs. (31)-(33), we can show that under the assumption of $d_{x^2-y^2}$ pairing they vanish identically. Indeed, each of the sums occurring in these equations vanishes identically due to the fact that the summands in the **q**-representation are odd functions. Consider for instance the first sum in Eq. (31),

$$\sum_{m\neq i} V_{im}\langle X_i^{\bar{\sigma}2}X_m^{\sigma 2}\rangle = \sum_{\mathbf{q}} V(\mathbf{q})\langle X_{\mathbf{q}}^{\bar{\sigma}2}X_{-\mathbf{q}}^{\sigma 2}\rangle.$$

In the right hand side, the sum over **q** remains invariant under those changes of the summation vector **q** which leave the Brillouin zone invariant, in particular under the permutation of the components q_x and q_y of **q** (in the tetragonal phase). Such a transform, however, leaves the interaction $V(\mathbf{q})$ invariant while resulting in the change of sign of the anomalous correlation function $\langle X_{\mathbf{q}}^{\bar{\sigma}2}X_{-\mathbf{q}}^{\sigma 2}\rangle$ having the $d_{x^2-y^2}$-wave symmetry. Thus, the sum over **q** equals zero, hence the correlation function at the left-hand side vanishes.

To calculate the site dependent contributions to the matrix, Eqs. (34)–(36), we should derive equation for the anomalous correlation function $\langle X_i^{02}N_j\rangle$. In Refs. [19, 21], to calculate it the Roth procedure was applied based on a decoupling of the Hubbard operators on the same lattice site by writing

the time-dependent correlation function in the form: $\langle c_{i\downarrow}(t)|c_{i\uparrow}(t')N_j(t')\rangle = \langle X_i^{0\downarrow}(t)|X_i^{\downarrow 2}(t')N_j(t')\rangle$. Since for the Hubbard operators we have the identity: $X_i^{\alpha\beta} = X_i^{\alpha\gamma}X_i^{\gamma\beta}$ for any intermediate state $|\gamma\rangle$, the decoupling of the operators on the same lattice site is not unique (as has been really observed in Refs. [19, 21]) and unreliable resulting in underestimation of single site strong correlations. However, a direct calculation of the correlation function $\langle X_i^{02}N_j\rangle$ can be performed if one consider the equation of motion of the corresponding commutator GF

$$L_{ij}(t-t') = \langle\langle X_i^{02}(t) \mid N_j(t')\rangle\rangle.$$

After differentiation with respect to the time variable t and use of the Fourier transform (6), we get the equation:

$$\begin{aligned}(\omega - E_2)\, L_{ij}(\omega) \;&\simeq\; 2\delta_{ij}\langle X_i^{02}\rangle + \sum_{m\neq i,\sigma} 2\sigma t_{im}^{12}\,[\,\langle\langle X_i^{0\bar\sigma}X_m^{0\sigma}|N_j\rangle\rangle_\omega \\ &-\; \langle\langle X_i^{\sigma 2}X_m^{\bar\sigma 2}|N_j\rangle\rangle_\omega\,]\,. \end{aligned} \tag{37}$$

Here we have neglected contributions from the intraband hopping integrals in the Hubbard Hamiltonian (2), while have retained the interband hopping which mediates the exchange interaction. This approximation can be proved if one takes into account that the pair excitation energy $|E_2| \simeq \Delta \gg |t_{ij}^{\alpha\beta}|$. Therefore, the intraband hopping integrals give only a small renormalization of the large excitation energy $|E_2|$, while the exchange interaction between subbands results in nonzero superconducting pairing in one subband. Eq. (37) with the condition (9) provides the expression of the GF of interest, $L_{ij}(\omega)$. The statistical average $\langle X_i^{02}N_j\rangle$ at sites $i \neq j$ can now be evaluated from the spectral representation theorem:

$$\begin{aligned}\langle X_i^{02}N_j\rangle = \int_{-\infty}^{+\infty} \frac{d\omega}{1-\exp(-\omega/T)} \sum_{m\neq i,\sigma} 2\sigma t_{im}^{12}\Big\{-\frac{1}{\pi}\mathrm{Im}\Big[\frac{1}{\omega - E_2 + i\varepsilon} \\ \times\Big(\langle\langle X_i^{0\bar\sigma}X_m^{0\sigma}|N_j\rangle\rangle_{\omega+i\varepsilon} - \langle\langle X_i^{\sigma 2}X_m^{\bar\sigma 2}|N_j\rangle\rangle_{\omega+i\varepsilon}\Big)\Big]\Big\}. \end{aligned} \tag{38}$$

We consider below the case of hole doping. Then the Fermi level (which defines the zero of the energy) stays in the singlet subband, hence in the Hamiltonian (2) the chemical potential $\mu \simeq \Delta$ and the energy parameters, $E_2 \simeq E_1 \simeq -\Delta$. The contribution to the above integral coming from $\delta(\omega - E_2)$ can be neglected since it is proportional to $\exp(-\Delta/T) \ll 1$. The one-hole subband Green function entering the Cauchy principal value integral can be estimated from its equation of motion to contribute a term

$$-\frac{1}{\pi}\mathrm{Im}\langle\langle X_i^{0\bar\sigma}X_m^{0\sigma}|N_j\rangle\rangle_{\omega+i\varepsilon} \simeq \delta_{mj}\langle X_i^{0\bar\sigma}X_j^{0\sigma}\rangle\delta(\omega - 2E_1),$$

therefore it is proportional to $\exp(-2\Delta/T) \ll 1$ and can be neglected as well. The only non-vanishing contribution to the Cauchy principal value integral in Eq. (38) comes from the Green function of the singlet subband:

$$\langle X_i^{02} N_j \rangle = -\frac{1}{\Delta} \sum_{m \neq i,\sigma} 2\sigma t_{im}^{12} \langle X_i^{\sigma 2} X_m^{\bar{\sigma} 2} N_j \rangle. \tag{39}$$

The exchange interaction is usually considered in the two-site approximation, which is obtained equating $m = j$ in Eq. (39). In this approximation, we get after summation over the spin σ:

$$\langle X_i^{02} N_j \rangle = -\frac{4t_{ij}^{12}}{\Delta} 2\sigma \langle X_i^{\sigma 2} X_j^{\bar{\sigma} 2} \rangle = \langle c_{i\downarrow} c_{i\uparrow} N_j \rangle \tag{40}$$

where we have used the identity for the Hubbard operators, $X_j^{\bar{\sigma}2} N_j = 2X_j^{\bar{\sigma}2}$ and the symmetry property of the anomalous averages: $\langle X_i^{\sigma 2} X_j^{\bar{\sigma} 2} \rangle = -\langle X_i^{\bar{\sigma} 2} X_j^{\sigma 2} \rangle$.

We have therefore proved that in the MFA the intersite anomalous correlation function is of the order of t_{ij}^{12}/Δ and it is proportional to the statistical average of the conventional electron (hole) pairs at neighboring lattice sites, $\langle X_i^{\sigma 2} X_j^{\bar{\sigma} 2} \rangle$. This finally allows us to write the expressions of the anomalous component Eq. (34) for the case of hole doping as following

$$\Delta_{ij\sigma}^{22} = \frac{1}{N} \sum_{\mathbf{q}} e^{i\mathbf{q}\cdot(\mathbf{i}-\mathbf{j})} \Delta_\sigma^{22}(\mathbf{q}) = J_{ij} \langle X_i^{\sigma 2} X_j^{\bar{\sigma} 2} \rangle. \tag{41}$$

This result recovers the exchange interaction contribution to the pairing, with an exchange energy parameter $J_{ij} = 4\,(t_{ij}^{12})^2/\Delta$. The anomalous component Eq. (35) for the case of hole doping can be neglected since its contribution to the gap equation (see Eq. (55))is extremely small, of the order of $\Delta_\sigma^{11}(\mathbf{q})/\Delta$.

In the case of electron doping, on the contrary, we can neglect the anomalous correlation function for the singlet subband, $\Delta_{ij\sigma}^{22}$, while an analogous calculation for the anomalous correlation function of the one-hole subband gives

$$\Delta_{ij\sigma}^{11} = J_{ij} \langle X_i^{0\bar{\sigma}} X_j^{0\sigma} \rangle. \tag{42}$$

We may therefore conclude that the anomalous contributions to the zero-order GF, Eq. (13), originate in conventional anomalous pairs of quasi-particles and their pairing in MFA is mediated by the exchange interaction which has been studied in the t-J model (see, e.g., [15, 18]). In view of this conclusion, the MFA nonzero superconducting pairing reported [19]-[21] in the frame of the conventional Hubbard model (1) can be inferred to stem from the exchange interaction, which equals $J_{ij} = 4t^2/U$ in this model. The exchange interaction vanishes in the limit $U \to \infty$, a feature which explains the disappearance of the pairing at large U [19]-[21].

