The paper is dedicated to Professor V.A. Moskalenko
on the occasion of his 80th birthday

SUPERCONDUCTIVITY IN STRONGLY CORRELATED ELECTRONIC SYSTEMS

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Abstract

A microscopic theory of superconducting pairing within the Hubbard model is discussed. A Dyson equation for the matrix thermodynamic Green function in the Nambu representation for Hubbard operators is derived by applying the Mori-type projection technique for the equation of motion method. The self-energy is calculated in the noncrossing approximation for electron scattering on spin and charge fluctuations induced by kinematic interaction for Hubbard operators. It is shown that superconducting pairing in strongly correlated electronic systems is determined by antiferromagnetic exchange caused by interband hopping and spin fluctuations due to hole motion in one subband.

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. A distinctive feature of high–T_c copper oxide superconductors is strong antiferromagnetic (AF) exchange interaction. The exchange binding energy of two holes with spin 1/2 in copper Cu($3d^9$) and oxygen O($2p^6$) ions comprises a value on the order of 1 eV, and the AF superexchange energy for copper spins is on the order of 0.13 eV which results in high Néel temperature $T_{\mathrm{N}} \simeq 300-500$ K. Anderson [1] was the first to stress the importance of the strong electron correlations in copper oxides. He proposed a theory of resonant valence bonds within the framework of the one-subband t-J model. Subsequently, superconducting pairing due to the AF exchange in the t-J model was considered by many researches (for review see [2, 3]).

However, the t-J model is usually derived from the two-subband Hubbard model by Schrieffer-Wolf transformation which excludes interband transitions that results in the instant exchange interaction. To prove the applicability of the t-J model for investigation of superconductivity one has to study the retardation effects in the exchange interaction by considering the original two-subband Hubbard model. Superconductivity in the Hubbard model has been extensively studied both by applying numerical simulations for finite clusters (see [4, 5]) and by various analytical methods (for reference see [3]). In the latter case, mostly the mean-field approximation was considered. A powerful diagram technique for the Hubbard model in the limit of strong correlations has been developed by Moskalenko et al. [6]. The method has been applied to study superconductivity in the Hubbard model [7].

In the present paper, we discuss superconducting pairing within the effective two-band Hubbard model for the CuO_2 plane [8]. We show that the AF exchange interaction and spin-fluctuation electron scattering induced by the kinematic interaction result in the singlet $d_{x^2-y^2}$-wave superconducting pairing. To treat rigorously strong correlations, the Hubbard operator technique within the projection method for the thermodynamic double-time Green functions [9] is used. An exact Dyson equation is derived with due regard for the two-subband nature of the Hubbard model in the limit of strong correlations. The self-energy represented by multi-particle GFs is calculated in the noncrossing approximation (NCA), which results in the strong-coupling Migdal-Eliashberg type theory.

In the next section, we briefly discuss the model and derivation of the Dyson equation and the self-energy in NCA. A self-consistent system of equations for a hole-doped case is considered in Sect. 3 where calculations of T_c are presented. Concluding remarks are given in Sect. 4.

2. General formulation

2.1. Hubbard model

To study electronic properties of the CuO_2 plane we consider the Hubbard model on a square lattice

$$H = E_1 \sum_{i,\sigma} X_i^{\sigma\sigma} + E_2 \sum_i X_i^{22} + \sum_{i\neq j,\sigma} t_{ij}\{X_i^{\sigma 0} X_j^{0\sigma} + X_i^{2\sigma} X_j^{\sigma 2} + \sigma(X_i^{2,\bar\sigma} X_j^{0\sigma} + \mathrm{H.c.})\}, \tag{1}$$

where $E_1 = \varepsilon_1 - \mu$ and $E_2 = 2E_1 + U_{\mathrm{eff}}$ are the energy levels of one- and two-hole states, where $U_{\mathrm{eff}} = \Delta_{pd}$ is the charge-transfer gap in cuprates. The Hubbard operators (HOs) $X_i^{\alpha\beta} = |i\alpha><i\beta|$ define transitions between four hole states: $\alpha,\beta = |0>, |\sigma>, |2> = |\uparrow\downarrow>$, $\sigma = \pm 1 = (\uparrow,\downarrow), \bar\sigma = -\sigma$. The bare electron dispersion is defined by the hopping parameters t_{ij} which are equal to t for the nearest neighbors (n.n.) and t', t'' for the next n.n. The $\mathbf{k}$-dependence of the hopping function is given by the equation

$$t(\mathbf{k}) = 4t\,\gamma(\mathbf{k}) + 4t'\,\gamma'(\mathbf{k}) + 4t''\,\gamma''(\mathbf{k}), \tag{2}$$

where $\gamma(\mathbf{k}) = (1/2)(\cos k_x + \cos k_y), \gamma'(\mathbf{k}) = \cos k_x \cos k_y$ and $\gamma''(\mathbf{k}) = (1/2)(\cos 2k_x + \cos 2k_y)$. The chemical potential μ depends on the average hole occupation number

$$n = <N_i>, \quad N_i = \sum_\sigma X_i^{\sigma\sigma} + 2X_i^{22}, \tag{3}$$

where $<...>$ denotes the statistical average. The spin operators in terms of HOs are defined as

$$S_i^\sigma = X_i^{\sigma\bar\sigma}, \quad S_i^z = (1/2)\sum_\sigma \sigma X_i^{\sigma\sigma}. \tag{4}$$

