Exchange and spin-fluctuation superconducting pairing in cuprates

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We propose a microscopical theory of superconductivity in CuO$_2$ layer within the effective two-band Hubbard model in the strong correlation limit. By applying a 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 conventional exchange interaction occurs. Allowing for the self-energy corrections due to kinematic interaction, a spin-fluctuation $d$-wave pairing is also obtained. $T_c$ dependence on the hole concentration and $k$-dependence of the gap function are derived. The results show that the exchange interaction (which stems from the interband hopping) prevails over the kinematic interaction (which stems from the intraband hopping).

I. INTRODUCTION

Recent experiment on field-induced superconductivity in infinite layer cuprate compound CaCuO$_2$ has proved that superconducting pairing is confined to the copper-oxygen plane both for electron and hole doping. Therefore to describe the mechanism of superconducting pairing in cuprates one should study interactions in one copper-oxygen plane. As was initially pointed out by Anderson, strong electron correlations in copper 3$d$-states play the most important role in explaining antiferromagnetic (AFM) and insulating properties of the undoped plane. These correlations in the electronic liquid of doped electrons or holes could be also responsible for superconducting pairing in the plane.

Electron correlations are usually considered within the framework of the Hubbard model or the so-called $t$-$J$ model which can be derived from the Hubbard model in the limit of strong correlations. Superconducting pairing mediated by AFM spin-fluctuations in the weak correlation limit of the Hubbard model has been proved by using different approaches: by applying AFM spin-wave models within the fluctuation exchange approximation (FLEX) (see, e.g. and the references therein), a renormalization group technique (see, e.g. and the references therein). A number of phenomenological models like the nearly AFM Fermi liquid was also proposed.

In the strong correlation limit a lot of numerical work has been done though the obtained results are still controversial. For instance, a robust $d$-wave pairing was observed for the $t$-$J$ model while absence of the long-range order was reported for the original Hubbard model. Concerning analytical calculations, usually a mean-field approximation (MFA) both for the $t$-$J$ model (see, e.g.) and for the Hubbard model were employed. Self-energy corrections were considered only for the $t$-$J$ model within an involved diagram technique or by using the Mori-type projection technique for the Green functions. A numerical solution of the Dyson equation in$^2$ revealed a non Fermi-liquid behavior in the normal state, while the $d$-wave superconductivity mediated by the exchange and spin-fluctuation pairing was observed. To clear up the origin of the controversial numerical results reported for the $t$-$J$ and Hubbard models and to elucidate the pairing mechanism in cuprates a comprehensive study of the Hubbard, or more general $p$-$d$ model beyond the MFA is very important.

In the present paper, we consider a microscopical theory of superconductivity in CuO$_2$ layer within the effective two-band Hubbard model in the strong correlation limit. We have proved, by a direct calculation of anomalous correlation functions in MFA that the $d$-wave pairing in the model is mediated by the conventional AFM exchange interaction as in the $t$-$J$ model. The retardation effects in the exchange interaction, which originate from the interband hopping with a large excitation energy, are negligible that results in the pairing of all the electrons (holes) in a conduction subband and a high $T_c$ proportional to the Fermi energy. Allowing for the self-energy corrections beyond the MFA, we consider also the spin-fluctuation pairing induced by kinematic interaction in the second order. The latter, acting in a narrow energy shell of the order of a spin-fluctuation energy $\omega_s$, results in a lower $T_c$.

The paper is organized as follows. In Sec. I, the general formalism and the Dyson equation for the matrix $\text{GF}$ in Nambu notation are derived for the two-band Hubbard model. Sec. II is devoted to the discussion of the superconducting pairing within MFA. The self-energy is calculated in Sec. III within the self-consistent Born approximation. Numerical results and their discussion are provided in Sec. IV. Conclusions are presented in Sec. V.
II. GENERAL FORMALISM

A distinctive property of cuprates is the strong antiferromagnetic superexchange interaction for copper spins that reaches a record value of 1500 K for transition metal compounds. It is caused by the strong pdO hybridization $t_{pd} \simeq 1.5$ eV for the 3d-copper states and the 2p-oxygen states and the small splitting energy of their atomic levels $\Delta_{pd} \simeq 3$ eV. At the same time strong Coulomb correlations for the 3d states of copper, $U_d \simeq 8$ eV, considerably increase the energy of two-hole 3d states and the lowest energy level at hole doping appears to be a Zhang-Rice singlet. These features of the electronic spectrum in CuO$_2$ plane can be described within the framework of the p-d model Hamiltonian (1):

$$H = \sum_{\sigma} \left\{ \epsilon_d \hat{d}^+_{i\sigma} \hat{d}_{i\sigma} + \epsilon_p c^+_{i\sigma} c_{i\sigma} \right\} + \sum_{i,j,\sigma} V_{ij} \left\{ \hat{d}^+_{i\sigma} c_{j\sigma} + \text{H.c.} \right\}. \quad \text{(1)}$$

Operators $\hat{d}^+_{i\sigma}$ and $c^+_{i\sigma}$ describe the creation of one-hole $d$ and $p$ states at sites $i$ of the square lattice in the CuO$_2$ plane with the energies $\epsilon_d$ and $\epsilon_p = \epsilon_d + \Delta_{pd}$, respectively. Because of the large Coulomb correlations, only singly occupied 3d states are taken into account: $d^+_{i\sigma} = d^+_{i\sigma}(1 - n^d_{i\sigma})$. For the bonding oxygen orbitals the Wannier representation is used that results in the narrow bandwidth $\Delta_{pd} = \Delta_{pd}(1)$ and then to apply a perturbation theory for the Coulomb repulsion $U$ in the conventional Hubbard model, the effective Hubbard model (2) corresponds to the strong correlation limit due to a large ratio of $\Delta$ to the band width: $\Delta/W \simeq 2$. Therefore at half-filling the Hamiltonian (2) describes the Mott-Hubbard insulating state (see Fig.1a in Ref.2).

In the present paper we have assumed a simple version of the p-d model (3) which has only two fitting parameters, $t_{pd}$ and $\Delta_{pd}$, in Eq. (1). Starting from a more general model which takes into account finite values of the Coulomb repulsion on $d$-sites $U_d$, on $p$-sites $U_p$, and between the nearest neighbor $d$ sites $U_{pd}$, and $p$-$p$ hybridization $t_{pp}$, one arrives to the same effective Hubbard model (3) but with renormalized hopping parameters $t_{ij}^{pd}$ and charge transfer energy $\Delta$ (see, e.g., Refs.2,3).

The Hubbard operators entering (3) obey the multiplication rules: $X_{i\sigma}^{nm} X_{k\bar{\sigma}}^{kl} = \delta_{m,k} X_{i\bar{\sigma}}^{nl}$ and the completeness relation

$$X_{i\sigma}^{00} + X_{i\sigma}^{1\sigma} + X_{i\sigma}^{2\bar{\sigma}} + X_{i\sigma}^{22} = 1. \quad \text{(3)}$$

The latter rigorously preserves the constraint of no double occupancy at each lattice site $i$ by any quantum state $|in\rangle$.

To discuss the quasi-particle (QP) spectrum and superconducting pairing within the model Hamiltonian (3), we introduce the two-time anticommutator retarded 4 × 4 matrix Green function (GF) in Zubarev notation (4)

$$\hat{G}_{ij\sigma}(t - t') = \langle \langle \hat{X}_{i\sigma}(|t) | \hat{X}^\dagger_{j\bar{\sigma}}(|t')) \rangle \rangle + \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} \sum_{q} e^{i\omega(t-t')} \frac{1}{N} \sum_{\bar{\sigma}} e^{iq\cdot(\bar{\sigma}-j)} \hat{G}_{\sigma}(\mathbf{q},\omega), \quad \text{(4)}$$

for the four-component Nambu operators $\hat{X}^\dagger_{i\sigma}$

$$\hat{X}^\dagger_{i\sigma} = (X_{i2\sigma} X_{i1\sigma} X_{i2\sigma} X_{i1\sigma}), \quad \text{(5)}$$

and $\hat{X}_{i\sigma}$ obtained from (3) by Hermitian conjugation. The GF (4) can thus be written as a 2 × 2 supermatrix of normal, $\hat{G}_{ij\sigma}(\omega)$, and anomalous, $\hat{F}_{ij\sigma}(\omega)$, 2 × 2 matrix components:

$$\hat{G}_{ij\sigma}(\omega) = \begin{pmatrix} \hat{G}_{ij\sigma}(\omega) & \hat{F}_{ij\sigma}(\omega) \\ \hat{F}^\dagger_{ij\sigma}(\omega) & -\hat{G}_{ij\sigma}^{-1}(\omega) \end{pmatrix}, \quad \text{(6)}$$

where the superscript (T) denotes the operation of transposition.