3.3 Spectrum in the mean-field approximation

Let us study at first the zero-order GF (13) in the normal state in MFA when it can be written in the form

$$\tilde{G}^0_\sigma(\mathbf{q},\omega) = \begin{pmatrix} \hat{G}^0_\sigma(\mathbf{q},\omega) & 0 \\ 0 & -\hat{G}^0_\sigma(-\mathbf{q},-\omega)^{(\mathrm{T})} \end{pmatrix}, \tag{43}$$

where the 2×2 matrix GF reads [22]:

$$\hat{G}^0_\sigma(\mathbf{q}\omega) = \{\omega\hat{\tau}_0 - \hat{E}_\sigma(\mathbf{q})\}^{-1} \begin{pmatrix} \chi_2 & 0 \\ 0 & \chi_1 \end{pmatrix}, \tag{44}$$

The $\mathbf{q}$-representation of the energy matrix is given by

$$\hat{E}_\sigma(\mathbf{q}) = \begin{pmatrix} \omega_2(\mathbf{q}) & W^{21}_\sigma(\mathbf{q}) \\ W^{12}_\sigma(\mathbf{q}) & \omega_1(\mathbf{q}) \end{pmatrix}. \tag{45}$$

The energy spectra of the unhybridized singlets and holes are defined by the equations

$$\begin{aligned} \omega_2(\mathbf{q}) &= E_1 + \Delta + a^{22}_\sigma/\chi_2 + V^{22}_\sigma(\mathbf{q})/\chi_2\,, \\ \omega_1(\mathbf{q}) &= E_1 + a^{22}_\sigma/\chi_1 + V^{11}_\sigma(\mathbf{q})/\chi_1\,, \end{aligned} \tag{46}$$

while the hybridization interaction is given by $\chi_2 W^{21}_\sigma = a^{21}_\sigma + V^{21}_\sigma(\mathbf{q}) = \chi_1 W^{12}_\sigma$. The effective interaction in these equations has the form

$$V^{\alpha\beta}_\sigma(\mathbf{q}) = \frac{t}{N}\sum_{k} \nu(\mathbf{k}) K^{\alpha\beta}_\sigma(\mathbf{k}\text{-}\mathbf{q})\,, \tag{47}$$

where $K^{\alpha\beta}_\sigma(\mathbf{q})$ denotes the Fourier transform of $K^{\alpha\beta}_{ij\sigma}$, Eqs. (27)-(29), while $\nu(\mathbf{q})$ is the geometrical structure factor with overlapping parameters of the Wannier oxygen states coming from the nearest and the next nearest neighbors

$$\nu(\mathbf{q}) = 2\sum_{j\neq 0} \nu_{0j} \mathrm{e}^{-i\mathbf{q}\cdot\mathbf{j}} \approx 8\nu_1\gamma(\mathbf{q}) + 8\nu_2\gamma'(\mathbf{q}), \tag{48}$$

where $\gamma(\mathbf{q}) = (1/2)(\cos q_x + \cos q_y)$, $\gamma'(\mathbf{q}) = \cos q_x \cos q_y$.

From Eqs. (44) and (45) we find that the off-diagonal matrix elements of the zero-order GF can be neglected since they are of the order $|t^{12}|/\Delta$ and appear to give a small contribution to the density of states [22]. We are thus left with the diagonal form of the zero-order GF,

$$\hat{G}^0_\sigma(\mathbf{q},\omega) = \begin{pmatrix} \chi_2/[\omega - \Omega_2(\mathbf{q})] & 0 \\ 0 & \chi_1/[\omega - \Omega_1(\mathbf{q})] \end{pmatrix}, \tag{49}$$

where the hybridized spectra $\Omega_\alpha(\mathbf{q})$ for singlets ($\alpha = 2$) and for holes ($\alpha = 1$) are given respectively by

$$\Omega_{2,1}(\mathbf{q}) = \frac{1}{2}[\omega_2(\mathbf{q}) + \omega_1(\mathbf{q})] \pm \frac{1}{2}\{[\omega_2(\mathbf{q}) - \omega_1(\mathbf{q})]^2 + 4W_\sigma^{21}W_\sigma^{12}\}^{1/2}. \quad (50)$$

To get a closed solution for the zero-order GF, the correlation functions entering (23) are calculated self-consistently. The energy shifts $a_\sigma^{\alpha\beta}$ (25) and (26) are readily calculated by using the spectral representation of the GF (49). However, the calculation of the two-particle correlation functions $K_{ij\sigma}^{\alpha\beta}$ in (27)–(29) requires the use of some approximations. In Refs. [19, 21], the Roth's procedure was used that resulted in the decoupling of the Hubbard operators at the same lattice site, e.g., $\langle X_i^{02}X_j^{20}\rangle = \langle X_i^{0\sigma}X_i^{\sigma 2}X_j^{20}\rangle$. As discussed in Sec. 3.2, it is possible to calculate this correlation function by using the equation of motion of the many-particle GF. Due to the large pair excitation energy $|E_2| \simeq \Delta$ the contribution of this correlation function appears to be small, of the order $(t_{ij}^{12}/\Delta)^2$, and can be neglected. Finally, to evaluate the correlation functions in Eq. (30), we neglect the charge correlations and decouple the product N_iN_j of the number operators N_i at different lattice sites $i \neq j$ to get

$$\chi_{ij}^{cs} \simeq (\chi_2)^2 + \langle \mathbf{S}_i\mathbf{S}_j\rangle. \quad (51)$$

For spin-singlet states without long-range magnetic order, the GF (49) and the one-hole spectrum (50) do not depend on spin. However, the short-range AFM spin-spin correlations are very important and, as calculations in Ref. [22] have shown, the spin-spin correlation functions $\langle \mathbf{S}_i\mathbf{S}_j\rangle$ in (51) bring significant contribution to the renormalization of the dispersion relation (50). Under large spin-spin correlations, one finds a next-nearest neighbor dispersion at small doping values. Under decreasing intensity of the spin-spin correlations, the dispersion changes to an ordinary nearest neighbor one with doping.

To summarize the study of MFA let us we consider a particular case of hole doping with the chemical potential in the singlet subband. In that case we can restrict our studies to the 2×2 matrix GF for the singlet subband:

$$\hat{G}_{ij,\sigma}^{22}(\omega) = \langle\langle \begin{pmatrix} X_i^{\sigma 2} \\ X_i^{2\bar{\sigma}} \end{pmatrix} \mid (X_j^{2\sigma}\ X_j^{\bar{\sigma}2})\rangle\rangle_\omega . \quad (52)$$

By taking into account the normal part of the GF in the diagonal form, Eq. (49), and the anomalous part of the frequency matrix for the singlet subband, Eq. (41), we can write the GF (52) in the form:

$$\hat{G}_\sigma^{22}(\mathbf{q},\omega) = \chi_2\{\omega\hat{\tau}_0 - \Omega_{2,\sigma}(\mathbf{q})\hat{\tau}_3 - \phi_\sigma^{22}(\mathbf{q})\hat{\tau}_1\}^{-1}, \quad (53)$$

where $\hat{\tau}_0$, $\hat{\tau}_1$, $\hat{\tau}_3$ are the Pauli matrices. Here we introduce the gap function in MFA for the singlet subband $\phi_\sigma^{22}(\mathbf{q}) = \Delta_\sigma^{22}(\mathbf{q})/\chi_2$ induced by the exchange interaction. From Eq. (41) we get

$$\phi_\sigma^{22}(\mathbf{q}) = \frac{1}{N\chi_2} \sum_{\mathbf{k}} J(\mathbf{k}-\mathbf{q}) \langle X_{-\mathbf{q}}^{2\bar{\sigma}} X_{\mathbf{q}}^{2\sigma} \rangle, \tag{54}$$

where we introduced the Fourier component for the nearest neighbor exchange interaction, $J(\mathbf{q}) = 4J\gamma(\mathbf{q})$. To compare our results derived for the Hubbard model with that ones for the t-J model we disregarded here off-diagonal anomalous parts of the frequency matrix, Eq. (36), which effectively gives only renormalization to the exchange interaction. Apparently, in the one subband t-J model off-diagonal anomalous correlation functions could not appear.