The HOs satisfy the completeness relation $X_i^{00} + X_i^{\uparrow\uparrow} + X_i^{\downarrow\downarrow} + X_i^{22} = 1$ and the multiplication rules $X_i^{\alpha\beta} X_i^{\gamma\delta} = \delta_{\beta\gamma} X_i^{\alpha\delta}$. From the latter follow the commutation relations

$$\left[X_i^{\alpha\beta}, X_j^{\gamma\delta}\right]_\pm = \delta_{ij}\left(\delta_{\beta\gamma} X_i^{\alpha\delta} \pm \delta_{\delta\alpha} X_i^{\gamma\beta}\right). \tag{5}$$

The upper sign pertains to Fermi-type operators like $X_i^{0\sigma}$ which change a number of particles and the lower sign pertains to Bose-type operators, for example, the particle number operator N_i in (3) or the spin operators S_i^α (4).

We emphasize here that in Hubbard model (1) there is no dynamical coupling of electrons (holes) to fluctuations of spins or charges. Instead, the *kinematic* interaction occurs induced by commutation relations (5). For example, the equation of motion for the HO $X_i^{\sigma 2}$ has the form

$$i\,dX_i^{\sigma 2}/\,dt = [X_i^{\sigma 2}, H] = (E_1 + U_{\text{eff}})X_i^{\sigma 2}$$
$$+\sum_{l\neq i,\sigma'} t_{il}\left(B_{i\sigma\sigma'}^{22}X_l^{\sigma' 2} - \sigma B_{i\sigma\sigma'}^{21}X_l^{0\bar{\sigma}'}\right) - \sum_{l\neq i} t_{il}\,X_i^{02}\left(X_l^{\sigma 0} + \sigma X_l^{2\bar{\sigma}}\right). \qquad (6)$$

$$B_{i\sigma\sigma'}^{22} = (X_i^{22} + X_i^{\sigma\sigma})\,\delta_{\sigma'\sigma} + X_i^{\sigma\bar{\sigma}}\,\delta_{\sigma'\bar{\sigma}} = (N_i/2 + S_i^z)\,\delta_{\sigma'\sigma} + S_i^{\sigma}\,\delta_{\sigma'\bar{\sigma}},$$
$$B_{i\sigma\sigma'}^{21} = (N_i/2 + S_i^z)\,\delta_{\sigma'\sigma} - S_i^{\sigma}\,\delta_{\sigma'\bar{\sigma}}\,, \qquad (7)$$

Here $B_{i\sigma\sigma'}^{\alpha\beta}$ are Bose-like operators related to the particle number operator N_i and spin operators S_i^{α} (4) which appear in commutation relations (5).

2.2. Dyson equation

To consider the superconducting pairing in Hubbard model (1), we define the thermodynamic Green function (GF) as a 4×4 matrix in Zubarev notation [9]

$$\mathrm{G}_{ij\sigma}(\omega) = \langle\langle \hat{X}_{i\sigma} \mid \hat{X}_{j\sigma}^{\dagger} \rangle\rangle_{\omega} = \begin{pmatrix} \hat{G}_{ij\sigma}(\omega) & \hat{F}_{ij\sigma}(\omega) \\ \hat{F}_{ij\sigma}^{\dagger}(\omega) & -\hat{G}_{ji\bar{\sigma}}(-\omega) \end{pmatrix}, \qquad (8)$$

where the four-component Nambu operator $\hat{X}_{i\sigma}$ and its conjugate operator $\hat{X}_{i\sigma}^{\dagger} = (X_i^{2\sigma}\;\; X_i^{\bar{\sigma}0}\;\; X_i^{\bar{\sigma}2}\;\; X_i^{0\sigma})$ are introduced. Because of the two-subband nature of model (1), the normal $\hat{G}_{ij\sigma}$ and anomalous $\hat{F}_{ij\sigma}$ components of the GF are 2×2 matrices which are coupled by the symmetry relations for the anticommutator retarded GF in (8).

To calculate GF (8) we use the method of equations of motion. Differentiating the GF with respect to the time t, the Fourier representation of it leads to the equation

$$\omega \mathrm{G}_{ij\sigma}(\omega) = \delta_{ij}\mathrm{Q} + \langle\langle [\hat{X}_{i\sigma}, H] \mid \hat{X}_{j\sigma}^{\dagger} \rangle\rangle_{\omega}\,, \qquad (9)$$

where

$$\mathrm{Q} = \langle \{\hat{X}_{i\sigma}, \hat{X}_{i\sigma}^{\dagger}\} \rangle = \hat{\tau}_0 \times \hat{Q}, \quad \hat{Q} = \begin{pmatrix} Q_2 & 0 \\ 0 & Q_1 \end{pmatrix}. \qquad (10)$$

Here $\hat{\tau}_0$ is the 2×2 unit matrix and in the paramagnetic state the coefficients $Q_2 = \langle X_i^{22} + X_i^{\sigma\sigma} \rangle = n/2$ and $Q_1 = \langle X_i^{00} + X_i^{\bar{\sigma}\bar{\sigma}} \rangle = 1 - Q_2$ depend on the occupation number of holes (3) only. In the Q matrix we neglect anomalous averages of the type $\langle X_i^{02} \rangle$, which make no contribution to the d-wave pairing.