To calculate the GF (4) we use the equation of motion method. Differentiation with respect to time $t$ of the
where \( \tilde{Z}_{i\sigma} = [\hat{X}_{i\sigma}, H] \) assuming that the system is in the paramagnetic state, \( \langle X_{i}^{\rho\sigma} \rangle = \langle X_{i}^{\bar{\rho}\bar{\sigma}} \rangle \), we get for the matrix \( \hat{\chi} = \{\{\tilde{X}_{i\sigma}, \tilde{X}_{j\sigma}\}\} \):

\[
\hat{\chi} = \begin{pmatrix}
\chi_2 & 0 & 0 & \chi_3 \\
0 & \chi_1 & \chi_3 & 0 \\
0 & \chi_3 & \chi_2 & 0 \\
\chi_3 & 0 & 0 & \chi_1 \\
\end{pmatrix} .
\] (8)

For the diagonal terms of the matrix we get \( \chi_2 = \langle X_{i}^{2\sigma} X_{i}^{\rho\sigma} \rangle = n/2, \chi_1 = \langle X_{i}^{0\sigma} + X_{i}^{\bar{\rho}\bar{\sigma}} \rangle = 1 - \chi_2 \) where \( n = 1 + \delta \) denotes the hole concentration. The anomalous correlation function \( \chi_3 = \langle X_{i}^{02} \rangle \) describes single-site pairing and for the \( d \)-wave symmetry it vanishes

\[
\chi_3 = \langle X_{i}^{02} \rangle = \langle c_{i\downarrow} c_{i\uparrow} \rangle = 0 .
\] (9)

Here we used the identity

\[
X_{i}^{02} = X_{i}^{0\uparrow} X_{i}^{1\downarrow} = c_{i\downarrow} c_{i\uparrow} ,
\] (10)

which results from the definitions of the Fermi annihilation operators: \( c_{i\sigma} = X_{i}^{\rho\sigma} + 2\tau X_{i}^{0\sigma} \) and the multiplication rules for the Hubbard operators, \( X_{i}^{\rho\sigma} X_{i}^{\bar{\rho}\bar{\sigma}} = 0, X_{i}^{\sigma\sigma} X_{i}^{\rho\rho} = 0, X_{i}^{0\uparrow} X_{i}^{1\downarrow} = X_{i}^{02} \).

The chemical potential \( \mu \) is calculated from the equation for the average number of holes,

\[
n = \langle N_{i} \rangle = \sum_{\sigma} \langle X_{i}^{\rho\sigma} \rangle + 2 \langle X_{i}^{2\sigma} \rangle .
\] (11)

Now by using the Mori-type projection technique we write the equation of motion for the operator \( \tilde{Z}_{i\sigma} \) in Eq. \( \ref{eq:Eq(12)} \) as a sum of a linear part and an irreducible part orthogonal to it, \( \tilde{Z}_{i\sigma}^{(ir)} \), which originates from the inelastic QP scattering:

\[
\tilde{Z}_{i\sigma} = [\hat{X}_{i\sigma}, H] = \sum_{\ell} \tilde{E}_{i\sigma} \hat{X}_{i\sigma} + \tilde{Z}_{i\sigma}^{(ir)} .
\] (12)

The orthogonality condition \( \langle \tilde{Z}_{i\sigma}^{(ir)}, \hat{X}_{j\sigma}^{\dagger} \rangle = 0 \) provides the definition of the \( s \) frequency matrix:

\[
\hat{E}_{i\sigma} = \hat{A}_{i\sigma} \tilde{\chi}^{-1} ,
\] (13)

\[
\hat{A}_{i\sigma} = \{\{\hat{X}_{i\sigma}, [\hat{X}_{j\sigma}, H], \tilde{X}_{j\sigma}^{\dagger}\}\} .
\] (14)

The frequency matrix \( \hat{A}_{i\sigma} \) defines the zero-order GF in the generalized MFA. In the \( (q, \omega) \)-representation, its expression is given by

\[
\tilde{G}_{i\sigma}^{0}(q, \omega) = \left( \omega \tilde{\tau}_0 - \hat{E}_{i\sigma}(q) \right)^{-1} \hat{\chi} ,
\] (15)

where \( \tilde{\tau}_0 \) is the \( 4 \times 4 \) unity matrix.

Differentiation of the many-particle GF \( \hat{G}_{i\sigma}(q, \omega) \) with respect to the second time \( t' \) and use of the same projection procedure as in \( \ref{eq:Eq(12)} \) result in the Dyson equation for the GF \( \hat{G}_{i\sigma}(q, \omega) \). In \( (q, \omega) \)-representation, the Dyson equation is

\[
\tilde{G}_{i\sigma}(q, \omega) = \left( \tilde{G}_{i\sigma}^{0}(q, \omega) \right)^{-1} - \tilde{\Sigma}_{i\sigma}(q, \omega) .
\] (16)

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

\[
\tilde{T}_{i\sigma}(q, \omega) = \tilde{\Sigma}_{i\sigma}(q, \omega) + \tilde{\Sigma}_{i\sigma}(q, \omega) \tilde{G}_{i\sigma}^{0}(q, \omega) \tilde{T}_{i\sigma}(q, \omega) ,
\] (17)

where \( \tilde{T}_{i\sigma}(q, \omega) = \chi^{-1} \langle \tilde{Z}_{q\sigma}^{(ir)} \mid \tilde{Z}_{q\sigma}^{(ir)} \rangle \rangle_{\omega} \chi^{-1} \) denotes the scattering matrix. From Eq. \( \ref{eq:Eq(17)} \) it follows that the self-energy operator is given by the \emph{proper} part of the scattering matrix that has no parts connected by the single-particle zero-order GF \( \tilde{G}_{i\sigma}^{0}(q, \omega) \):

\[
\tilde{\Sigma}_{i\sigma}(q, \omega) = \chi^{-1} \langle \tilde{Z}_{q\sigma}^{(ir)} \mid \tilde{Z}_{q\sigma}^{(ir)} \rangle \rangle_{\omega}^{\text{prop}} \chi^{-1} .
\] (18)

The equations \( \ref{eq:Eq(13)} \), \( \ref{eq:Eq(14)} \), and \( \ref{eq:Eq(18)} \) provide an exact representation for the single-particle GF \( \hat{G}_{i\sigma}(q, \omega) \). Its calculation, however, requires the use of some approximations for the many-particle GF in the self-energy matrix \( \tilde{\Sigma}_{i\sigma}(q, \omega) \) which describes the finite lifetime effects (inelastic scattering of electrons on spin and charge fluctuations).

### III. MEAN-FIELD APPROXIMATION

#### A. Spectrum in the normal state

Let us consider at first the QP spectrum in the generalized MFA given by the zero-order GF \( \tilde{G}_{i\sigma}^{0}(q, \omega) \). The latter is defined by the frequency matrix \( \hat{A}_{i\sigma} \) which can be readily calculated by writing down equations of motion for the Hubbard operators in Eq. \( \ref{eq:Eq(12)} \) and performing necessary commutations in the matrix \( \hat{A}_{i\sigma} \), Eq. \( \ref{eq:Eq(13)} \). As a result of these calculations, which are presented at greater length in the Appendix A, the matrix \( \hat{A}_{i\sigma} \) can be written in the form

\[
\hat{A}_{i\sigma} = \begin{pmatrix}
\tilde{\omega}_{i\sigma} & \hat{\Delta}_{i\sigma} \\
\hat{\Delta}_{i\sigma}^{\dagger} & -\tilde{\omega}_{i\sigma}^{\dagger} \\
\end{pmatrix} ,
\] (19)

where \( \tilde{\omega}_{i\sigma} \) and \( \hat{\Delta}_{i\sigma} \) are \( 2 \times 2 \) matrices. The diagonal parts of the matrix defines the normal state QP spectrum:

\[
\tilde{\omega}_{i\sigma} = \delta_{ij} \left( E_{1} + \Delta \right) \chi_{2} + a_{\sigma}^{22} a_{\bar{\sigma}}^{21} - a_{\bar{\sigma}}^{21} E_{1} \chi_{1} + a_{\sigma}^{22} \right)
\]

\[
+ (1 - \delta_{ij}) V_{ij} \left( K_{ij}^{22} - K_{ij}^{11} \right) ,
\] (20)

while the off-diagonal matrices determine the superconducting pairing:
\[ \Delta_{ij\sigma} = \delta_{ij} \left( \begin{array}{cc} b_{\sigma}^{22} & b_{\sigma}^{21} \\ -b_{\sigma}^{21} & b_{\sigma}^{11} \end{array} \right) \]

\[ + (1 - \delta_{ij})V_{ij} \left( \begin{array}{cc} L_{ij\sigma}^{22} & L_{ij\sigma}^{21} \\ -L_{ij\sigma}^{21} & L_{ij\sigma}^{11} \end{array} \right). \]  \tag{21}

In Eq. (20), the quantities \( a_{\alpha\beta} \) determine energy shifts (renormalization of the chemical potential), while the coefficients \( K_{ij\sigma}^{\alpha\beta} \) define renormalized hopping parameters. The site-independent anomalous correlation functions, \( b_{\sigma}^{22} \), \( b_{\sigma}^{21} \), \( b_{\sigma}^{11} \), and the site-dependent ones, \( L_{ij\sigma}^{22} \), \( L_{ij\sigma}^{21} \), \( L_{ij\sigma}^{11} \), in Eq. (21) determine superconducting pairing in MFA. Explicit values of the coefficients in Eq. (20) and Eq. (21) are given in the Appendix A, Eqs. (A17)–(A18).