The anomalous correlation function for the singlet subband now can be calculated self-consistently from the anomalous part of the GF (53) that results in the following BCS-type equation for gap function (54) in the MFA:

$$\phi_\sigma^{22}(\mathbf{q}) = \frac{1}{N} \sum_{\mathbf{k}} J(\mathbf{k}-\mathbf{q}) \frac{\phi_\sigma^{22}(\mathbf{k})}{2E_2(\mathbf{k})} \tanh \frac{E_2(\mathbf{k})}{2T}, \tag{55}$$

with the quasiparticle energy $\mathcal{E}_2(\mathbf{k}) = [\Omega_{2,\sigma}(\mathbf{k})^2 + \phi_\sigma^{22}(\mathbf{k})^2]^{1/2}$. This equation is identical to the MFA results for the t-J model (see, e.g., [15, 18]).

Analogous equations can be obtained for the electron doped case, $n < 1$, with the chemical potential in the one-hole band by considering GF for the Hubbard operators $X_i^{0\sigma}$, $X_i^{\bar{\sigma}0}$.

4 Self-energy corrections

4.1 Self-consistent Born approximation

The starting point for the calculation of self-energy corrections is the $(\mathbf{r}, t)$-representation of the self-energy (16):

$$\tilde{\Sigma}_{ij\sigma}(t-t') = \tilde{\chi}^{-1} \langle\langle \hat{Z}_{i\sigma}^{(ir)}(t) \,|\, \hat{Z}_{j\sigma}^{(ir)\dagger}(t') \rangle\rangle^{(prop)} \tilde{\chi}^{-1}. \tag{56}$$

The operators $Z^{(ir)}$ are obtained from Eqs. (17)–(18) by substituting the Bose-like operators $B_{i\sigma\sigma'}^{\alpha\beta}$ by their fluctuating parts: $\delta B_{i\sigma\sigma'}^{\alpha\beta} = B_{i\sigma\sigma'}^{\alpha\beta} - \langle B_{i\sigma\sigma'}^{\alpha\beta} \rangle$ which describe charge and spin fluctuations around the averages following from Eqs. (19)–(21). The terms which contain X_i^{02} operators, whose contribution to the low energy dynamics of the system is assumed to be small (since it involves large charge fluctuations at one site) can be disregarded.

The self-energy (56) is calculated below in the self-consistent Born approximation (SCBA) (or the non-crossing approximation). In SCBA, the propagation of the Fermi-like and Bose-like excitations in the many-particle GF in (56) are assumed to be independent of each other and therefore the SCBA results from the decoupling of the corresponding operators in the time-dependent correlation functions as follows:

$$\langle B_{1'}(t)X_1(t)B_{2'}(t')X_2(t')\rangle \simeq \langle X_1(t)X_2(t')\rangle\langle B_{1'}(t)B_{2'}(t')\rangle. \tag{57}$$

Using the spectral theorem, the SCBA results in the following decoupling relation for the emerging GF in the $(\mathbf{r},\omega)$-representation:

$$\langle\langle B_{1'}X_1 \,|\, B_{2'}X_2\rangle\rangle_\omega \simeq \frac{1}{\pi^2}\int\limits_{-\infty}^{+\infty}\int\limits_{-\infty}^{+\infty}\frac{\mathrm{d}\omega_1\mathrm{d}\omega_2}{\omega-\omega_1-\omega_2}$$

$$\times\frac{1}{2}\left(\tanh\frac{\omega_1}{2T}+\coth\frac{\omega_2}{2T}\right)\mathrm{Im}\langle\langle X_1 \,|\, X_2\rangle\rangle_{\omega_1}\mathrm{Im}\langle\langle B_{1'} \,|\, B_{2'}\rangle\rangle_{\omega_2}. \tag{58}$$

Within this approximation, the GF associated to the irreducible operators in Eq. (56) can be evaluated and we get the self-energy in the $(\mathbf{r},\omega)$-representation,

$$\tilde{\Sigma}_{ij\sigma}(\omega) = \tilde{\chi}^{-1}\begin{pmatrix}\hat{M}_{ij\sigma}(\omega) & \hat{\Phi}_{ij\sigma}(\omega)\\ \hat{\Phi}^{\dagger(\mathrm{T})}_{ij\sigma}(\omega) & -\hat{M}^{(\mathrm{T})}_{ij\bar{\sigma}}(-\omega)\end{pmatrix}\tilde{\chi}^{-1}, \tag{59}$$

where the 2×2 matrices $\hat{M}$ and $\hat{\Phi}$ denote the normal and anomalous contributions to the self-energy respectively:

$$\hat{M}_{ij\sigma}(\omega) = \begin{pmatrix}M^{22}_{ij\sigma} & M^{21}_{ij\sigma}\\ M^{12}_{ij\sigma} & M^{11}_{ij\sigma}\end{pmatrix} = \left\langle\!\!\left\langle\begin{pmatrix}(Z^{\sigma 2}_i)^{(ir)}\\ (Z^{0\bar{\sigma}}_i)^{(ir)}\end{pmatrix}\middle|\left(\left(Z^{2\sigma}_j\right)^{(ir)}\left(Z^{\bar{\sigma}0}_j\right)^{(ir)}\right)\right\rangle\!\!\right\rangle_\omega,$$

$$\hat{\Phi}_{ij\sigma}(\omega) = \begin{pmatrix}\Phi^{22}_{ij\sigma} & \Phi^{21}_{ij\sigma}\\ \Phi^{12}_{ij\sigma} & \Phi^{11}_{ij\sigma}\end{pmatrix} = \left\langle\!\!\left\langle\begin{pmatrix}(Z^{\sigma 2}_i)^{(ir)}\\ (Z^{0\bar{\sigma}}_i)^{(ir)}\end{pmatrix}\middle|\left(\left(Z^{\bar{\sigma}2}_j\right)^{(ir)}\left(Z^{0\sigma}_j\right)^{(ir)}\right)\right\rangle\!\!\right\rangle_\omega.$$

The GF (5) can thus be written as a 2×2 super-matrix of normal, $\hat{G}_{ij\sigma}(\omega)$, and anomalous, $\hat{F}_{ij\sigma}(\omega)$, 2×2 matrix components:

$$\tilde{G}_{ij\sigma}(\omega) = \begin{pmatrix}\hat{G}_{ij\sigma}(\omega) & \hat{F}_{ij\sigma}(\omega)\\ \hat{F}^{\dagger}_{ij\sigma}(\omega) & -\hat{G}^{(\mathrm{T})}_{ij\bar{\sigma}}(-\omega)\end{pmatrix}. \tag{60}$$

Eqs. (59) and (60) provide a closed self-consistent system of equations for the self-energy and GF within the SCBA (58).

To get a tractable problem, this system is simplified using diagonal approximations for the GF solution, while the matrix elements of $\hat{M}_{ij\sigma}(\omega)$ and $\hat{\Phi}_{ij\sigma}(\omega)$ are calculated keeping the leading terms only in V_{ij}. Use of Fourier transforms similar to (6) results in the $(\mathbf{q},\omega)$-representation of the contributions to the normal and anomalous parts of the self-energy [25]:

$$\hat{M}_\sigma(\mathbf{q},\omega) = \frac{1}{N}\sum_{\mathbf{k}}\int_{-\infty}^{+\infty} d\omega_1 K^{(+)}(\omega,\omega_1|\mathbf{k},\mathbf{q}-\mathbf{k}) \times \{-\frac{1}{\pi}\mathrm{Im}[\hat{P}_2^{(+)}G_\sigma^{22}(\mathbf{k},\omega_1) + \hat{P}_1^{(+)}G_\sigma^{11}(\mathbf{k},\omega_1)]\}\,, \tag{61}$$

$$\hat{\Phi}_\sigma(\mathbf{q},\omega) = \frac{1}{N}\sum_{\mathbf{k}}\int_{-\infty}^{+\infty} d\omega_1 K^{(-)}(\omega,\omega_1|\mathbf{k},\mathbf{q}-\mathbf{k}) \times \{-\frac{1}{\pi}\mathrm{Im}[\hat{P}_2^{(-)}F_\sigma^{22}(\mathbf{k},\omega_1) - \hat{P}_1^{(-)}F_\sigma^{11}(\mathbf{k},\omega_1)]\}\,, \tag{62}$$

where

$$\hat{P}_2^{(\pm)} = \begin{pmatrix} K_{22}^2 & \pm 2\sigma K_{21}K_{22} \\ 2\sigma K_{21}K_{22} & \pm K_{21}^2 \end{pmatrix}, \quad \hat{P}_1^{(\pm)} = \begin{pmatrix} K_{21}^2 & \pm 2\sigma K_{21}K_{11} \\ 2\sigma K_{21}K_{11} & \pm K_{11}^2 \end{pmatrix}.$$