In the Hubbard model, there is no well-defined quasiparticle (QP) excitations specified by noninteracting propagation. Therefore, it is convenient to choose the mean-field contribution to the energy of QPs in the equations of motion (9) as the zeroth-order QP energy. To identify this contribution, we use the Mori-type projection method. To this aim, we write the operator $\hat{Z}_{i\sigma} = [\hat{X}_{i\sigma}, H]$ in (9) as a sum of the linear part, proportional to the original operator $\hat{X}_{i\sigma}$, and the irreducible part $\hat{Z}_{i\sigma}^{(ir)}$ orthogonal to $\hat{X}_{i\sigma}$

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

The orthogonality conditions $\langle \{\hat{Z}_{i\sigma}^{(ir)}, \hat{X}_{j\sigma}^{\dagger}\} \rangle = \langle \hat{Z}_{i\sigma}^{(ir)}\hat{X}_{j\sigma}^{\dagger} + \hat{X}_{j\sigma}^{\dagger}\hat{Z}_{i\sigma}^{(ir)} \rangle = 0$ determine the linear part, the frequency matrix

$$\mathrm{E}_{ij\sigma} = \langle \{[\hat{X}_{i\sigma}, H], \hat{X}_{j\sigma}^{\dagger}\} \rangle\, \mathrm{Q}^{-1}, \qquad (12)$$

which defines the QP spectrum in the generalized MFA. Differentiating the multiparticle GF $<<\hat{Z}_{i\sigma}(t)\,|\,\hat{X}^{\dagger}_{j\sigma}(t')>>$ in (9) with respect to the second time t' and using the same projection procedure as in (11) leads to the Dyson equation for GF (8). Passing to the Fourier representation in the $(\mathbf{q},\omega)$ space, we write the Dyson equation as

$$\mathrm{G}_{\sigma}(\mathbf{k},\omega)=\left\{\omega\tilde{\tau}_0-\mathrm{E}_{\sigma}(\mathbf{k})-\Sigma_{\sigma}(\mathbf{k},\omega)\right\}^{-1}\mathrm{Q}, \tag{13}$$

where $\tilde{\tau}_0$ is the 4×4 unit matrix. The self-energy operator $\Sigma_{\sigma}(\mathbf{q},\omega)$ is defined by the *proper* part of the scattering matrix

$$\Sigma_{\sigma}(\mathbf{q},\omega)=<<\hat{Z}^{(ir)}_{\mathbf{q}\sigma}|\hat{Z}^{(ir)\dagger}_{\mathbf{q}\sigma}>>^{(prop)}_{\omega}\,\mathrm{Q}^{-1}. \tag{14}$$

Dyson equations (12)–(14) give the exact representation for GF (8). To obtain the closed system of equations, we must evaluate the multiparticle GF in the self-energy operator (14) which describes processes of inelastic scattering of electrons (holes) on charge and spin fluctuations due to the kinematic interaction.

2.3. Mean-Field Approximation

The superconducting pairing in the Hubbard model already occurs in the MFA and is caused by the kinetic exchange interaction as proposed by Anderson [1]. It is therefore reasonable to consider the MFA separately. Using commutation relations for HOs (5), frequency matrix (12) takes the form

$$\mathrm{E}_{ij\sigma}=\begin{pmatrix}\hat{\varepsilon}_{ij\sigma} & \hat{\Delta}_{ij\sigma}\\ \hat{\Delta}^{*}_{ji\sigma} & -\hat{\varepsilon}_{ji\bar{\sigma}}\end{pmatrix},\quad \text{or}\quad \mathrm{E}_{\sigma}(\mathbf{k})=\begin{pmatrix}\hat{\varepsilon}_{\sigma}(\mathbf{k}) & \hat{\Delta}_{\sigma}(\mathbf{k})\\ \hat{\Delta}^{*}_{\sigma}(\mathbf{k}) & -\hat{\varepsilon}_{\bar{\sigma}}(\mathbf{k})\end{pmatrix}. \tag{15}$$

The matrix $\hat{\varepsilon}_{\sigma}(\mathbf{k})$ determines the QP spectrum in the two Hubbard subbands in the normal phase (for details see [10])

$$\varepsilon_{1,2}(\mathbf{k})=(1/2)[\omega_2(\mathbf{k})+\omega_1(\mathbf{k})]\mp(1/2)\Lambda(\mathbf{k}),$$
$$\Lambda(\mathbf{k})=\{[\omega_2(\mathbf{k})-\omega_1(\mathbf{k})]^2+4W(\mathbf{k})^2\}^{1/2}, \tag{16}$$

where $\omega_1(\mathbf{k})=4t\,\alpha_1\gamma(\mathbf{k})+4t'\,\beta_1\gamma'(\mathbf{k})-\mu$, $\omega_2(\mathbf{k})=4t\,\alpha_2\gamma(\mathbf{k})+4t'\,\beta_2\gamma'(\mathbf{k})+U_{eff}-\mu$, and $W(\mathbf{k})=4t\,\alpha_{12}\gamma(\mathbf{k})+4t'\,\beta_{12}\gamma'(\mathbf{k})$. The kinematic interaction renormalizes the spectrum: $\alpha_{1(2)}=Q_{1(2)}[1+C_1/Q^2_{1(2)}]$, $\beta_{1(2)}=Q_{1(2)}[1+C_2/Q^2_{1(2)}]$, $\alpha_{12}=\sqrt{Q_1Q_2}[1-C_1/Q_1Q_2]$, $\beta_{12}=\sqrt{Q_1Q_2}[1-C_2/Q_1Q_2]$. Here we go beyond the Hubbard I renormalization of hopping parameters given by the factors $Q_{1(2)}$ and take into consideration the renormalization caused by spin correlation functions for the n. n. and the next n. n., respectively

$$C_1=<\mathbf{S}_i\mathbf{S}_{i\pm a_x/a_y}>,\quad C_2=<\mathbf{S}_i\mathbf{S}_{i\pm a_x\pm a_y}>. \tag{17}$$

However, we neglected charge correlations in the renormalization by using the approximation $<N_iN_j>=<N_i><N_j>$ which should be reasonable in the limit of strong electron correlations.