The QP spectrum in the normal state of the single-hole Hubbard model \( \mathcal{H} \) within the MFA has been studied in detail by Plakida et al. \[ \text{Eq. (3)} \]. Therefore here we give only the results of the calculations which will be used further in discussion of superconducting pairing in the model \( \mathcal{H} \). The QP spectrum is described by the normal state components of the zero-order GF \( \tilde{G}_{\sigma}^{0}(q, \omega) \):

\[ \tilde{G}_{\sigma}^{0}(q, \omega) = \left( \begin{array}{cc} \tilde{G}_{\sigma}^{\alpha}(q, \omega) & 0 \\ 0 & -\tilde{G}_{\sigma}^{\alpha}(-q, -\omega) \end{array} \right), \]

where the \( 2 \times 2 \) matrix GF reads

\[ \tilde{G}_{\sigma}^{0}(q, \omega) = \{ \omega \tilde{\sigma} - E_{\sigma}(q) \}^{-1} \left( \begin{array}{cc} \chi_{2} & 0 \\ 0 & \chi_{1} \end{array} \right). \]  \tag{23}

The \( q \)-representation of the energy matrix is given by

\[ E_{\sigma}(q) = \left( \begin{array}{cc} \omega_{2}(q) & W_{\sigma}^{21}(q) \\ W_{\sigma}^{12}(q) & \omega_{1}(q) \end{array} \right). \]  \tag{24}

The energy spectra for the unhybridized singlet and one-hole excitations are defined by the equations

\[ \omega_{2}(q) = E_{1} + \Delta + a_{\sigma}^{22} / \chi_{2} + V_{\sigma}^{22}(q) / \chi_{2}, \]

\[ \omega_{1}(q) = E_{1} + a_{\sigma}^{22} / \chi_{1} + V_{\sigma}^{12}(q) / \chi_{1}, \]

while the hybridization interaction is given by

\[ \chi_{2} W_{\sigma}^{21} = a_{\sigma}^{21} + V_{\sigma}^{22}(q), \quad \chi_{1} W_{\sigma}^{12} = \chi_{2} W_{\sigma}^{21}. \]  \tag{26}

The effective interaction in (25), (26) has the form

\[ V_{\sigma}^{\alpha\beta}(q) = \frac{t_{pd}}{N} \sum_{k} \nu(k) K_{\sigma}^{\alpha\beta}(k - q), \]

where the Fourier transform of \( K_{ij\sigma}^{\alpha\beta} \) in Eq. (29) is

\[ \nu(k) = 2 \sum_{j \neq 0} \nu_{ij} e^{-i a_{j}} \equiv 8 \nu_{1} \gamma(q) + 8 \nu_{2} \gamma^{*}(q), \]  \tag{28}

where

\[ \gamma(q) = \frac{1}{2}(\cos q_{x} + \cos q_{y}), \quad \gamma^{*}(q) = \cos q_{x} \cos q_{y}. \]  \tag{29}

As was shown in Ref. 2, the off-diagonal matrix elements of the zero-order GF can be neglected since they give a small contribution of the order of \( t_{pd}^{2} / \Delta \) to the density of states (see Fig. 2 in Ref. 3). Therefore, the zero-order GF \( \tilde{G}_{\sigma}^{0}(q, \omega) \) can be written in the diagonal form

\[ \tilde{G}_{\sigma}^{0}(q, \omega) = \left( \begin{array}{cc} \chi_{2}/[\omega - \Omega_{2}(q)] & 0 \\ 0 & \chi_{1}/[\omega - \Omega_{1}(q)] \end{array} \right), \]  \tag{30}

where the hybridized spectra \( \Omega_{\alpha}(q) \) for singlet \((\alpha = 2)\) and for one-hole \((\alpha = 1)\) excitations are given by

\[ \Omega_{2,1}(q) = \frac{1}{2}[\omega_{2}(q) + \omega_{1}(q)] \pm \frac{1}{2}\{[\omega_{2}(q) - \omega_{1}(q)]^{2} + 4W_{\sigma}^{21}W_{\sigma}^{12}\}^{1/2}. \]  \tag{31}

In these equations and in what follows, the spin dependence of the QP energies is omitted.

To obtain a closed solution for the zero-order GF, the correlation functions entering Eq. (20) are calculated self-consistently. The energy shifts \( a_{\alpha\beta} \) depending on single-particle correlation functions are readily calculated by using the spectral representation of the GF \( \mathcal{G}^{0} \). However, the calculation of the functions \( K_{ij\sigma}^{\alpha\beta} \) depending on the density-density and spin-spin correlation function (see Eq. (A12)) requires the use of some approximations.

In Ref. 1, the Roth procedure was used which involved uncontrollable decoupling of the Hubbard operators at the same lattice site, as e.g., \( \langle X_{i}^{t2}X_{j}^{20} \rangle = \langle X_{i}^{t0}X_{i}^{t2}X_{j}^{20} \rangle \). Here in the calculation of the effective hopping parameters \( K_{ij\sigma}^{\alpha\beta} \) we apply a simple approximation by neglecting the charge-charge correlations \( N_{i}N_{j} \) at different lattice sites \( i \neq j \) (as in the Hubbard I approximation) but fully take into account the spin-spin correlations:

\[ \chi_{ij}^{c} = \frac{1}{4}(N_{i}N_{j}) + \langle S_{i}S_{j} \rangle \simeq (\chi_{2})^{2} + \langle S_{i}S_{j} \rangle \]  \tag{32}

For a spin-singlet state without long-range magnetic order, the GF \( \mathcal{G}^{0} \) and the one-hole spectrum \( \mathcal{G}^{1} \) do not depend on spin. However, the short-range AFM spin-spin correlations are very important and, as calculations in Ref. 2 have shown, the spin-spin correlation functions \( \langle S_{i}S_{j} \rangle \) in Eq. (23) bring significant contribution to the renormalization of the dispersion relation \( \mathcal{G}^{1} \). For large spin-correlations at small doping values one finds a next-nearest neighbor dispersion. With doping, by decreasing the spin correlations, the dispersion changes to the nearest-neighbor one which is conventional to the overdoped case (see Fig. 1 in Ref. 2). The corresponding Fermi surface appears to be large even for a small doping as it is shown in Sec. 3. Therefore, the present model reproduces the most important features of the electronic spectra of cuprates: insulating state of the undoped CuO2 plane and a strong reduction of the band width of single-particle excitations in the doped metallic state with the doping dependent dispersion. Concerning a non-Fermi
liquid behavior and a pseudogap formation in the underdoped region one has to study more accurately the self-energy corrections as has been done within the t-J model in Refs. [37,38].

**B. Superconducting pairing**

Let us consider the anomalous part \( \Delta_{ij\sigma} \), Eq. (21), of the frequency matrix. The site independent anomalous correlation functions \( b_i^{\alpha\beta} \), Eqs. (A13)-(A18), vanishes for the \( d_{x^2-y^2} \) pairing. It can be easily proved by considering the \( \mathbf{q} \)-dependent representation of the correlation functions, as e.g., \( \sum_{m\neq i} V_{im} \langle X_{im}^{\sigma\sigma} X_{m\sigma}^{\sigma\sigma} \rangle = \sum_{q} V(q) \langle X_{iq}^{\sigma\sigma} X_{q\sigma}^{\sigma\sigma} \rangle \). While the interaction \( V(q) \) is invariant under the permutation of the components \( q_x \) and \( q_y \) (in the tetragonal phase) the anomalous correlation function having the \( d_{x^2-y^2} \)-wave symmetry changes the sign that results in vanishing of the sum over \( q \).

To calculate the site dependent contributions \( L_{ij\alpha\beta} \), Eqs. (A10)-(A18), we have to derive an estimate of the anomalous correlation function \( \langle X_{i\alpha}^{02} N_j \rangle \). The approach followed in Refs. [37,38] for its calculation employed the Roth procedure which decouples the Hubbard operators at the same lattice site by writing the time-dependent correlation function in the form: \( \langle c_{i\downarrow}(t)c_{i\uparrow}(t')N_j(t') \rangle = \langle X_{i\downarrow}^{0i}(t)X_{i\uparrow}^{2i}(t')N_j(t') \rangle \). In view of the identity satisfied by the Hubbard operators: \( X_{ij}^{\alpha\beta} = X_{ij\alpha}^{\gamma\delta}X_{ij\gamma}^{\sigma\delta} \) for any intermediate state \( |\gamma\rangle \), the decoupling of the operators at the same lattice site is not unique and therefore unreliable (a feature already noticed in Refs. [37,38]).