The kernel of the integral equations for the self-energy operators is defined in the standard way:

$$K^{(\pm)}(\omega,\omega_1|\mathbf{k},\mathbf{q}-\mathbf{k}) = t^2\,|\nu(\mathbf{k})|^2 \int_{-\infty}^{+\infty} \frac{d\omega_2}{\omega-\omega_1-\omega_2} \times \frac{1}{2}\left(\tanh\frac{\omega_1}{2T} + \coth\frac{\omega_2}{2T}\right)[-\frac{1}{\pi}\mathrm{Im}D^{(\pm)}(\mathbf{q}-\mathbf{k},\omega_2)]\,, \tag{63}$$

with a spectral density of spin-charge fluctuations given by the commutator GF

$$D^{(\pm)}(\mathbf{q},\omega) = \langle\langle \mathbf{S_q}|\mathbf{S_{-q}}\rangle\rangle_\omega \pm \frac{1}{4}\langle\langle \delta N_\mathbf{q}|\delta N_\mathbf{-q}\rangle\rangle_\omega = \chi^s(\mathbf{q},\omega) \pm \chi^c(\mathbf{q},\omega)\,, \tag{64}$$

and $\nu(\mathbf{k})$ is given by Eq. (48). The QP energies $\bar{\Omega}_\alpha(\mathbf{q})$ of the normal state for the diagonal GF in Eqs. (61) and (62) are evaluated from

$$\bar{\Omega}_{\alpha,\sigma}(\mathbf{q}) = \Omega_\alpha(\mathbf{q}) - \chi_\alpha^{-1}M_\sigma^{\alpha\alpha}(\mathbf{q},\omega=\Omega_\alpha(\mathbf{q})), \tag{65}$$

where the MFA energy $\Omega_\alpha(\mathbf{q})$ is defined by Eq. (50).

4.2 Weak coupling approximation

Once the self-energy corrections (61) and (62) have been calculated in SCBA and the exchange corrections to the GF, Eqs. (53) and (54), have been estimated, we can replace the result in the Dyson equation (14) to get the one-particle matrix GF. An important simplification of the Dyson equation (14) occurs if we observe that the off-diagonal normal and anomalous matrix elements of the GF, Eq. (60), are small as compared to the diagonal ones. Neglecting the small matrix elements, the inversion of the GF matrix in (14) results in simple enough analytical formulas.

In spite of these simplification, the numerical complexity of the resulting integral equations which define the critical temperature predicted by the two-band singlet-hole model is enormous. Before embarking to the full solution of such a problem, we study a simplified, yet meaningful, limit case offered by the weak coupling approximation (WCA), which assumes that the behavior of the physical system is dominated by the interactions around the Fermi level.

Within WCA, the interaction kernel (63) at frequencies (ω, ω_1) close to the Fermi surface is factorized in the form

$$K^{(\pm)}(\omega, \omega_1 | \mathbf{k}, \mathbf{q}-\mathbf{k}) \simeq -\frac{1}{2} \tanh\left(\frac{\omega_1}{2T}\right) \lambda^{(\pm)}(\mathbf{k}, \mathbf{q}-\mathbf{k}) \,, \tag{66}$$

for $|\omega, \omega_1| \leq \omega_s \ll W$ where ω_s is a characteristic pairing energy and W is the band width. In this approximation, the effective interaction is defined by the static susceptibility

$$\begin{aligned} \lambda^{(\pm)}(\mathbf{k}, \mathbf{q}-\mathbf{k}) &= t^2 \, |\nu(\mathbf{k})|^2 \int_{-\infty}^{+\infty} \frac{\mathrm{d}\omega_2}{\omega_2} [-\frac{1}{\pi} \mathrm{Im} D^{(\pm)}(\mathbf{q}-\mathbf{k}, \omega_2)] \\ &= -t^2 \, |\nu(\mathbf{k})|^2 \mathrm{Re} D^{(\pm)}(\mathbf{q}-\mathbf{k}, \omega_2 = 0)] \,. \end{aligned} \tag{67}$$

The WCA is suitable for the band which crosses the FS. For the another band, which is far away from the FS at an energy of the order of the band gap, $\omega_1 \simeq \Delta$, an integration over ω_1 in Eqs.(61) and (62) is straightforward.

For a slightly doped hole system, $n = 1 + \delta \geq 1$, the chemical potential is in the singlet band, $\mu \simeq \Delta$, and we can write the dispersion relations for the two bands in the normal state, Eq. (65), as follows

$$\bar{\Omega}_2(\mathbf{q}) \simeq \Delta - \mu + \epsilon_2(\mathbf{q}) \simeq \epsilon_2(\mathbf{q}) \,, \bar{\Omega}_1(\mathbf{q}) \simeq -\mu + \epsilon_1(\mathbf{q}) \simeq -\Delta + \epsilon_1(\mathbf{q}) \,, \tag{68}$$

with the zero of the energy fixed at the Fermi wave-vector $\epsilon_2(\mathbf{q}_F) = 0$. Integration over ω_1 in (62) gives the following system of equations for the diagonal components of the self-energy, $\Phi^{\alpha\alpha}(\mathbf{q}) = 2\sigma \Phi^{\alpha\alpha}_{\sigma}(\mathbf{q}, \omega = 0)$,

$$\begin{aligned} \Phi^{22}(\mathbf{q}) &= -K^2_{22} \mathcal{S}_2(\mathbf{q}) + K^2_{12} \mathcal{S}_1(\mathbf{q}) \,, \\ \Phi^{11}(\mathbf{q}) &= K^2_{12} \mathcal{S}_2(\mathbf{q}) - K^2_{11} \mathcal{S}_1(\mathbf{q}) \,. \end{aligned} \tag{69}$$

The sum $\mathcal{S}_2(\mathbf{q})$ for the singlet band at the FS is given by

$$\mathcal{S}_2(\mathbf{q}) = \frac{1}{N}\sum_{\mathbf{k}} \lambda^{(-)}(\mathbf{k}, \mathbf{q}-\mathbf{k}) \frac{\Phi^{22}(\mathbf{k})}{2\bar{\mathcal{E}}_2(\mathbf{k})} \tanh \frac{\bar{\mathcal{E}}_2(\mathbf{k})}{2T} , \tag{70}$$

with the integration over $\mathbf{k}$ restricted to an energy shell around the Fermi energy of the order of a characteristic energy ω_s of the spin (charge) fluctuations. The quasiparticle energy is given by

$$\bar{\mathcal{E}}_2(\mathbf{q}) = [\bar{\Omega}_2^2(\mathbf{q}) + \mid \chi_2^{-1}\Phi^{22}(\mathbf{q}) \mid^2]^{1/2} , \tag{71}$$

where $\bar{\Omega}_2(\mathbf{q})$ is the quasi-particle dispersion in the normal state, Eq. (65).

The one-hole band lies below the FS at an energy of the order $\Delta \gg W$. The integration over ω_1 in Eq. (62) can therefore be done by neglecting the dispersion in this band in Eq. (68) as well as the superconducting gap in the anomalous GF in Eq. (62). This results in the estimate

$$\mathcal{S}_1(\mathbf{q}) = \frac{1}{N}\sum_{\mathbf{k}} t^2 |\nu(\mathbf{k})|^2 \frac{\Phi^{11}(\mathbf{k})}{\Delta^2} \chi_{sc}^{(-)}(\mathbf{k}-\mathbf{q}). \tag{72}$$

In this equation, the spin-charge correlation function

$$\chi_{sc}^{(-)}(\mathbf{q}) = \langle \mathbf{S}_{\mathbf{q}} \mathbf{S}_{-\mathbf{q}} \rangle - \frac{1}{4}\langle N_{\mathbf{q}} N_{-\mathbf{q}} \rangle .$$

resulted from the integration over ω_2 in Eq. (63).