Now we calculate the anomalous component $\hat{\Delta}_{ij\sigma}$ of matrix (16), which determines the superconducting gap. In what follows, we consider only the singlet d-wave pairing, which is determined by the anomalous averages at noncoincident sites, $(i\neq j)$. The diagonal matrix components have the forms

$$\Delta^{22}_{ij\sigma}=-\sigma t_{ij}<X^{02}_iN_j>/Q_2,\quad \Delta^{11}_{ij\sigma}=\sigma t_{ij}<N_jX^{02}_i>/Q_1. \tag{18}$$

Expressing the Fermi operators in terms of the Hubbard operators as $a_{i\sigma}=X^{0\sigma}_i+\sigma X^{\bar{\sigma}2}_i$, we can write the anomalous averages in (18) as $<X^{02}_iN_j>=<X^{0\downarrow}_iX^{\downarrow 2}_iN_j>=<a_{i\downarrow}\,a_{i\uparrow}N_j>$, because other products of the HOs do not contribute due to the multiplication rules. This representation of the anomalous averages in terms of Fermi operators shows that the pairing occurs at a single site but in different Hubbard subbands.

The anomalous averages $< X_i^{02} N_j >$ can be calculated directly by using an equation for the pair commutator GF $L_{ij}(t-t') =<< X_i^{02}(t) \,|\, N_j(t') >>$ without *any decoupling* approximations [8]. This results in the following equation for the pair correlation function of the two-hole band

$$< X_i^{02} N_j > = -\frac{1}{U_{\text{eff}}} \sum_{m \neq i,\sigma} \sigma t_{im} < X_i^{\sigma 2} X_m^{\bar{\sigma} 2} N_j > \simeq -\frac{4 t_{ij}}{U_{\text{eff}}} \sigma < X_i^{\sigma 2} X_j^{\bar{\sigma} 2} > . \tag{19}$$

The last equation is obtained in the two-site approximation, $m = j$, which is typically used in a derivation of the t-J model. As a result, the equation for the superconducting gap in formulae (18) in the case of hole doping, $n = 1+\delta > 1$, can be written as

$$\Delta_{ij\sigma}^{22} = -\sigma\, t_{ij} < X_i^{02} N_j > /Q_2 = J_{ij} < X_i^{\sigma 2} X_j^{\bar{\sigma} 2} > /Q_2 . \tag{20}$$

This is equivalent to the gap equation in the t-J model which describes pairing due to the exchange interaction $J_{ij} = 4(t_{ij})^2/U_{\text{eff}}$. A similar gap equation can be obtained for the one-hole Hubbard band: $\Delta_{ij\sigma}^{11} = J_{ij} < X_i^{0\bar{\sigma}} X_j^{0\sigma} > /Q_1$. We thus conclude that anomalous averages (18) in the Hubbard model correspond to the anomalous averages in one of the Hubbard subbands (depending on the position of the chemical potential) in the t-J model. Therefore, this is just conventional pairing mediated by the exchange interaction which has been extensively studied within the t-J model (see, e.g., [11] and references therein).

The same anomalous pair correlation functions (18) were obtained in MFA for the original Hubbard model (1) in Refs. [12–14]. To calculate the anomalous correlation function $< c_{i\downarrow} c_{i\uparrow} N_j >$ in [12, 14] the Roth procedure was applied based on a decoupling of the operators on the same lattice site in the time-dependent correlation function: $< c_{i\downarrow}(t) \,|\, c_{i\uparrow}(t') N_j(t') >$. However, the decoupling of the Hubbard operators on the same lattice site is not unique (as it has been really observed in Refs. [12, 14]) and is unreliable. To avoid the uncontrollable decoupling, kinematical restrictions were imposed on the correlation functions for the Hubbard operators in Ref. [13]. However, it has not produced a unique solution for the superconducting equations either.

2.4. Self-energy operator

Self-energy operator (14) can be conveniently written in the same form as GF (8)

$$\Sigma_{ij\sigma}(\omega) = \begin{pmatrix} \hat{M}_{ij\sigma}(\omega) & \hat{\Phi}_{ij\sigma}(\omega) \\ \hat{\Phi}^{\dagger}_{ij\sigma}(\omega) & -\hat{M}_{ji\bar{\sigma}}(-\omega) \end{pmatrix} \mathrm{Q}^{-1}, \tag{21}$$

where the matrices $\hat{M}$ and $\hat{\Phi}$ denote the respective normal and anomalous components of the self-energy operator.