Here we perform a direct calculation of the correlation function \( \langle X_{i\alpha}^{02} N_j \rangle \) without any decoupling by considering the equation for the corresponding commutator GF

\[
L_{ij}(t-t') = \langle \langle X_{i\alpha}^{02}(t) | N_j(t') \rangle \rangle.
\]

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

\[
(\omega - E_2) L_{ij}(\omega) = 2\delta_{ij} \langle X_{i\alpha}^{02} \rangle + \sum_{m\neq i} 2\sigma t_{im}^{12} \left\{ \langle X_{i\alpha}^{0\sigma} X_{m\sigma}^{0\alpha} | N_j \rangle \rangle - \langle X_{i\sigma}^{\gamma\sigma} X_{m\sigma}^{\gamma\sigma} | N_j \rangle \rangle \right\} - \frac{1}{\pi} \text{Im} \left\{ \frac{1}{\omega - E_2 + i\varepsilon} \left[ \langle X_{i\alpha}^{0\sigma} X_{m\sigma}^{0\alpha} | N_j \rangle \rangle + \langle X_{i\sigma}^{\gamma\sigma} X_{m\sigma}^{\gamma\sigma} | N_j \rangle \rangle \right] \right\}.
\]

The statistical average \( \langle X_{i\alpha}^{02} N_j \rangle \) at sites \( i \neq j \) can now be evaluated from the spectral representation theorem:

\[
\langle X_{i\alpha}^{02} N_j \rangle = \int_{-\infty}^{+\infty} \frac{d\omega}{1 - \exp(-\omega/T)} \sum_{m\neq i} 2\sigma t_{im}^{12} \left\{ \langle X_{i\alpha}^{0\sigma} X_{m\sigma}^{0\alpha} | N_j \rangle \rangle - \langle X_{i\sigma}^{\gamma\sigma} X_{m\sigma}^{\gamma\sigma} | N_j \rangle \rangle \right\} - \frac{1}{\pi} \text{Im} \left\{ \frac{1}{\omega - E_2 + i\varepsilon} \left[ \langle X_{i\alpha}^{0\sigma} X_{m\sigma}^{0\alpha} | N_j \rangle \rangle + \langle X_{i\sigma}^{\gamma\sigma} X_{m\sigma}^{\gamma\sigma} | N_j \rangle \rangle \right] \right\}.
\]

We consider below a particular case of hole doping when the Fermi level stays in the singlet subband: \( \mu \simeq \Delta \), 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 contribution from the anomalous correlation function \( \langle X_{i\alpha}^{02} N_j \rangle \rangle \) can be estimated from its equation of motion as follows:

\[
-\frac{1}{\pi} \text{Im} \left\{ \langle X_{i\alpha}^{0\sigma} X_{m\sigma}^{0\alpha} | N_j \rangle \rangle + \langle X_{i\sigma}^{\gamma\sigma} X_{m\sigma}^{\gamma\sigma} | N_j \rangle \rangle \right\} \delta_m \langle X_{i\alpha}^{0\sigma} X_{j\sigma}^{\alpha\sigma} \rangle \delta(\omega - 2E_1).
\]

Therefore it gives also an exponentially small contribution \( \exp(-2\Delta/T) \ll 1 \). The only non vanishing contribution in Eq. (34) comes from the Green function of the singlet subband:

\[
\langle X_{i\alpha}^{02} N_j \rangle \rangle \simeq -\frac{1}{\Delta} \sum_{m\neq i,\sigma} 2\sigma t_{im}^{12} \langle X_{i\sigma}^{\gamma\sigma} X_{m\sigma}^{\gamma\sigma} N_j \rangle. \tag{35}
\]

Here the retardation effect, the frequency dependence in the denominator \( 1/(\omega - E_2) \), is ignored since the interband excitation energy is much larger than the QP excitation energy in the singlet subband: \( |E_2| \simeq \Delta \gg |t_{ij}^{22}| \). The exchange interaction is usually considered in the two-site approximation, which is obtained equating \( m = j \) in Eq. (35). In this approximation, we get after summation over the spin \( \sigma \):

\[
\langle X_{i\alpha}^{02} N_j \rangle = N \sum_{\mathbf{q}} e^{i\mathbf{q}\cdot(r_{ij})} \langle \langle X_{i\alpha}^{0\sigma} X_{j\sigma}^{\alpha\sigma} \rangle \rangle = -\frac{4i}{\Delta} t_{ij}^{12} 2\sigma \langle X_{i\alpha}^{\alpha\sigma} X_{j\sigma}^{\alpha\sigma} \rangle. \tag{36}
\]

where we have used the identity for the Hubbard operators, \( X_{i\sigma}^{\alpha\sigma} N_j = 2X_{i\sigma}^{\sigma\sigma} \), and Eq. (11).

This finally allows us to write the expressions of the anomalous component \( \Delta_{ij\sigma}^{22} \) for the case of hole doping as follows:

\[
\Delta_{ij\sigma}^{22} = \frac{1}{N} \sum_{\mathbf{q}} e^{i\mathbf{q}\cdot(r_{ij})} \Delta_{ij\sigma}^{22}(\mathbf{q}) = J_{ij} \langle X_{i\alpha}^{0\sigma} X_{j\sigma}^{\alpha\sigma} \rangle. \tag{37}
\]

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 \( \Delta_{ij\sigma}^{11} \) for the case of hole doping can be neglected since its contribution to the gap equation is extremely small, of the order of \( \Delta_{ij\sigma}^{11}(\mathbf{q})/\Delta \).

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

\[
\Delta_{ij\sigma}^{11} = J_{ij} \langle X_{i\alpha}^{0\sigma} X_{j\sigma}^{\alpha\sigma} \rangle. \tag{38}
\]

We have therefore proved that in the MFA the interband anomalous correlation function is of the order of \( t_{ij}^{12}/\Delta \) and it is proportional to the statistical average of the conventional electron (hole) pairs at neighboring lattice sites in the Hubbard subband which intersects
the Fermi level. As a consequence, the anomalous contributions to the zero-order GF, Eq. (15), 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., [3][4]. In view of this conclusion, the MFA nonzero superconducting pairing reported in the frame of the conventional Hubbard model [4] can be inferred from the exchange interaction which equals to \( J_{ij} = 4t^2/U \) in this model. The exchange interaction vanishes in the limit \( U \to \infty \), a feature which explains the disappearance of the pairing at large \( U \) [4] [13].

To summarize the study of the MFA, let us write down a closed system of equations for the particular case of hole doping with the chemical potential in the singlet subband. The \( 2 \times 2 \) matrix GF for the singlet subband writes:

\[
\hat{G}^{22}_{ij,\sigma}(\omega) = \left( \begin{pmatrix} X^{\sigma_2}_i & X^{\sigma_2}_j \end{pmatrix} \right) \omega . \quad (39)
\]

By taking into account the normal part of the GF in the diagonal form, Eq. (39), and the anomalous part of the frequency matrix for the singlet subband, Eq. (37), we can write the GF (39) in the form:

\[
\hat{G}^{22(0)}_{\sigma}(q, \omega) = \chi (\omega \hat{\tau}_0 - \Omega_2(q) \hat{\tau}_3 - \phi^{22}_{\sigma}(q) \hat{\tau}_3)^{-1} , \quad (40)
\]

where \( \hat{\tau}_0, \hat{\tau}_1, \hat{\tau}_3 \) are the Pauli matrices. Here we introduced the gap function in MFA for the singlet subband \( \phi^{22}_{\sigma}(q) = \Delta^{22}_{\sigma}(q)/\chi_2 \) induced by the exchange interaction. From Eq. (40), and equation for the GF (37), we get a self-consistent BCS-type equation for the gap function in the MFA:

\[
\phi^{22}_{\sigma}(q) = \frac{1}{N} \sum_k J(q-k) \phi^{22}_{\sigma}(k) \frac{\tan \xi_2(k)}{2T} , \quad (41)
\]

where \( J(q) = 4J\gamma(q) \) is the Fourier component of the nearest neighbor exchange interaction and \( \xi_2(k) = \sqrt{\Omega_2(k)^2 + |\phi^{22}_{\sigma}(k)|^2}^{1/2} \) denotes the QP energy. 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 \( X^{\pi_1}_i, X^{\pi_0}_i \).

The obtained results for the gap equation in MFA for superconducting pairing mediated by AFM exchange interaction are identical to the MFA results for the t-J model (see, e.g., [4][13]). However, we have derived these results from the original two subband Hubbard model [13] which has allowed an understanding of the role of retardation effects in the exchange pairing. We have proved that they can be neglected due to the large interband excitation energy in comparison with the QP intraband excitation energy. We also obtained a more general, three-site representation for the anomalous correlation function [13] which can be used to study the many-particle exchange pairing.

### IV. SELF-ENERGY CORRECTIONS

#### A. Self-consistent Born approximation

To study the finite life-time effects and renormalization of the QP spectra caused by inelastic scattering one should calculate the self-energy [13] induced by many-particle excitations. A general representation for the self-energy in the \( (r, \omega) \)-representation reads

\[
\hat{\Sigma}_{ij\sigma}(\omega) = \chi^{-1} \left( \hat{M}_{ij\sigma}(\omega) - \frac{\hat{\Phi}_{ij\sigma}(\omega)}{\hat{\Phi}_{ij\sigma}(\omega) - M_{ij\sigma}^{(T)}(-\omega)} \right) \chi^{-1} , \quad (42)
\]

where the \( 2 \times 2 \) matrices \( \hat{M} \) and \( \hat{\Phi} \) denote the normal and anomalous contributions to the self-energy, respectively (see Appendix B, Eqs. (44), (45)).