A simple estimate shows that the sum $\mathcal{S}_1(\mathbf{q})$ gives a small contribution, of the order $(t_{eff}/\Delta)^2 \Phi^{11}(\mathbf{q}) \simeq 10^{-2}\Phi^{11}(\mathbf{q})$, and it can be neglected in the system of equations (69). By taking into account the contribution due to the exchange interaction in MFA, Eq. (55), the equation for the singlet gap in the WCA can be written as follows:

$$\Phi^{22}(\mathbf{q}) = \frac{1}{N}\sum_{\mathbf{k}} [J(\mathbf{k}-\mathbf{q}) - K_{22}^2 \lambda^{(-)}(\mathbf{k}, \mathbf{q}-\mathbf{k})] \frac{\Phi^{22}(\mathbf{k})}{2\bar{\mathcal{E}}_2(\mathbf{k})} \tanh \frac{\bar{\mathcal{E}}_2(\mathbf{k})}{2T} . \tag{73}$$

Although the one-hole band brings negligible contribution to Eqs. (69), the band coupling may result in a nonzero gap in the one-hole band, $\Phi^{11}(\mathbf{q}) \simeq K_{12}^2 \mathcal{S}_2(\mathbf{q})$, as shown by the second equation (69).

Similar considerations hold true for an electron doped system, $n = 1+\delta \leq 1$ when $\mu \simeq 0$ in (68). In that case, the significant WCA equation involves the gap $\Phi^{11}(\mathbf{q})$ and critical T_c defined by the second equation (69), with proper inclusion of an exchange interaction term similar to that occurring in Eq. (73).

5 Numerical results and discussion

To solve the gap equations, a model for the bosonic GF in the effective interaction (67) is needed. The charge-charge fluctuations are small as compared to the spin-spin fluctuations and they are neglected. To evaluate the spin-spin fluctuations, a model representation of the spin-fluctuation susceptibility is necessary. We used the following expression which has been suggested in numerical studies: [29]

$$\begin{aligned} \chi_s''(\mathbf{q},\omega) &= -\frac{1}{\pi}\mathrm{Im}\langle\langle \mathbf{S}_q \mid \mathbf{S}_{-q}\rangle\rangle_{\omega+i\delta} = \chi_s(\mathbf{q})\chi_s''(\omega) \\ &= \frac{\chi_0}{1+\xi^2[1+\gamma(\mathbf{q})]} \tanh\frac{\omega}{2T}\frac{1}{1+(\omega/\omega_s)^2} \end{aligned} \tag{74}$$

with $\gamma(\mathbf{q}) = (1/2)(\cos q_x + \cos q_y)$. Thus, the effective coupling due to spin fluctuations, Eq. (67), reduces to

$$\lambda_s(\mathbf{k},\mathbf{q}-\mathbf{k}) = t^2|\nu(\mathbf{k})|^2\chi_s(\mathbf{q}-\mathbf{k})F_s(0)\,, \tag{75}$$

where

$$F_s(z) = \int_0^\infty \frac{2\omega \mathrm{d}\omega}{\omega^2+z^2} \tanh\frac{\omega}{2T}\frac{1}{1+(\omega/\omega_s)^2}\,.$$

The parameters of the model susceptibility (74) are fixed under conditions specific to the present model. The $\mathbf{q}$-dependent part has a peak at the AFM wave vector with its intensity defined by the short-range AFM correlation length ξ. The typical values of ξ are in the range from one to three (in lattice constant units) and ξ is taken for a fitting parameter of the model. The constant $\chi_0(\xi)$ defines the intensity of the spin fluctuations at the AFM wave vector $\mathbf{Q} = (\pi,\pi)$ when $1+\gamma(\mathbf{Q}) = 0$. It is found from the normalization condition for $n = 1+\delta \geq 1$:

$$\begin{aligned} \frac{1}{N}\sum_i \langle \mathbf{S_i}\mathbf{S_i}\rangle &= \frac{1}{N}\sum_{\mathbf{q}}\chi_s(\mathbf{q})\int_{-\infty}^{+\infty}\frac{\mathrm{d}z}{\exp(z/T)-1}\chi_s''(z) = \frac{\pi\omega_s}{2N}\sum_{\mathbf{q}}\chi_s(\mathbf{q}) \\ &= \frac{3}{4}(2-n), \end{aligned}$$

which gives $\langle \mathbf{S_q}\mathbf{S_{-q}}\rangle = \pi\omega_s\chi_s(\mathbf{q})/2$ and $\chi_0 = 3(2-n)/(2\pi\omega_s C_1)\,, \quad C_1 = (1/N)\sum_{\mathbf{q}}\{1+\xi^2[1+\gamma(\mathbf{q})]\}^{-1}$. At large ξ, $\chi_0 \propto \xi^2/\ln\xi$. For the frequency-dependent part, we choose the scaling function with an enhanced intensity at frequencies $\omega \leq T$ and a large cut-off energy ω_s of the order of the exchange energy J.

In the neighborhood of T_c, the gap equation (73) can be linearized by neglecting the gap function in (71). We start with the derivation of an analytical

estimation of the superconducting T_c mediated by the spin fluctuation coupling $\lambda_s(\mathbf{k}, \mathbf{q}-\mathbf{k})$ only. For the $d_{x^2-y^2}$-wave pairing symmetry we assume the conventional $\mathbf{q}$-dependence of the gaps:

$$\Phi^{\alpha\alpha}(\mathbf{q}) = \phi_\alpha(\cos q_x - \cos q_y) = \phi_\alpha \eta(\mathbf{q}) \,. \tag{76}$$

Then integrating over $\mathbf{q}$ both sides of the equation (73) multiplied by $\eta(\mathbf{q}) = (\cos q_x - \cos q_y)$ we get the following equation for T_c:

$$\frac{K_{22}^2}{N^2} \sum_{\mathbf{q},\mathbf{k}} \lambda_s(\mathbf{k}, \mathbf{q}-\mathbf{k}) \frac{\eta(\mathbf{q})\eta(\mathbf{k})}{2\bar{\Omega}_{2,\mathbf{k}}} \tanh \frac{\bar{\Omega}_{2,\mathbf{k}}}{2T_c} = -1 \,. \tag{77}$$

Since the sign of the susceptibility term $\chi_s(\mathbf{q}-\mathbf{k})$ in $\lambda_s(\mathbf{k}, \mathbf{q}-\mathbf{k})$ remains constant over the summation domain, the sum over $\mathbf{q}$ in Eq. (77) can be evaluated by the mean value theorem. Taking into consideration the symmetry of the $\mathbf{k}$ vectors around the AFM wave-vector $\mathbf{Q} = (\pi, \pi)$ (the S symmetry point of the BZ), it results that the mean value theorem yields the optimal estimate

$$\frac{1}{N} \sum_{\mathbf{q}} \eta(\mathbf{q}) \chi_s(\mathbf{q}-\mathbf{k}) \simeq \eta(\mathbf{k}+\mathbf{Q}) \frac{1}{N} \sum_{\mathbf{q}} \chi_s(\mathbf{q}) = -\eta(\mathbf{k}) \chi_0 C_1. \tag{78}$$