The system of equations for the (4×4) matrix GF (8) and the self-energy (21) can be reduced to a system of equations for the normal $\hat{G}_\sigma(\mathbf{k},\omega)$ and anomalous $\hat{F}_\sigma(\mathbf{k},\omega)$ (2×2) matrix components. By using representations for the frequency matrix (12) and the self-energy (21), we derive for these components the following system of matrix equations

$$\hat{G}_\sigma(\mathbf{k},\omega) = (\hat{G}_N(\mathbf{k},\omega)^{-1} + \hat{\varphi}_\sigma(\mathbf{k},\omega)\, \hat{G}_N(\mathbf{k},-\omega)\, \hat{\varphi}^*_\sigma(\mathbf{k},\omega))^{-1}\, \hat{Q}, \tag{22}$$

$$\hat{F}^*_\sigma(\mathbf{k},\omega) = -\hat{G}_N(\mathbf{k},-\omega)\, \hat{\varphi}^*_\sigma(\mathbf{k},\omega)\, \hat{G}_\sigma(\mathbf{k},\omega). \tag{23}$$

In (22) we introduced the normal state matrix GF and the matrix superconducting gap function

$$\hat{G}_N(\mathbf{k},\omega) = (\omega\hat{\tau}_0 - \hat{\varepsilon}(\mathbf{k}) - \hat{M}(\mathbf{k},\omega)/\hat{Q})^{-1}, \quad (24)$$

$$\hat{\varphi}_\sigma(\mathbf{k},\omega) = \hat{\Delta}_\sigma(\mathbf{k}) + \hat{\Phi}_\sigma(\mathbf{k},\omega)/\hat{Q}. \quad (25)$$

To calculate the self-energy matrix (14) we used the non-crossing (NCA) or the self-consistent Born approximation (SCBA). In this approximation, Fermi-like excitations described by operators $X_j = X_j^{0\sigma}\,(X_j^{\bar{\sigma}2})$ and Bose-like excitations described by operators B_i (7) in multiparticle GF (14) are considered as propagating independently. Therefore, their correlation functions at noncoincident lattice sites $(i \neq j, l \neq m)$ can be factored into a product of the corresponding functions

$$< B_i(t)X_j(t)B_l(t')X_m(t') > \simeq < X_j(t)X_m(t') >< B_i(t)B_l(t') > . \quad (26)$$

Using the spectral representation for these correlation functions we get in the NCA the following expressions for the normal $M_\sigma^{\alpha\alpha}(\mathbf{q},\omega)$ and anomalous $\Phi_\sigma^{\alpha\alpha}(\mathbf{q},\omega)$ diagonal components of the self-energy

$$M_\sigma^{22}(\mathbf{k},\omega) = \frac{1}{N}\sum_{\mathbf{q}}\int_{-\infty}^{+\infty} dz\, K^{(+)}(\omega,z\,|\,\mathbf{q},\mathbf{k}-\mathbf{q})\left\{-\frac{1}{\pi}\mathrm{Im}\left[G_\sigma^{22}(\mathbf{q},z) + G_\sigma^{11}(\mathbf{q},z)\right]\right\}, \quad (27)$$

$$\Phi_\sigma^{22}(\mathbf{k},\omega) = \frac{1}{N}\sum_{\mathbf{q}}\int_{-\infty}^{+\infty} dz\, K^{(-)}(\omega,z\,|\,\mathbf{q},\mathbf{k}-\mathbf{q})\left\{-\frac{1}{\pi}\mathrm{Im}\left[F_\sigma^{22}(\mathbf{q},z) - F_\sigma^{11}(\mathbf{q},z)\right]\right\}, \quad (28)$$

where $G_\sigma^{\alpha\alpha}(\mathbf{q},z)$ and $F_\sigma^{\alpha\alpha}(\mathbf{q},z)$ are given by the diagonal components of the matrices (22) and (23). The kernel of integral equations (8) and (9) is given by the functions

$$K^{(\pm)}(\omega,z\,|\,\mathbf{q},\mathbf{k}-\mathbf{q}) = |\,t(\mathbf{q})\,|^2\,\frac{1}{2}\int_{-\infty}^{+\infty}\frac{d\Omega}{\omega - z - \Omega}\left(\tanh\frac{z}{2T} + \coth\frac{\Omega}{2T}\right) \times\frac{1}{\pi}\mathrm{Im}\,\chi_{sc}^{(\pm)}(\mathbf{k}-\mathbf{q},\Omega). \quad (29)$$

We emphasize here that the interaction is defined by the hopping parameter $t(\mathbf{q})$ (2) and therefore no fitting parameter for the spin-electron interaction is used. The spectral density of bosonic excitations in (29) is determined by the dynamic susceptibility of the Bose-like operators $B_i(t)$, the spin and number (charge) fluctuations

$$\chi_{sc}^{(\pm)}(\mathbf{q},\omega) = \chi_s(\mathbf{q},\omega) \pm \chi_c(\mathbf{q},\omega) = -[<< \mathbf{S}_\mathbf{q}\,|\,\mathbf{S}_{-\mathbf{q}} >>_\omega \pm (1/4) << \delta N_\mathbf{q}\,|\,\delta N_{-\mathbf{q}} >>_\omega], \quad (30)$$

where we introduced the commutator GF for the spin $\mathbf{S}_\mathbf{q}$ and the number $\delta N_\mathbf{q} = N_\mathbf{q} - < N_\mathbf{q} >$ operators. The renormalized QP spectrum in the two-hole subband in the normal state is determined by equation (24): $\tilde{\varepsilon}_2(\mathbf{k}) \simeq \varepsilon_2(\mathbf{k}) + \mathrm{Re}M_\sigma^{22}(\mathbf{q},\omega = \tilde{\varepsilon}_2(\mathbf{k}))/Q_2$, and gap function (25) is defined as $\varphi_{2,\sigma}(\mathbf{k},\omega) = \Delta_\sigma^{22}(\mathbf{k}) + \Phi_\sigma^{22}(\mathbf{k},\omega)/Q_2$.