Here we consider the self-consistent Born approximation (SCBA) (or the non-crossing approximation) which is proved to be quite reliable in studies of the t-J model [13]. In SCBA, the propagation of the Fermi-like excitation, \( X_1(t) \), and Bose-like excitation, \( B_1(t) \), (spin or charge - see Appendix A, Eq. [13]) in the many-particle GF in [12] are assumed to be uncorrelated. In the diagram technique SCBA is represented by a skeleton loop diagram without vertex corrections. Therefore the SCBA results from the decoupling of the corresponding operators in the many-particle time-dependent correlation functions for lattice sites \( (n \neq n' , \; 2 \neq 2') \) as follows:

\[
\langle B_{1'}(t) X_1(t) B_{2'}(t') X_2(t') \rangle \simeq \langle B_{1'}(t) B_{2'}(t') \rangle \langle X_1(t) X_2(t') \rangle \simeq \langle B_{1'}(t) B_{2'}(t') \rangle \langle X_1(t) X_2(t') \rangle \simeq \langle B_{1'}(t) B_{2'}(t') \rangle \langle X_1(t) X_2(t') \rangle . \quad (43)
\]

Using the spectral theorem, the SCBA results in the following decoupling relation for the many-particle GF:

\[
\langle B_{1'} X_1 | B_{2'} X_2 \rangle \omega \simeq \frac{1}{\pi} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \frac{d\omega_1 d\omega_2}{\omega - \omega_1 - \omega_2} \times \frac{N(\omega_1, \omega_2)}{N(\omega_1, \omega)} \Im \langle X_1 | X_2 \omega_1 \rangle \Im \langle B_{1'} | B_{2'} \rangle \omega_2 , \quad (44)
\]

where \( N(\omega_1, \omega_2) = (1/2) | \tan (\omega_1/2T) + \coth (\omega_2/2T) | \). Within this approximation we obtain a self-consistent system of equations for the self-energy [12] and single-particle GF [13]. However, to get a tractable problem, we simplify this system by using a diagonal approximation for the GF as has been assumed for the zero-order GF [12]. Consequently, keeping only the diagonal self-energy components, \( M_{M_{\alpha}}^{\alpha} \) and \( \Phi_{\alpha}^{\alpha} \) in Eq. (42), we can solve the \( 4 \times 4 \) matrix Dyson equation (10) in the form of two independent \( 2 \times 2 \) matrices for GF for the singlet and one-hole subbands. The diagonal approximation gives the lowest order contribution to the self-energy in the small hybridization parameter \( (\gamma_2^2/\Delta) \).

By taking into account the zero-order \( 2 \times 2 \) matrix GF for the singlet subband, Eq. (11), we derive the following Dyson equation for GF (39).
Here the normal, \( M_{\sigma}^{22}(q, \omega) \), and anomalous, \( \Phi_{\sigma}^{22}(q, \omega) \), parts of the self-energy for the singlet subband in the SCBA approximation can be written in the form:

\[
M_{\sigma}^{22}(q, \omega) = \frac{1}{N} \sum_{k} \int_{-\infty}^{+\infty} \mathrm{d}\omega_1 K^{(+)}(\omega, \omega_1 | k, q - k) \times \left\{ -\frac{1}{\pi} \text{Im} \left[ K_{22}^{2} G_{\sigma}^{22}(k, \omega_1) + K_{12}^{2} G_{\sigma}^{11}(k, \omega_1) \right] \right\} ,
\]

\[
\Phi_{\sigma}^{22}(q, \omega) = \frac{1}{N} \sum_{k} \int_{-\infty}^{+\infty} \mathrm{d}\omega_1 K^{(-)}(\omega, \omega_1 | k, q - k) \times \left\{ -\frac{1}{\pi} \text{Im} \left[ K_{22}^{2} F_{\sigma}^{22}(k, \omega_1) - K_{12}^{2} F_{\sigma}^{11}(k, \omega_1) \right] \right\} .
\]

The kernel of the integral equations for the self-energy is defined by the equation

\[
K^{(\pm)}(\omega, \omega_1 | k, q - k) = t_{pd}^2 |\nu(q)|^2 \times \int_{-\infty}^{+\infty} \frac{\mathrm{d}\omega_2}{\omega - \omega_1 - \omega_2} \left[ \frac{1}{\pi} \text{Im} \chi_{sc}^{(\pm)}(q - k, \omega_2) \right] ,
\]

where \( \nu(q) \) is given by Eq. (28). The spectral density of spin-charge fluctuations is defined by the corresponding dynamical susceptibilities which are given by the commutator GF

\[
\chi_{sc}^{(\pm)}(q, \omega) = \chi_{s}(q, \omega) \pm \chi_{c}(q, \omega) = \langle \{ \mathbf{S}_q \mathbf{S}_{-q} \} \rangle_\omega \pm \frac{1}{4} \langle \{ \delta N_q \delta N_{-q} \} \rangle_\omega .
\]

Analogous expression for the GF in terms of the Hubbard operators \( \lambda^{0\sigma}, \lambda^{\sigma 0} \), and the corresponding self-energy components can be written for the one-hole subband in the case of electron doping (see Appendix B, Eqs. (50)-(52)).

### B. Weak coupling approximation

Self-consistent numerical solution of the coupled system of equations for the GF (43) and the self-energy (45), (46) is rather complicated (see, e.g. calculations in Ref. [2]). To estimate the role of the kinematic interaction in superconducting pairing and its contribution to superconducting \( T_c \) beyond the MFA, we study below a simplified approach based on the weak coupling approximation (WCA). In WCA, it is assumed that the behavior of an electron liquid is dominated by the interactions around the Fermi level and therefore the interaction kernel (45) at frequencies \( (\omega, \omega_1) \) close to the Fermi surface (FS) can be factorized in the form

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

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

\[
\lambda^{(\pm)}(k, q - k) = t_{pd}^2 |\nu(q)|^2 \times \int\frac{\mathrm{d}\omega_2}{\omega_2} \left[ \frac{1}{\pi} \text{Im} \chi_{sc}^{(\pm)}(q - k, \omega_2) \right]
\]

\[
= t_{pd}^2 |\nu(q)|^2 \text{Re} \chi_{sc}^{(\pm)}(q - k, \omega_2 = 0) .
\]

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 \( \omega_1 \) in Eqs. (48) and (49) is straightforward.

For a hole doped 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 as follows

\[
\Omega_2(q) = \Omega_2(q) + \chi_{1}^{-1} M_{22}^{22}(q, \omega = \Omega_2(q)) \simeq \Delta - \mu + \epsilon_2(q) \simeq \epsilon_2(q) ,
\]

\[
\Omega_1(q) = \Omega_1(q) + \chi_{1}^{-1} M_{11}^{11}(q, \omega = \Omega_1(q)) \simeq -\mu + \epsilon_1(q) \simeq -\Delta + \epsilon_1(q) ,
\]

where the MFA energy \( \Omega_{0}(q) \) is defined by Eq. (31). The zero of the energy in the singlet band is fixed at the Fermi wave-vector \( \epsilon_2(q_F) = 0 \).

Integration over \( \omega_1 \) in (49) gives the following equation for the anomalous component of the self-energy

\[
\Phi_{\sigma}^{22}(q, \omega \simeq 0) = -K_{22}^{2} S_{2,\sigma}(q) + K_{12}^{2} S_{1,\sigma}(q) .
\]

The sum \( S_{2,\sigma}(q) \) for the singlet band at the FS is given by

\[
S_{2,\sigma}(q) = \frac{1}{N} \sum_{k} \lambda^{(-)}(k, q - k) \frac{\bar{\Phi}^{22}_{\sigma}(k)}{2\bar{\varepsilon}_{\sigma}(k)} \tanh \frac{\bar{\varepsilon}_{\sigma}(k)}{2T} ,
\]

where \( \bar{\Phi}^{22}_{\sigma}(k) = \phi^{22}_{\sigma}(k) + \Phi^{22}_{\sigma}(q, 0) \chi_{sc}^{-1} \) is an effective gap function. The integration over \( k \) is restricted here to an energy shell around the Fermi energy of the order of a characteristic energy \( \omega_s \) of the spin (charge) fluctuations defined by the susceptibility (49). The quasiparticle energy is given by

\[
\bar{\varepsilon}_{\sigma}(q) = [\bar{\Omega}_{\sigma}^{2}(q) + |\bar{\Phi}^{22}_{\sigma}(q)|^2]^{1/2} .
\]

The one-hole band lies below the FS at an energy of the order \( \Delta \gg W \). Therefore, integration over \( \omega_1 \) in Eq. (49) for the anomalous GF \( F_{\sigma}^{11}(k, \omega_1) \) can be done by neglecting for the QP excitation energy in this band...
the dispersion in Eq. [54] as well as the superconducting gap: \( F_{s}^{2}(k, \omega_{s}) \simeq \phi_{s}^{2}(k)/(\omega_{s}^{2} - \Delta^{2}) \).

This results in the estimate

\[
S_{1,s}(q) = \frac{1}{N} \sum_{k} t_{pd}[\nu(k)]^{2} \phi_{s}^{2}(k) L_{sc}^{-1}(k - q). \quad (57)
\]

In this equation, the spin-charge static correlation function \( L_{sc}^{-1}(q) = (S_{q}S_{-q}) - \frac{1}{2} \delta N_{d} \delta N_{e} \) resulted from the integration over \( \omega_{2} \) in Eq. [55]. A simple estimate shows that the sum \( S_{1,s}(q) \) gives a small contribution, of the order \( (t_{eff}/\Delta)^{2} \phi_{s}^{2}(k) \simeq 10^{-2} \phi_{s}^{2}(k) \), and it can be neglected in Eq. [54].