Replacing it in Eq. (77) and averaging over the direction of the wave-vector $\mathbf{k}$, we get the following equation for T_c mediated by spin fluctuation:

$$\frac{\lambda_{s,22}}{N} \sum_{\mathbf{k}} \frac{1}{2\bar{\Omega}_2(\mathbf{k})} \tanh \frac{\bar{\Omega}_2(\mathbf{k})}{2T_c} = 1 \,, \tag{79}$$

with an effective spin-fluctuation coupling

$$\lambda_{s,22} \simeq \chi_0 C_1 F_s(0) \frac{K_{22}^2 t^2}{N} \sum_{\mathbf{k}} \eta(\mathbf{k})^2 |\nu(\mathbf{k})|^2 \simeq \frac{t_{eff}^2}{\omega_s} \,, \tag{80}$$

where $t_{eff} = K_{22} 2\nu_1 t$ and we assumed $F_s(0) \simeq 1$. The estimates (78) and (80) are reliable for $\xi \gg 1$. In the logarithmic approximation, Eq. (79) yields

$$\frac{\lambda_{s,22}}{N} \sum_{\mathbf{q}} \frac{1}{2\epsilon_2(\mathbf{q})} \tanh \frac{\epsilon_2(\mathbf{q})}{2T_c} \simeq \lambda_{s,22} N(0) \ln(1.13 \frac{\omega_s}{T_c}) \,, \tag{81}$$

where $N(0)$ is the density of states at the Fermi energy for the singlet band. To derive a numerical estimate, we assume the model parameters [22]: $K_{11} \simeq -0.89$, $K_{22} \simeq -0.48$, $K_{12} \simeq 0.83$, for the energy $\Delta = 2t = 3$ eV. A reasonable value for the density of states is inferred to be $N(0) \simeq 1$ (eV $\cdot$ spin)$^{-1}$, which

follows from the numerical calculations discussed below, while for the spin-fluctuation energy we suppose $\omega_s = 0.15$ eV – the characteristic exchange energy in cuprates, $\omega_s \ll W \simeq t$. This set of parameter values leads to the estimate $\lambda_{s,22} \simeq 0.27$ eV, which results in a weak coupling, $V_{s,22} = \lambda_{s,22} N(0) \simeq 0.27$. However, due to a large spin-fluctuation energy ω_s, a high critical temperature for the singlet band is inferred:

$$T_c \simeq \omega_s \exp\{-1/V_{s,22}\} \simeq 0.03\,\omega_s \simeq 50 \text{ K}. \tag{82}$$

The superconducting gap ϕ_1 in the one-hole band induced, according to Eqs. (69), by the gap in the singlet band, is quite large: $\phi_1/\phi_2 \simeq -(K_{12}/K_{22})^2 \simeq -3$. However, its contribution to the superconducting density of state is negligible, of the order of $(\phi_1/\Delta)^2$ at the energy $\omega \simeq -\Delta$.

Similar estimations can be done for the electron doped case, $n = 1+\delta \leq 1$, where $\mu \simeq 0$. In this case, the dominating contribution to T_c comes from the integral $\mathcal{S}_1$. For a symmetric Hubbard model with equal hopping integrals, $K_{11} = K_{22}$, we will have the electron-hole symmetry and a same T_c. In the reduced p-d model (2), the effective coupling constant $V_{s,11} = \lambda_{s,11} N_1(0)$ can be smaller due to lower density of state, whence a lower T_c, as observed in cuprates. The uncertainty associated to the value of $N_1(0)$ prevents other considerations on T_c in this case.

More precise results concerning the relative weights of the contributions to the critical temperature coming from the kinematic and exchange interactions follow from the numerical solution of the gap equation (73) (linearized as $T \to T_c$) under the constraint of no-double-occupancy in the upper and lower Hubbard subbands:

$$\langle X_i^{\sigma 2} X_i^{\bar{\sigma} 2} \rangle = \langle X_i^{0\bar{\sigma}} X_i^{0\sigma} \rangle = 0.$$

These constraints are automatically satisfied by the order parameter with $\mathrm{d}_{x^2-y^2}$ symmetry of a square lattice. The discretization of this Fredholm integral equation results in an eigenvalue problem for the gap parameter $\Phi^{22}(\mathbf{q})$ of the singlet band. The temperature at which the largest eigenvalue equals one, while the corresponding eigenvector shows $\mathrm{d}_{x^2-y^2}$ symmetry, will be taken for the critical temperature T_c. We note that the eigenvalues of the integral equation are discrete (since the kernel is compact) and real (since the kernel can be made symmetric). The numerical results reported below have been derived under the following parameter values. The antiferromagnetic correlation length was equated to the typical value $\xi = 3$, which was kept constant over the whole domain of the investigated hole concentrations. The other parameters resulting in the effective spin fluctuation coupling $\lambda_{s,22}(\mathbf{k}, \mathbf{q}-\mathbf{k})$ are those defined above in this section. For the exchange interaction, we assumed the value $J = 0.4 t_{eff}$, usually considered in the t-J model.

Fig. 1 shows the dependence of the critical temperature T_c (in $t_{eff} \simeq K_{22} 2\nu_1 t \simeq 0.14t \simeq 0.2$ eV units) on the doping parameter δ. The kinematic interaction alone results in a lower T_c (the solid line in Fig. 1) as compared to the exchange interaction (the dashed line). The highest T_c (dotted line) is obtained when both interactions are included in Eq. (73). The maximum values of T_c are quite high in all cases. They vary from $T_c^{max} \simeq 0.12 t_{eff} \simeq 270$ K at optimum doping $\delta_{opt} \simeq 0.13$ in the highest curve to $T_c^{max} \simeq 0.04 t_{eff} \simeq 90$ K at $\delta_{opt} \simeq 0.07$ in the lowest curve. There is a reasonable agreement of the latter value with the crude analytical estimate (82). It is important to note that the WCA results overestimate T_c because of the neglect of the strong inelastic scattering, the effect of which would be a marked T_c damping [18]. At smaller antiferromagnetic correlation lengths, the numerical solution suggested a strong decrease of the contribution of the kinematic interaction to T_c. This feature stems from the decrease of the parameter χ_0 which controls the magnitude of the electron-electron coupling induced by the spin-fluctuations. However, the parabolic behavior of T_c with δ, showing a maximum at some optimum doping, is similar to the experimental data. This behavior of $T_c(\delta)$ originates in the occurrence of a strong dependence of the density of states on the doping, with a marked peak at the optimum value δ_{opt}, as shown in Ref. [22] for the Hubbard model with narrow bands.

Further insight is obtained from the analysis of the various factors which control the temperature dependence of the behavior of the order parameter $\Phi^{22}(\mathbf{k})$ inside BZ and the investigation of the relationship established via these factors with the Fermi surface of the sample. To this aim, we considered several temperature and doping sampling and computed in each case the $\mathbf{q}$-dependence of the gap under the inclusion in the gap equation of the kinematic interaction term alone, of the exchange term alone, and of both contributions to the superconducting pairing. Fig. 2 provides excerpts from the obtained data, under consideration of the kinematic interaction term alone in Eq. (73), at three temperatures, $T = 0$, $T = 0.5T_c$ and $T = 0.9T_c$, at optimum doping ($\delta = 0.07$) and in the "overdoped"case $\delta = 0.2$. For comparison, Fig. 3 provides similar excerpts from the solution of the complete gap equation (73) at the same temperature sampling, at optimum doping ($\delta = 0.13$) and in the "overdoped"case $\delta = 0.2$. The occurrence of a superconducting state with $d_{x^2-y^2}$ symmetry is observed, with a $\mathbf{q}$-dependence pattern of the gap shown by isolines. This dependence is much more complicated than that depicted by the simple analytical model (76). The inspection of the temperature dependence of the Fermi surface at optimum doping reveals the occurrence of different behaviors in Fig. 2 (a)–(c) and Fig. 3 (a)–(c). As $T \to T_c$, the kinematic interaction results in a shift away of the FS from the star of the $(\pi, 0)$ point of the BZ. The

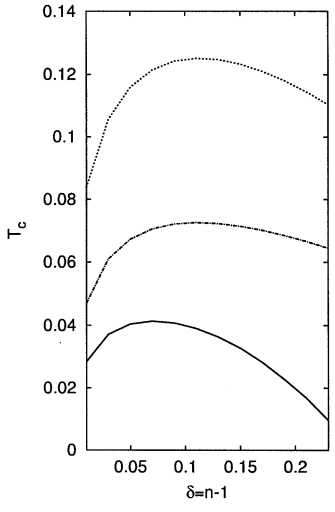

Рис. 1: Dependence of the solution T_c (in t_{eff} units) of the gap equation (73) on the doping parameter δ: (i) under consideration of the kinematic interaction, $\lambda^{(-)}(\mathbf{k}, \mathbf{q}-\mathbf{k})$ (with $\xi = 3$), only (solid line); (ii) under consideration of the exchange interaction, $J = 0.4t_{eff}$, only (dashed line); (iii) under consideration of both contributions (dotted line).

inclusion of the exchange interaction results in an opposite trend of the FS variation. The comparison of the isolines occurring in figures 2 and 3 shows that, while the kinematic interaction term alone results in gap maxima placed inside the BZ (see Fig. 2), the inclusion of the exchange interaction as well (Fig. 3) shifts the maxima towards the $(\pi, 0)$-type points of the BZ, which are close to the FS too ("hot spots"). The shift of the optimum doping value from the smaller value $\delta = 0.07$, in Fig. 2 to the higher value $\delta = 0.13$, in Fig. 3 shows that the inclusion of the exchange term is essential for the achievement of an optimum doping close to those experimentally observed in cuprates. The features of the kinematic interaction come from its specific wave-vector dependence through the factor $|\nu(\mathbf{k})|^2$ in Eq. (75), where from it results that the main contribution due to the nearest neighbor hopping damps quadratically in the neighborhood of the lines $|k_x| + |k_y| = \pi$. Therefore, there is no contribution of the kinematic interaction to the pairing at larger doping where there are significant regions of the FS close to those lines. On the contrary, in Eq. (73), the exchange interaction gives the largest contribution close to the "hot spots", such that the larger FS at higher hole concentrations results in higher T_c.