In the NCA the vertex corrections are neglected as in the Migdal-Eliashberg theory. The kinematic interaction induced by the intra-band hopping is of the same order as the bandwidth and vertex corrections may be important in obtaining quantitative results. However, in the NCA the self-energy is calculated self-consistently allowing us to consider a strong coupling limit which plays a key role both in renormalization of QP spectra and in superconducting pairing. Thus, this approach can be considered as a first reasonable approximation.

3. Results and discussion

3.1. Self-consistent system of equations

In this section we consider a self–consistent system of equations for the GFs (22)–(25) and the self-energy (27), (28) for the two-hole subband at hole doping, $n = 1+\delta > 1$. Normal GF (24) can be approximately written as

$$G_N^{22}(\mathbf{k},\omega) = [1-b(\mathbf{k})]G_2(\mathbf{k},\omega) + b(\mathbf{k})G_1(\mathbf{k},\omega), \tag{31}$$

$$G_{1(2)}(\mathbf{k},\omega) = \frac{1}{\omega - \varepsilon_{1(2)}(\mathbf{k}) - \Sigma(\mathbf{k},\omega)}, \tag{32}$$

where the hybridization parameter $b(\mathbf{k}) = [\varepsilon_2(\mathbf{k}) - \omega_2(\mathbf{k})]/[\varepsilon_2(\mathbf{k}) - \varepsilon_1(\mathbf{k})]$. The self-energy in (31) can be approximated by the same diagonal component for the both subbands

$$\Sigma(\mathbf{k},\omega) = \frac{1}{N}\sum_{\mathbf{q}}\int_{-\infty}^{+\infty} dz K^{(+)}(\omega,z\,|\,\mathbf{q},\mathbf{k}-\mathbf{q})(-\frac{1}{\pi}\operatorname{Im}[G_1(\mathbf{q},z)+G_2(\mathbf{q},z)]). \tag{33}$$

Gap equation (25) for the diagonal component for the two-hole subband can be written as

$$\varphi_{2,\sigma}(\mathbf{k},\omega) = \frac{1}{N}\sum_{\mathbf{q}}\int_{-\infty}^{+\infty} dz\,[J(\mathbf{k}-\mathbf{q})\frac{1}{2}\tanh\frac{z}{2T} + K^{(-)}(\omega,z\,|\,\mathbf{q},\mathbf{k}-\mathbf{q})](-\frac{1}{\pi Q_2})\operatorname{Im}F_{\sigma}^{22}(\mathbf{q},z). \tag{34}$$

Here gap equation (20) in MFA for the exchange interaction $J(\mathbf{q}) = 4J\,\gamma(\mathbf{q})$ was used, where J is the exchange energy for the n. n. spins. In (34), a contribution from the one-hole subband $F_{\sigma}^{11}(\mathbf{q},z)$ was neglected, since the gap function is vanishingly small in this filled band located much below the Fermi level. To determine the superconducting T_c it is sufficient to solve a linear equation for the gap (34) by using the linearized anomalous GF (23)

$$F_{\sigma}^{22}(\mathbf{k},\omega) = -G_N^{22}(\mathbf{k},-\omega)\,\varphi_{2,\sigma}(\mathbf{k},\omega)\,G_N^{22}(\mathbf{k},\omega)\,Q_2\,. \tag{35}$$

To close the system of equations we should specify a model for the spin-charge susceptibility (30) in kernel (29). Below we take into account only the spin-fluctuation contribution $\chi_s(\mathbf{q},\omega) = -\langle\langle \mathbf{S}_q\,|\,\mathbf{S}_{-q}\rangle\rangle_\omega$ for which we adopt the following model

$$\operatorname{Im}\chi_s(\mathbf{q},\omega+i0^+) = \chi_s(\mathbf{q})\,\chi_s''(\omega) = \frac{\chi_0}{1+\xi^2(1+\gamma(\mathbf{q}))}\tanh\frac{\omega}{2T}\frac{1}{1+(\omega/\omega_s)^2}. \tag{36}$$

The $\mathbf{q}$-dependence in $\chi_s(\mathbf{q})$ is determined by the AF correlation length ξ while a frequency dependence is determined by a continuous spin-fluctuation spectrum in $\chi_s''(\omega)$ with a cut-off energy of the order of the exchange energy $\omega_s \sim J$. The two fitting parameters, however, do not fix the strength of the spin-fluctuation interaction given by the static susceptibility χ_0 at the AF wave vector $\mathbf{Q} = (\pi,\pi)$. This parameter is fixed by the normalization condition

$$\langle \mathbf{S}_i^2 \rangle = \frac{1}{N}\sum_i \langle \mathbf{S}_i\mathbf{S}_i \rangle = \frac{1}{\pi}\int_{-\infty}^{+\infty}\frac{dz}{\exp(z/T)-1}\chi_s''(z)\,\frac{1}{N}\sum_{\mathbf{q}}\chi_s(\mathbf{q}), \tag{37}$$

which gives the following value for this constant: $\chi_0 = (2\langle \mathbf{S}_i^2\rangle/\omega_s)\times$ $\times\{(1/N)\sum_{\mathbf{q}} 1/[1+\xi^2(1+\gamma(\mathbf{q}))]\}^{-1}$, where $\langle \mathbf{S}_i^2\rangle = (3/4)(1-\delta)$.