By taking into account the contribution due to the exchange interaction in MFA, Eq. [51], the equation for the effective gap in the singlet subband can be written as follows:

\[
\bar{\phi}_{s}^{22}(q) = \frac{1}{N} \sum_{k} \left[ J(k - q) - K_{22} \chi_{s}(k, q - k) \right] \times \frac{\bar{\phi}_{s}^{22}(k)}{2 \omega_{s}(k)} \tanh \frac{\tilde{\varepsilon}_{2}(k)}{2T}. \quad (58)
\]

In this equation integration over \( k \) for the exchange interaction is performed without any restriction on the QP energy, while for the spin-fluctuation contribution, \( \chi_{s}(k, q - k) \), the energy of the pairing quasi-particles is confined to a narrow energy shell of the order of \( \omega_{s} \) close to the FS as pointed out in Eq. [53].

Similar considerations hold true for an electron doped system, \( n = 1 + \delta \leq 1 \) when \( \mu \simeq 0 \) in [53]. In that case, the significant WCA equation involves the gap \( \bar{\phi}_{s}^{22}(q) \) and critical \( T_{c} \) defined by the corresponding equation analogous to Eq. [58].

Thus, we have proved that in the strong correlation limit of the effective Hubbard model [2], the equations of the gap functions of the two subbands: singlet and one-hole, can be solved independently since the self-energy corrections (both the normal and anomalous components) from the another subband give a vanishingly small contribution due to the large interband gap \( \Delta \gg W \).

V. NUMERICAL RESULTS AND DISCUSSION

We start with an analytical estimation of the superconducting \( T_{c} \) mediated by the exchange interaction and spin fluctuations in the gap equation [58] for a hole doped case. The charge-charge fluctuations contribution is small due to their large energy as compared to the spin-spin fluctuations and they are neglected. Therefore the effective interaction mediated by spin fluctuations in Eq. [51] can be written in the form

\[
\lambda_{s}(k, q - k) = t_{pd}^{2}|\nu(k)|^{2} \chi_{s}(q - k), \quad (59)
\]

where \( \chi_{s}(q - k) \) is the static spin susceptibility. It can be evaluated from a dynamical spin susceptibility suggested in numerical studies[24] as follows:

\[
\chi_{s}(q) \simeq \frac{1}{\omega_{s}} \langle S_{q}S_{-q} \rangle = \frac{\chi_{0}(q)}{1 + \xi^{2}[1 + \gamma(q)]}, \quad (60)
\]

There are two fitting parameters in the model: a short-range AFM correlation length \( \xi \) of the order of a few lattice spacing and a cut-off energy of spin-fluctuations \( \omega_{s} \) of the order of the exchange energy \( J \). The spin susceptibility \( \bar{\phi}_{s}^{22}(q) \) has a maximum value \( \chi_{0}(q) \) at the AFM wave vector \( Q = (\pi, \pi) \) when \( 1 + \gamma(Q) = 0 \). Its value is fixed by the normalization condition for \( n = 1 + \delta \geq 1: \)

\[
\frac{1}{N} \sum_{q} (S_{q}S_{-q}) = \frac{3}{4}(1 - \delta), \quad (61)
\]

which gives \( \chi_{0}(q) \simeq (3(1 - \delta)/(4 \omega_{s}C(q))) \) where \( C(q) \simeq (1/N) \sum_{q} [1 + \xi^{2}[1 + \gamma(q)]^{-1} \). At large \( \xi \), \( \chi_{0}(q) \sim \xi^{2}/\ln \xi \).

For an analytical estimation of superconducting \( T_{c} \) we consider the linearized Eq. [54] where for the gap we assume the \( d_{x^{2}-y^{2}} \)-wave symmetry in the conventional form:

\[
\bar{\phi}_{s}^{22}(q) = \phi_{s}^{22}(\cos qx - \cos qy) = \phi_{s}^{22} \eta(q). \quad (62)
\]

Then integrating over \( q \) both sides of Eq. [58] multiplied by \( \eta(q) \) we get the following equation for \( T_{c} \):

\[
1 = \frac{1}{N} \sum_{k} \frac{1}{2 \Omega_{2}(k)} \tanh \frac{\Omega_{2}(k)}{2T_{c}} \times \left[ J \eta(k)^{2} + \lambda_{s}(4\gamma(k))^{2} \eta(k)^{2} \right]. \quad (63)
\]

For the exchange interaction \( J(q - k) = 4J_{q}(q - k) \) integration over \( q \) gives \( (4/N) \sum_{q} \gamma(k - q) \eta(q) = J_{q}(k) \). In \( q \)-integration of the static spin susceptibility in Eq. [58] we have taken into account that it is positive and shows a strong peak at the AFM wave-vector \( q - k = Q = (\pi, \pi) \). Therefore the sum over \( q \) was evaluated at this wave vector: \( (1/N) \sum_{q} \gamma(k - q) \eta(q) \simeq -\eta(k) \sum_{q} \chi_{s}(q') = -\eta(k) 3(1 - \delta)/4\omega_{s} \). The effective coupling constant for spin-fluctuation pairing in Eq. [63] is given by \( \lambda_{s} = (K_{22} t_{pd}^{2} 2\nu_{l})^{2} 3(1 - \delta)/4\omega_{s} \simeq t_{eff}^{2}/\omega_{s} \).

Now we can perform integration over the QP energy \( \Omega_{2}(k) \) in Eq. [63] by introducing an effective density of electronic states (DOS) for two interactions:

\[
N_{d}(\varepsilon) = \frac{1}{N} \sum_{k} \eta(k)^{2} \delta(\varepsilon - \Omega_{2}(k)), \quad (64)
\]

\[
N_{s}(\varepsilon) = \frac{1}{N} \sum_{k} \eta(k)^{2}(4\gamma(k))^{2} \delta(\varepsilon - \Omega_{2}(k)). \quad (65)
\]

They are normalized to unity since \( (1/N) \sum_{k} \eta(k)^{2} = 1 \) and \( (1/N) \sum_{k} \eta(k)^{2}(4\gamma(k))^{2} = 1 \). The resulting equation for \( T_{c} \) takes the form:

\[
1 \simeq \int_{-\mu}^{W} f(\varepsilon) \frac{d\varepsilon}{2\varepsilon} \tanh \frac{\varepsilon}{2T_{c}} \times [JN_{d}(\varepsilon) + \theta(\omega_{s} - |\varepsilon|)\lambda_{s}N_{s}(\varepsilon)], \quad (66)
\]
and having weaker coupling should be lower than $J \approx J_N (\pi, 0)$ points, while for the spin-fluctuation interaction the corresponding DOS is strongly suppressed since the kinematic interaction which is proportional to $\nu (k)$ vanishes along the lines $|k_x| + |k_y| = \pi$. The effect of vanishing of spin-fluctuation pairing close to the AFM Brillouin zone, $|k_x| + |k_y| = \pi$, was first mentioned by Schrieffer in his remarks concerning the model of nearly AFM Fermi liquid.

These specific properties of interactions result in a lower $T_c$ mediated by spin-fluctuations in comparison with the exchange interaction though the coupling constant are comparable: $J \simeq 0.15 \text{ eV}$, while $\lambda_s \simeq t_{c,ff}^2/\omega_s \simeq 0.27 \text{ eV} \text{ for } t_{c,ff} \simeq 0.2 \text{ eV}$ and $\omega_s \simeq 0.15 \text{ eV}$. To demonstrate this we solve Eq. (60) by applying the conventional logarithmic approximation since $T_c \ll \omega_s \ll \mu$. Then we get the following estimate for $T_c$ mediated by the exchange interaction

$$T_c^{se} \simeq 1.14 \sqrt{\mu (W - \mu)} \exp (-1/J N_d (\delta)),$$

where $N_d (\delta)$ is an average DOS for a hole concentration $\delta$. The superconducting $T_c^{se}$ peaks at an optimal doping for the chemical potential $\mu = W/2$ and being proportional to a large electronic energy $\mu = EF$ even for a weak coupling reaches a high value. For instance, by assuming the model parameters: $E_F = \bar{W}/2 \simeq 0.35 \text{ eV}$, $J \simeq 0.15 \text{ eV}$, and $N_d (\delta) \simeq 2$ (eV·spin)$^{-1}$, we get $J N (\delta) \simeq 0.3$ and $T_c \simeq 170 \text{ K}$.

For the spin-fluctuation pairing we obtain the BCS-like formula

$$T_c^{sf} \simeq 1.14 \omega_s \exp (-1/\lambda_s N_{sf} (0)),$$

where $N_{sf} (0)$ is DOS for the FS. For a large FS, close to the lines $|k_x| + |k_y| = \pi$, it is rather small as pointed out above that results in a weak effective coupling. Therefore $T_c^{sf}$, being proportional to $\omega_s \ll \mu$, and having weaker coupling should be lower than $T_c^{se}$, Eq. (65). It should be stressed that in comparison with phenomenological models for spin-fluctuation pairing, as e.g. in Ref.11, the coupling constant $\lambda_s N_{sf} (0)$ in Eq. (65) is defined by the original microscopic parameters of the Hubbard model. For a conventional Hubbard model with only one hopping integral $t_{ij}$ we will have the electron-hole symmetry and a same $T_c$. In the reduced $p-d$ model (2), the bandwidth for the singlet subband (proportional to $t_{ij}^2$) and the one-hole subband (proportional to $t_{ij}^1$) and the corresponding coupling constants are different that results in different $T_c(\delta)$ curves as observed in experiment.