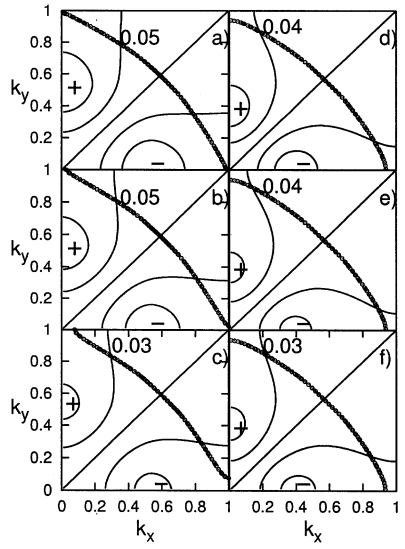

Рис. 2: Contribution of the kinematic interaction to the temperature dependence of the order parameter $\Phi^{22}(\mathbf{k})$ [solution of Eq. (73) at $J = 0$] over the first quadrant of the BZ (k_x, k_y in π/a units): at optimum doping ($\delta = 0.07$) $\{T = 0\,(a);\ 0.5T_c\,(b);\ 0.9T_c\,(c)\}$ and at overdoping ($\delta = 0.2$) $\{T = 0\,(d);\ 0.5T_c\,(e);\ 0.9T_c\,(f)\}$. The circles plot the Fermi surface. The $+/-$ denote gap signs inside octants. The numbers in graphs show the maximum isoline value.

When comparing the contributions of the exchange and spin-fluctuation interactions to Eq. (73), another point which deserves attention is the elucidation of the reason why the former results in a T_c which is twice as large as the T_c resulting from the latter. The interactions are of the same second order in the hopping matrix elements. In our calculations, the exchange interaction parameter $J = 0.4t_{eff} \simeq 0.08$ eV is roughly three times smaller than the parameter of the spin-fluctuation coupling, Eq. (80), $\lambda_{s,22} \simeq 0.27$ eV. There are, however, two opposite features which change the overall effect in favor of the exchange interaction. The first is the particular wave-vector dependence of the two interactions mentioned above, which suppresses the spin-fluctuation coupling at the "hot spots", while securing maximum contribution from the exchange interaction. A second factor is the width of the energy shell of the effective interaction. The exchange interaction, being mediated by the interband hopping, $\propto (t_{ij}^{12})^2$, with large energy transfer and negligible retardation effects, couples the charge carriers in a broad energy shell, of the order of the bandwidth $W = 8t_{eff}$. The spin-fluctuation interaction, $\propto (t_{ij}^{22})^2$, acting in

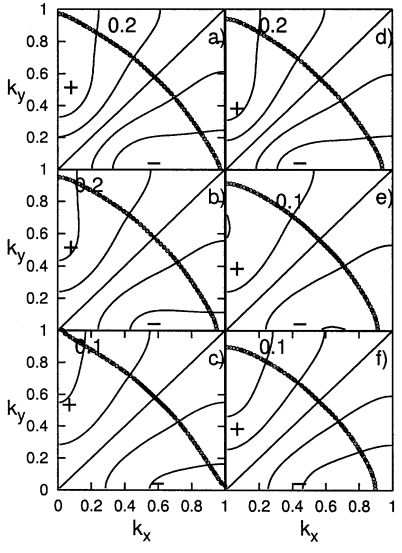

Рис. 3: Combined effect of the kinematic and exchange interactions to the temperature dependence of the order parameter $\Phi^{22}(\mathbf{k})$ [solution of Eq. (73)] over the first quadrant of the BZ: at optimum doping ($\delta = 0.13$) $\{T = 0\,(a);\ 0.5T_c\,(b);\ 0.9T_c\,(c)\}$ and at overdoping ($\delta = 0.2$) $\{T = 0\,(d);\ 0.5T_c\,(e);\ 0.9T_c\,(f)\}$. Other notations are detailed in Fig. 2. The step in-between the equally spaced isolines is the same on both figures.

the subband which crosses the Fermi surface, couples the holes (electrons) in a much narrower energy shell, $\omega_s \ll W$ and that results in lower T_c.

Therefore, the most important pairing interaction in the strong correlation limit of the Hubbard model (2) is the exchange interaction, while the spin-fluctuation coupling mediated by the kinematic interaction results only in a moderate enhancement of T_c. The same result has been obtained in studies of the $t-J$ model beyond the WCA in Ref. [18]. This observation could explain why the numerical simulations of the $t-J$ model usually predict a much stronger pairing tendency than the original Hubbard model [2, 4].

From Fig. 2 and Fig. 3 we can also infer the ratio between the maximum gap value at the Fermi surface and kT_c. For our model we have $2\Phi_{22}(\mathrm{FS})/kT_c \approx 3.5$ at any doping, which is close the BCS ratio. It is to be emphasized that our approach is a mean-field type theory in which the phase of the order parameter is fixed — the gaps are taken to be real and the problem of the phase coherence of the superconducting order parameter [30] is beyond the scope of our theory. This remark also explains why we have obtained the pairing long-range or-

der (LRO) for the two-dimensional Hubbard model while it can be rigorously proved, within the Bogoliubov-Mermin-Wagner theory, a nonexistence of this LRO [31]. A finite 3D coupling will stabilize the phase fluctuations and implement the LRO. As observed in cuprates, the T_c dependence on the inter-layer coupling is rather weak which can occur only for strong intra-layer pairing.

6 Conclusions

A microscopical theory of the superconducting pairing has been developed within the reduced two-band $p-d$ Hubbard model (2) with two microscopical parameters only, the $p-d$ hybridization parameter t and the charge-transfer gap Δ. Making use of the projection technique [28] for the two-time GF in terms of the Hubbard operators, we obtained the Dyson equation for the 4×4 matrix GF (14) with the corresponding matrix self-energy (16). In the zero-order approximation for GF, Eq. (53), we have obtained d-wave superconducting pairing of conventional hole (electron) pairs in one Hubbard subband which is mediated by the exchange interaction given by the interband hopping: $J_{ij} = 4(t_{ij})^2/\Delta$. The normal and anomalous components of the self-energy matrix were calculated in the self-consistent Born approximation for the electron–spin-fluctuation scattering, Eqs. (61) and (62) mediated by kinematic interaction of the second order of the intraband hopping. It is to be stressed that, within the present model, the electron-electron coupling is induced by the exchange and kinematic interactions resulting from non-fermionic commutation relations, as pointed out first by Hubbard [6], without needing additional fitting parameters to accommodate that interaction.

The self-consistent system of equations of the two diagonal gap parameters for the lower and upper Hubbard subbands was obtained in the weak coupling approximation, Eq. (69). Analytical and numerical estimates of the superconducting T_c have been derived under the use of a model antiferromagnetic spin-fluctuation susceptibility, Eq. (74). Simple analytical evaluations proved a possibility of the $d_{x^2-y^2}$-wave pairing with moderate T_c even for a low density of states, Eq. (82), outside the van Hove singularity. It is important to note that the superconducting pairing due to kinematic interaction in the second order occurs in one subband even in the limit $\Delta \to \infty$, which corresponds to $U \to \infty$ in the original Hubbard model (1) when the exchange interaction $J \propto (t_{ij}^{12})^2/\Delta$ vanishes. However, in this limit the spin-fluctuations, Eq. (74), may be suppressed and that prevents the quasiparticle formation and the occurrence of the corresponding superconducting pairing.