The spin correlation functions (17) in the single-particle excitation spectra (16) in MFA are defined by equations $C_1 = (1/N)\sum_{\mathbf{q}} C_{\mathbf{q}}\,\gamma(\mathbf{q}),\quad C_2 = (1/N)\sum_{\mathbf{q}} C_{\mathbf{q}}\,\gamma'(\mathbf{q})$. The static correlation function $C_{\mathbf{q}}$ can be calculated from the same model (17) as follows $C_{\mathbf{q}} = \langle \mathbf{S}_{\mathbf{q}}\mathbf{S}_{-\mathbf{q}}\rangle =$

$=C(\xi)/[1+\xi^2(1+\gamma(\mathbf{q}))]$, where the factor $C(\xi)=\chi_0(\omega_s/2)$. The doping dependence of the AF correlation length $\xi(\delta)$ at low temperature was evaluated from comparison of the correlation function C_1 with numerical results of an exact diagonalization for finite clusters [15]. It was found that $\xi=3-2$ for $\delta=0.05-0.15$, accordingly.

The electronic spectra in the normal state in the hole-doped case have been extensively studied in Ref. [10] where dispersion of single-particle excitations, spectral functions, and the Fermi surface in the normal state have been reported in the limit of strong correlations for $U_{\text{eff}}=8t$. Therefore, below we discuss the superconducting properties only within Hubbard model (1).

3.2. Equation for superconducting gap and T_c

Let us consider superconducting gap (34) and T_c at hole doping. For the linearized anomalous GF (35) the gap equation in the Matsubara frequency representation, $\omega_n=i\pi T(2n+1)$, can be written as

$$\begin{gathered}\varphi_{2,\sigma}(\mathbf{k},i\omega_n)=\frac{T}{N}\sum_{\mathbf{q}}\sum_{m}\{\,J(\mathbf{k}-\mathbf{q})+\lambda^{(-)}(\mathbf{q},\mathbf{k}-\mathbf{q}\,|\,i\omega_n-i\omega_m)\}\\ \times G_N^{22}(\mathbf{q},-i\omega_m)\,G_N^{22}(\mathbf{q},i\omega_m)\,\varphi_{2,\sigma}(\mathbf{q},i\omega_m).\end{gathered}\tag{38}$$

Here the interaction function for the spin susceptibility model (37) is given by the equation $\lambda(\mathbf{q},\mathbf{k}-\mathbf{q}\,|\,i\omega_\nu)=-|t(\mathbf{q})|^2\chi_s(\mathbf{k}-\mathbf{q})F_s(\omega_\nu)$ where $F_s(\omega_\nu)$ is defined by the function $\chi_s''(\omega)$. To calculate T_c and to find the gap function one should solve linear equation (38) in $(\mathbf{k},\omega_n)$-space for the eigenvalue and the eigenfunction. In the strong-coupling limit within the Eliashberg-type theory, the full normal-state GFs (31) and (32) calculated self-consistently taking into consideration the self-energy (33) should be used. This program has been implemented for the single-band t-J model in [11]. However, two-subband form of GFs (31) and (32) in the Hubbard model presents some complications in numerical solution which will be considered elsewhere.

Therefore, as a first step, a weak-coupling approximation (WCA) for the gap function (34) can be considered. In the WCA, function (29) in (34) is approximated by its value near the Fermi energy for $|\omega,z|\ll\mu$ as follows: $K(\omega,z\,|\,\mathbf{q},\mathbf{k}-\mathbf{q})=$ $=-|t(\mathbf{q})|^2\,\chi(\mathbf{k}-\mathbf{q})\,(1/2)\tanh(z/2T)$, where $\chi(\mathbf{q})=\operatorname{Re}\chi(\mathbf{q},\Omega=0)$ is the static susceptibility. In the WCA the self-energy contribution in normal-state GF (32) is neglected that results in the following equation for the gap function at the Fermi energy $\Delta(\mathbf{k})=\varphi_{2,\sigma}(\mathbf{k},\omega=0)$

$$\begin{gathered}\Delta(\mathbf{k})=\frac{1}{N}\sum_{\mathbf{q}}(J(\mathbf{k}-\mathbf{q})-|t(\mathbf{q})|^2\,\chi(\mathbf{k}-\mathbf{q}))\\ \times([\frac{(1-b(\mathbf{q}))^2}{2\varepsilon_2(\mathbf{q})}+\frac{b(\mathbf{q})(1-b(\mathbf{q})}{\varepsilon_1(\mathbf{q})+\varepsilon_2(\mathbf{q})}]\tanh\frac{\varepsilon_2(\mathbf{q})}{2T}\\ +[\frac{b(\mathbf{q})^2}{2\varepsilon_1(\mathbf{q})}+\frac{b(\mathbf{q})(1-b(\mathbf{q})}{\varepsilon_1(\mathbf{q})+\varepsilon_2(\mathbf{q})}]\tanh\frac{\varepsilon_1(\mathbf{q})}{2T})\,\Delta(\mathbf{q}).\end{gathered}\tag{39}$$