A substantial proof of the analytical results given above is provided by a numerical study of the original gap equation using a direct summation in $k$-space. The numerical solution of the gap equation was performed under the condition of no double occupation at each lattice site $i$ by a quantum state $|in\rangle$ in the upper, $n = 2$, or lower, $n = \sigma$, Hubbard subbands:

$$\langle X^\sigma (k) X^{\sigma^*} (k) \rangle = \langle X^\sigma (k) X^{\sigma^*} (k) \rangle = 0,$$

which automatically follows from the Hubbard operator multiplication rules. The condition is satisfied by the order parameter with $d_{x^2-y^2}$ symmetry for a square lattice because the anomalous correlation functions $\langle X^k_{x} X^{x*}_{-k} \rangle$ or $\langle X^k_{y} X^{y*}_{-k} \rangle$ having the $d_{x^2-y^2}$-wave symmetry change the sign under the permutation of the components $k_x$ and $k_y$ that results in vanishing of the sum over $k$ in the equation: $\langle X^{20} (k) X^{20^*} (k) \rangle = (1/N) \sum_{k} \langle X^{20} (k) X^{20^*} (k) \rangle = 0$.

The discretization of the Fredholm integral equation results in an eigenvalue problem for the gap equation (58) resulting in an eigenvalue problem for the gap function $\bar{\Phi}_\sigma (q)$ of the singlet subband. The temperature at which the largest eigenvalue equals one, while the corresponding eigenvector shows $d_{x^2-y^2}$ 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: $\Delta_{pd} = 2t_{pd} = 3 \text{ eV}$, $t_{c,ff} \simeq K_{22} 2m_\perp \simeq 0.14 t_{pd} \simeq 0.2 \text{ eV}$. For the exchange interaction, we assumed the parameter $J = 0.4 t_{c,ff}$, usually considered in the $t-J$ model. In the model for the static spin susceptibility $\bar{\xi} (q)$ the antiferromagnetic correlation length was equated to the typical value $\xi = 3$ which was kept independent of $\delta$ and for the cut-off frequency we took $\omega_s = 0.15 \text{ eV}$.

Fig. 1 shows the dependence of the critical temperature $T_c$ (in $t_{c,ff}$ units) on the doping parameter $\delta$. 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. (68). The maximum values of $T_c$ are quite high in all cases. They vary from $\Delta_{p} = 0.12 t_{c,ff} \simeq 270 \text{ K}$ at optimum doping $\delta_{opt} \simeq 0.13$ in the highest curve $T_c^{max} \simeq 0.4 t_{c,ff} \simeq 90 \text{ K}$ at $\delta_{opt} \simeq 0.07$ in the lowest curve. There is a reasonable agreement of these values with the crude analytical estimates (67), (68). It is important to note that the WCA results overestimate $T_c$ because of the neglect of the inelastic scattering which strongly suppresses $T_c$, as was proved for the $t-J$ model.
superconducting state with $d_T$ in Eq.(58) and the subsequent numerical solution at the lines. This dependence is much more complicated than with a $q_\delta$ doping ($\delta \rightarrow 0$), the BZ, (0 $\rightarrow$ $\pi/a$ units), at optimum value $\delta_{opt}$, as shown in Fig. 2 in Ref. [2] for the Hubbard model (2). At doping values $\delta \rightarrow 0$, the superconducting $T_c$ vanishes. However, at low doping a phase transition to AFM state should occur and therefore we do not show $T_c(\delta)$ for $\delta \rightarrow 0$. Moreover, at low doping a pseudogap formation should be taken into account that further suppresses $T_c$.

Further insight is obtained from the analysis of the $k$-dependence of the gap $\Phi^{22}(k)$ inside the BZ at different temperatures. In Fig. 2 a typical wave-vector dependence of the gap is shown in the first quadrant of the BZ, ($0 \leq k_x$, $k_y \leq 1$, in $\pi/a$ units), at optimum doping ($\delta = 0.13$) at three temperatures, $T = 0$ (a), $T = 0.5T_c$ (b) and $T = 0.9T_c$ (c). The occurrence of a superconducting state with $d_{x^2-y^2}$ symmetry is observed, with a $q$-dependence pattern of the gap shown by isolines. This dependence is much more complicated than that depicted by the simple analytical model (2).

Consideration of the kinematic interaction term alone in Eq.(58) and the subsequent numerical solution at the specific optimum doping value $\delta = 0.07$, resulted in gap maxima inside the BZ, while inclusion of the exchange interaction as well and numerical solution at the higher optimum doping value $\delta = 0.13$ resulted in the shift of the maxima towards the ($\pi$,0)-type points of the BZ, which are close to the large FS, as shown in Fig. 4. The particular behavior of the spin-fluctuation pairing is explained by vanishing of the kinematic interaction along the lines $|k_x| + |k_y| = \pi$, close to the large FS, as discussed above. These results show that the inclusion of the exchange term is essential for the achievement of experimentally observed in cuprates wave-vector dependence of the gap and an optimum doping values. An additional experimental evidence for AFM exchange pairing mechanism in cuprates comes from the $T_c$ dependence on the lattice constants or an external pressure. While in electron-phonon superconductors $T_c$ decreases with an increasing applied pressure, in cuprates $T_c$ (at optimum doping) increases with pressure [3]. As was shown recently, the AFM exchange pairing model for $T_c$, (67) describes quite well the experimentally observed $T_c$ dependence on the lattice constants in the CuO$_2$-plane in mercury cuprates.

Therefore, we may conclude that 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 [3]. However, the super-
conducting exchange pairing in the t-J model is realized already in the simplest MFA for the nearest neighbor particles, while in the Hubbard model a more complicated three-particle anomalous correlation functions, Eq. (33), are induced by a dynamical second order interband hopping responsible for the exchange interaction. This observation may explain why numerical simulations for the t-J model usually predict a much stronger pairing tendency than for the original Hubbard model since in the latter more complicated dynamical processes should be accounted for.

VI. CONCLUSIONS

A microscopical theory of the superconducting pairing has been proposed within the reduced two-band p-d Hubbard model with two microscopical parameters only, the p-d hybridization parameter $t_{pd}$ and the charge-transfer gap $\Delta_{pt}$. By applying the projection technique for the two-time GF in terms of the Hubbard operators, one obtains the Dyson equation for the $4 \times 4$ matrix GF (16) with the corresponding matrix self-energy (18).

In the zero-order approximation for GF, Eq. (20), we have proved that the $d$-wave superconducting pairing of conventional hole (electron) pairs in one Hubbard subband occurs that is mediated by the interband hopping as in the $t$-$J$ model. Contrary to Refs. [24]-[27] the anomalous correlation function in MFA $\langle N_i^\sigma N_j^\sigma \rangle = \langle c_i^\dagger c_j^\sigma N_j^\sigma \rangle$ was calculated without any decoupling approximation (see Sec. IV). We have also proved that retardation effects in the exchange interaction are negligible that results in pairing of all electrons (holes) in the conduction band and a high-$T_c$ proportional to the Fermi energy, Eq. (61).

Spin-fluctuation pairing was studied in the second order of the intraband hopping within the self-consistent Born approximation for the self-energy (17). The observed spin-fluctuation $d$-wave pairing in the Hubbard model is mediated by the kinematic interaction which vanishes inside the BZ along the lines $|k_x| + |k_y| = \pi$ and produces pairing only in a narrow energy shell of the order of spin-fluctuation energy close to the FS: $\omega_s \ll E_F$. These specific properties of the interaction results in a lower $T_c$ mediated by spin-fluctuations, Eq. (68), in comparison with the exchange interaction, Eq. (58). Numerical solution of the gap equation (58) confirms the analytical estimations for the superconducting $T_c$ and reproduces experimentally observed $T_c(\delta)$ dependence with a maximum at the optimum doping $\delta_{opt} \approx 0.13$, Fig. 4. The $d$-wave symmetry of the gap function with a complicated $k$- dependence, Fig. 5 is also proved by the numerical solution.

It is to be stressed that, within the Hubbard model in the limit of strong correlations, the electron-electron coupling induced by the exchange and kinematic interactions are caused by the non-fermionic commutation relations for the Hubbard operators, and therefore no additional fitting parameters are needed to accommodate that interactions. These mechanisms of superconducting pairing are absent in the fermionic models as was pointed out by Anderson. However, they are different: while the AFM exchange pairing originates in the lowering of kinetic energy of electron (hole) pairs caused by the interband hopping as suggested by Anderson, the spin-fluctuation pairing is of the conventional nature: the pairing is due to attraction in the $d$-wave channel caused by the spin-fluctuation exchange.

The weak point of the argument is the derivation of the reported results in the weak coupling approximation for the superconducting equations. To substantiate the present results, more rigorous self-consistent numerical solution of the strong coupling Dyson equations in the $(q, \omega)$-space, as done for the $t$-$J$ model, should be elaborated. In this connection we can mention papers [24]-[27] where superconducting pairing in the Hubbard model was investigated within the non-crossing approximation for the self-energy in the 4-cluster model in the dynamical mean field theory.