More accurate results for the gap in the singlet subband have been obtained from the numerical solution of the integral equation (73). The insight gained

from these computations points to the relative importance of the exchange interaction versus the spin-fluctuation coupling. The former is shown to be the most important pairing interaction in the Hubbard model in the strong correlation limit, while the latter results only in a moderate enhancement of T_c. The smaller weight of the spin-fluctuation coupling comes from two specific features of it: its vanishing inside the BZ along the lines $|k_x|+|k_y| = \pi$ pointing towards the hot spots and the existence of a small energy shell within which the pairing is effective. By contrast, the exchange interaction is maximal along the above-mentioned lines inside BZ and it couples the electrons (holes) in a much broader energy shell, of the order of the bandwidth $W = 8t_{eff}$, due to the interband hopping where the retardation effects are unimportant.

The T_c exhibits parabolic dependence on the doping parameter δ (Fig. 1). The optimum doping values δ_{opt} as well as the maximum values reached by T_c at δ_{opt} show a marked dependence on the coupling interactions included in the model. Sampling at several temperatures of the wave-vector behavior of the order parameters $\Phi^{22}(\mathbf{k})$ over the first quadrant of the BZ (Fig. 2 and Fig. 3) show the occurrence of a peculiar $d_{x^2-y^2}$-wave gap pattern which strongly depends on the type of the involved interactions as well.

In conclusion, the present investigation points to the existence of a singlet $d_{x^2-y^2}$-wave superconducting pairing for holes or electrons in the two-band Hubbard model mediated by the exchange interaction and antiferromagnetic spin-fluctuation scattering induced by the kinematic interaction, characteristic to the Hubbard model. These mechanisms of superconducting pairing are absent in the fermionic models (for a discussion, see Anderson [32]). The pairing interaction occurs in the second order of small hopping parameters: the exchange interaction is mediated by the iterband hopping, while the kinematic interaction is induced by the intraband hopping. The weak point of the argument is the derivation of the reported results in the weak coupling approximation of the superconducting equations. To substantiate the present results, more rigorous inferences emerging from the direct numerical solution of strong coupling Eliashberg-type equations in the $(\mathbf{q}, \omega)-$space, as done recently for the $t-J$ model, [18] should be elaborated.

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Список литературы

[1] C.C. Tsuei, J.R. Kirtley, M. Rupp, et al., Science, **271**, 329 (1996).

[2] For a review see D.J. Scalapino, Phys. Reports, **250**, 329 (1995); arXiv:cond-mat/9908287.

[3] N.M. Plakida, *High-Temperature Superconductivity. Experiment and Theory* (Spinger-Verlag, Berlin, Heidelberg, 1995).

[4] E. Dagotto, Rev. Mod. Phys., **66**, 763 (1994).

[5] P.W. Anderson, Science, **235**, 1196 (1987); P.W. Anderson, *The theory of superconductivity in the high-T_c cuprates* (Princeton University Press, Princeton, New Jersey, 1997).

[6] J. Hubbard, Proc. Roy. Soc. A (London) **276** 238 (1963).

[7] Pao Chien-Hua and N.E. Bickers,, Phys. Rev. Lett., **72**, 1870 (1994); Phys. Rev. B, **51**, 16310 (1995).

[8] P. Monthoux and D.J. Scalapino, Phys. Rev. Lett., **72**, 1874 (1994).

[9] S.T. Lenck, J.P. Carbotte, and R.C. Dynes, Phys. Rev. B, **50**, 10149 (1994).

[10] T. Dahm and L. Tewordt, Phys. Rev. Lett. **74**, 793 (1995).

[11] J.R. Schrieffer, J. Low Temp. Phys. **99**, 397 (1995).

[12] R.O. Zaitsev and V.A. Ivanov, Soviet Phys. Solid State, **29**, 2554 (1987); *ibid.*, 3111 (1987); Physica C, **153-155**, 1295 (1988).

[13] N.M. Plakida and I.V. Stasyuk, Modern Phys. Lett., **2**, 969 (1988).

[14] D.N. Zubarev, Sov. Phys. Usp. **3**, 320 (1960).

[15] N.M. Plakida, V.Yu. Yushankhai, and I.V. Stasyuk, Physica C, **160**, 80 (1989).

[16] V.Yu. Yushankhai, N.M. Plakida, and P. Kalinay, Physica C, **174**, 401 (1991).

[17] Yu.A. Izyumov and B.M. Letfulov, Intern. J. Modern Phys. B, **6**, 3771 (1992).

[18] N.M. Plakida and V.S. Oudovenko, Phys. Rev. B **59**, 11949 (1999).

[19] J. Beenen and D.M. Edwards, Phys. Rev. B, **52**, 13636 (1995).

[20] A. Avella, F. Mancini, D. Villani, and H. Matsumoto, Physica C, **282-287**, 1757 (1997); T. Di Matteo, F. Mancini, H. Matsumoto, and V.S. Oudovenko, Physica B, **230 - 232**, 915 (1997).

[21] T.D. Stanescu, I. Martin, and Ph. Phillips, Phys. Rev. B **62**, 4300 (2000).

[22] N.M. Plakida, R. Hayn, and J.-L. Richard, Phys. Rev. B **51**, 16599 (1995).

[23] L.F. Feiner, J.H. Jefferson, and R. Raimondi, Phys. Rev. B **53**, 8751 (1996); R. Raimondi, J.H. Jefferson, and L.F. Feiner, Phys. Rev. B **53**, 8774 (1996).

[24] V.J. Emery, Phys. Rev. Lett. **58**, 2794 (1987); C.M. Varma, S. Schmitt-Rink, and E. Abrahams, Solid State Commun. **62**, 681 (1987).

[25] N.M. Plakida, Physica C **282-287**, 1737 (1997).

[26] Th. Maier, M. Jarrel, Th. Pruschke, and J. Keller, Phys. Rev. Lett.**85**, 1524 (2000).

[27] A.I. Lichtenstein and M.I. Katsnelson, Phys. Rev. B **62**, R9283 (2000).

[28] N.M. Plakida, Phys. Lett. A **43**, 481 (1973).

[29] J. Jaklič and B. Prelovsėk, Phys. Rev. Lett **74**, 3411 (1995); *ibid.* **75**, 1340 (1995).

[30] G. Deutscher, Nature, **397**, 410 (1999).

[31] Gang Su and M. Suzuki, Phys. Rev. B **58**, 117 (1998).

[32] P.W. Anderson, Adv. in Physics **46**, 3 (1997).

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Плакида Н.М. и др. E17-2001-59
Обменное и спин-флуктуационное сверхпроводящее спаривание
в модели Хаббарда в пределе сильных корреляций

Предложена микроскопическая теория сверхпроводимости в двухзонной, синглет-дырочной модели Хаббарда в пределе сильных электронных корреляций. На основе проекционной техники для матричной функции Грина от операторов Хаббарда получено уравнение Дайсона. Показано, что уже в приближении среднего поля возникает d-волновое сверхпроводящее спаривание для стандартных электронных (дырочных) пар, обусловленное обменным взаимодействием. Получена также система уравнений для сверхпроводящих щелей в двух хаббардовских подзонах при учете собственно энергетических поправок, обусловленных кинематическим взаимодействием. Численное и аналитическое решение уравнений предсказывает существование синглетного d-волнового спаривания в дырочной и синглетной подзонах. Вычислены зависящие от волнового вектора щелевые функции и температура T_c при различной концентрации дырок. Полученные результаты показывают, что обменное взаимодействие (обусловленное межзонными перескоками) дает бóльший вклад в сверхпроводящее спаривание, чем кинематическое взаимодействие (обусловленное внутризонными перескоками).

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Plakida N.M. et al. E17-2001-59
Exchange and Spin-Fluctuation Superconducting Pairing
in the Hubbard Model in the Strong Correlation Limit

A microscopic theory of superconductivity within the two-band singlet-hole Hubbard model in the strong correlation limit is developed. Making use of the projection technique for the matrix Green function in terms of the Hubbard operators, the Dyson equation is derived. It is proved that in the mean-field approximation d-wave superconducting pairing mediated by the exchange interaction occurs for conventional electron (hole) pairs. Allowing for the self-energy corrections due to kinematic interaction, a coupled system of equations for the superconducting gaps in the two Hubbard subbands is obtained. The derived numerical and analytical solutions predict the occurrence of singlet d-wave pairing both in the one-hole and singlet Hubbard subbands. The wave-vector dependent gap functions and T_c are calculated for different hole concentrations. The results show that in pairing the exchange interaction (which stems from the interband hopping) prevails over the kinematic interaction (which stems form the intraband hopping).

The investigation has been performed at the Bogoliubov Laboratory of Theoretical Physics, JINR.

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