In this equation, only the first term $\propto[(1-b(\mathbf{q}))^2/2\varepsilon_2(\mathbf{q})]\tanh(\varepsilon_2(\mathbf{q})/2T)$ shows a divergence at the Fermi surface (FS) for $\varepsilon_2(\mathbf{q})\to 0$, while other terms with the energy $\varepsilon_1(\mathbf{q})\sim U_{\text{eff}}$ in the denominators make much smaller contribution. This suggests that for estimation of T_c one can take into consideration only contribution from the two-hole subband on the FS. A numerical solution of this reduced equation has been obtained in Ref. [8] in the limit of weak hybridization, $b(\mathbf{q}) \ll 1$. The d-wave pairing with high $T_c^{\max} \sim 200$ K was found. In the strong-coupling limit a certain reduction of $T_c^{\max}$ in comparison with WCA should be observed.

Concerning the mechanism of pairing in the Hubbard model, we can draw the following general conclusions. As follows from gap equations (38) or (39), there are two channels of pairing. The first one is mediated by inter-subband hopping and is determined by the AF exchange interaction $J(\mathbf{k}-\mathbf{q})$ which is usually considered in the RVB-type theories [1]. There are no retardation effects for the exchange pairing because of a large hopping energy $U_{\text{eff}} \gg t$ that results in pairing of all electrons in the conduction subband. The second contribution comes from the spin-fluctuation pairing $\propto \chi(\mathbf{k}-\mathbf{q})$ induced by intra-subband hopping which is only possible in a range of energies $\pm\omega_s$ near the FS, as in the BCS theory. This type of pairing is usually considered in phenomenological spin-fermion models [16]. The spin-fluctuation interaction is repulsive and can produce pairing only for an alternating-sign gap on the FS, as the d-wave gap.

To estimate both contributions, we consider the equation for the d-wave gap $\Delta(\mathbf{k}) = \Delta_0 (\cos k_x - \cos k_y) \equiv \Delta_0\, \eta(\mathbf{k})$ in the WCA in a conventional BCS form

$$1 = \int_{-\mu}^{\widetilde{W}-\mu} \frac{d\varepsilon}{2\varepsilon} \tanh\frac{\varepsilon}{2T_c} [\lambda_{ex}\, N(\varepsilon) + \theta(\omega_s - |\,\varepsilon\,|)\, \lambda_{sf}\, N(\varepsilon)]. \tag{40}$$

where $N(\varepsilon)$ is the density of electronic states and $\widetilde{W}$ is the renormalized band width of the conduction band. The effective exchange and spin-fluctuation coupling constants are given by the corresponding interactions averaged over the FS: $\lambda_{ex} = J < \eta^2(\mathbf{k}) >_{\text{FS}} \simeq J,\, \lambda_{sf} = < t^2(\mathbf{k})\eta^2(\mathbf{k}) >_{\text{FS}} /\omega_s \le t^2/\omega_s$. By solving this equation in the standard logarithmic approximation, we obtain for the exchange pairing $T_{c,ex} = \sqrt{\mu(\widetilde{W}-\mu)}\,\exp(-1/V_{ex})$, and for the spin-fluctuation pairing $T_{c,sf} = \omega_s \exp(-1/V_{sf})$ where the effective coupling constants $V_{ex} \sim J\, N(0)$ and $V_{sf} \sim \lambda_{sf}\, N(0)$. It is remarkable, that $T_{c,ex}$ is proportional to the Fermi energy μ and can be large even for a weak coupling. Taking into account both contributions, the superconducting temperature can be written as

$$T_c = \omega_s \exp(-1/\widetilde{V}_{sf}), \quad \widetilde{V}_{sf} = V_{sf} + \frac{V_{ex}}{1 - V_{ex} \ln(\mu/\omega_s)}. \tag{41}$$

Whereas the spin-fluctuation interaction for a weak coupling results in low $T_{c,sf} \sim 10$ K for $V_{sf} \sim 0.2$ and $\omega_s \sim J \sim 0.13$ eV, a large value of T_c can be obtained due to enhancement of the spin-fluctuation coupling constant $\tilde{V}_{sf}$ by the second term with a large logarithm for $\mu \gg \omega_s$.

4. Conclusions

In the present paper, we consider superconductivity for Hubbard model (1) in the strong correlation limit. By employing the Mori-type projection technique, we derived the self-consistent system of equations for the thermodynamic GF and the self-energy for two Hubbard subbands, Eqs. (22)–(25). The self-energy was calculated in the noncrossing approximation which is similar to the Migdal-Eliashberg strong-coupling approximation. It was shown that AF correlations play an important role in the renormalization of quasi-particle electronic spectra, both due to AF short-range static correlations considered in MFA, Eqs. (16), and caused by dynamic AF spin-fluctuations determining the self-energy, Eqs. (27) and (28). We have shown that AF correlations mediate the superconducting d-wave pairing as well, the AF exchange pairing within MFA, as in RVB theory [1], and the spin-fluctuation pairing as in the phenomenological spin-fermion models [16]. It is important to point out that AF correlations in the Hubbard model are induced by the kinematic interaction, which is characteristic of strongly correlated electronic systems and is absent in the fermionic models (for a discussion, see Ref. [17]). Therefore, we believe that the magnetic mechanism of superconducting pairing in the Hubbard model considered here is a relevant mechanism of high-temperature superconductivity in copper-oxide materials.

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