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APPENDIX A: FREQUENCY MATRIX

To calculate the frequency matrix (13) one needs to consider the equations of motion of the Hubbard operators:

$$Z_{i}^{\sigma^{2}} = \left[ X_{i}^{\sigma^{2}}, H \right] = (E_i + \Delta)X_{i}^{\sigma^{2}}$$
$$+ \sum_{l \neq i, \sigma} \left( t_{il}^{22} B_{i \sigma \sigma}^{22} X_{l}^{\sigma^{2}} - 2t_{il}^{21} B_{i \sigma \sigma}^{21} X_{l}^{\sigma^{2}} \right)$$
$$- \sum_{l \neq i} X_{i}^{\sigma^{0}} \left( t_{il}^{11} X_{l}^{\sigma^{0}} + 2\sigma t_{il}^{21} X_{l}^{\sigma^{5}} \right), \quad (A1)$$

$$Z_{i}^{\sigma^{0}} = \left[ X_{i}^{\sigma^{0}}, H \right] = E_{i} X_{i}^{\sigma^{0}}$$
$$+ \sum_{l \neq i, \sigma} \left( t_{il}^{21} B_{i \sigma \sigma}^{21} X_{l}^{\sigma^{0}} - 2\sigma t_{il}^{12} B_{i \sigma \sigma}^{12} X_{l}^{\sigma^{2}} \right)$$
$$- \sum_{l \neq i} X_{i}^{\sigma^{2}} \left( t_{il}^{22} X_{l}^{\sigma^{2}} + 2\sigma t_{il}^{12} X_{l}^{\sigma^{0}} \right), \quad (A2)$$

$$Z_{i}^{2\sigma} = - (Z_{i}^{\sigma^{2}})^{\dagger}, \quad Z_{i}^{\sigma^{0}} = - (Z_{i}^{\sigma^{0}})^{\dagger}. \quad (A3)$$
Here, $B^{i\sigma\sigma'}_\alpha$ are Bose-like operators describing the number (charge) and spin fluctuations:

$$B^{22}_{i\sigma\sigma'} = (X^{22}_i + X^{22}_i \delta_{\sigma\sigma})\delta_{\sigma\sigma'} + X^{22}_i \delta_{\sigma\sigma'},$$

$$B^{21}_{i\sigma\sigma'} = \left( \frac{1}{2} N_i + S^i_\sigma \right) \delta_{\sigma\sigma'} + S^i_\sigma \delta_{\sigma\sigma'},$$

$$B^{11}_{i\sigma\sigma'} = \delta_{\sigma\sigma'} - B^{21}_{i\sigma\sigma'},$$

where we have used the completeness relation (3), and the definition of the number operator $N_i$, Eq. (11) and the spin operators $S^i_\sigma = \sum_{i\sigma} X^{i\sigma}_\sigma$, $S^i_\sigma = \bar{X}^{i\sigma}_\sigma$. Performing necessary commutations of the operators $Z^{\sigma\sigma}_i$ and $Z^{\sigma\sigma}_i$ in the matrix $A_{ij\sigma}$, Eq. (14), we get for the quantities $a^{\sigma\beta}_\alpha$ in Eq. (20) the following equations:

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

$$a^{2\sigma}_\sigma = -\sum_{m \neq i} V_{im} \left( K_{22} \left( X^{20}_i X^{20}_m \right) + K_{11} \left( X^{20}_m X^{20}_i \right) \right),$$

$$-2\sigma \sum_{m \neq i} V_{im} K_{12} \left( \left( X^{20}_i X^{20}_m \right) - \left( X^{20}_m X^{20}_i \right) \right).$$

For the renormalized hopping parameters $K^{\sigma\beta}_{ij\sigma}$ in the matrix (21) analogous calculations give the results:

$$K^{22}_{ij\sigma} = K_{22} \chi^{CS}_{ij\sigma} - K_{11} \left( X^{20}_i X^{20}_j \right),$$

$$K^{11}_{ij\sigma} = K_{11} \left( \chi^{CS}_{ij\sigma} + 1 - n \right) - K_{22} \left( X^{20}_i X^{20}_j \right),$$

$$K^{21}_{ij\sigma} = 2\sigma K_{12} \left( \chi^{CS}_{ij\sigma} - \frac{1}{2} n \right),$$

where $\chi^{CS}_{ij\sigma}$ stands for the static charge and spin correlation functions:

$$\chi^{CS}_{ij\sigma} = \frac{1}{4} \langle N_i N_j \rangle + \langle S_i S_j \rangle.$$ (A12)

In Eq. (21), the site independent anomalous correlation functions are given respectively by:

$$b^{22}_{\sigma} = \sum_{m \neq i} V_{im} \left( K_{22} \left( X^{20}_i X^{20}_m \right) - X^{20}_m X^{20}_i \right),$$

$$-2\sigma K_{12} \left( \left( X^{20}_i X^{20}_m \right) + X^{20}_m X^{20}_i \right),$$

$$b^{11}_{\sigma} = \sum_{m \neq i} V_{im} \left( K_{11} \left( X^{20}_i X^{20}_m \right) - X^{20}_m X^{20}_i \right),$$

$$-2\sigma K_{12} \left( \left( X^{20}_i X^{20}_m \right) + X^{20}_m X^{20}_i \right),$$

$$b^{21}_{\sigma} = \sum_{m \neq i} V_{im} \left( K_{22} \left( X^{20}_i X^{20}_m \right) + X^{20}_m X^{20}_i \right),$$

$$-2\sigma K_{12} \left( \left( X^{20}_i X^{20}_m \right) - X^{20}_m X^{20}_i \right).$$

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

$$L^{22}_{ij\sigma} = -2\sigma K_{21} \langle X^{02}_{i} N_{j} \rangle,$$ (A16)

$$L^{11}_{ij\sigma} = -2\sigma K_{21} \langle (2 - N_{j}) X^{02}_{i} \rangle,$$ (A17)

$$L^{11}_{ij\sigma} = \frac{1}{2} \left( K_{22} \langle X^{02}_{i} N_{j} \rangle - K_{11} \langle (2 - N_{j}) X^{02}_{i} \rangle \right).$$ (A18)

According to Eq. (40), the anomalous correlation functions describe the pairing at one lattice site but in different subbands: $\langle X^{02}_{i} N_{j} \rangle = \langle X^{01}_{i} X^{12}_{i} \rangle = \langle \bar{c}_{i\downarrow} c_{i\uparrow} N_{j} \rangle$.

**APPENDIX B: SELF-ENERGY**

The starting point for the calculation of self-energy corrections is the $K$, $t'$-representation of the self-energy [13]:

$$\tilde{\Sigma}_{ij\sigma}(t - t') = \tilde{\chi}^{-1} \langle \tilde{Z}^{(ir)}_{ij\sigma}(t) | \tilde{Z}^{(ir)\dagger}(t') \rangle \langle \text{prop} \rangle \tilde{\chi}^{-1}. \tag{B1}$$

The operators $Z^{(ir)}$ are obtained from Eqs. (A1)-(A3) according to definition, Eq. (12). Neglecting the terms which contain $X^{02}$ operators, whose contribution to the low energy dynamics of the system is assumed to be small (since it involves large charge fluctuations), we get:

$$Z^{(ir)}_{i,ij\sigma} = \sum_{l \neq i,\sigma'} \left( t^{22}_{il} \delta B^{22}_{i\sigma\sigma'} X^{l2}_i - 2\sigma t^{22}_{il} \delta B^{21}_{i\sigma\sigma'} X^{i2}_i \right), \tag{B2}$$

$$Z^{(ir)}_{i,ij\sigma} = \sum_{l \neq i,\sigma'} \left( t^{11}_{il} \delta B^{11}_{i\sigma\sigma'} X^{i0}_l - 2\sigma t^{12}_{il} \delta B^{12}_{i\sigma\sigma'} X^{i2}_l \right). \tag{B3}$$

Here, $\delta B^{\alpha\beta}_{i\sigma\sigma'} = B^{\alpha\beta}_{i\sigma\sigma'} - (B^{\alpha\beta}_{i\sigma\sigma'})^*$ are Bose-like operators describing charge and spin fluctuations as follows from Eqs. (A4)-(A6).

The many-particle GF in Eq. (B1), associated to the irreducible operators, Eqs. (B2), (B3), give the following $2 \times 2$ matrices $\tilde{M}$ and $\Phi$ for the normal and anomalous contributions to the self-energy, respectively:

$$\tilde{M}_{ij\sigma}(\omega) = \begin{pmatrix} M^{22}_{ij\sigma}(\omega) & M^{21}_{ij\sigma}(\omega) \\ M^{12}_{ij\sigma}(\omega) & M^{11}_{ij\sigma}(\omega) \end{pmatrix}$$

$$\Phi_{ij\sigma}(\omega) = \begin{pmatrix} \Phi^{22}_{ij\sigma}(\omega) & \Phi^{21}_{ij\sigma}(\omega) \\ \Phi^{12}_{ij\sigma}(\omega) & \Phi^{11}_{ij\sigma}(\omega) \end{pmatrix}$$

In the diagonal approximations for the GF the self-energy matrix elements $\tilde{M}_{ij\sigma}(\omega)$ (B4) and $\Phi_{ij\sigma}(\omega)$ (B5) within the SCBA (44) in the $(q, \omega)$-representation are given by the equations:

$$\tilde{M}_{\sigma}(q, \omega) = \frac{1}{N} \sum_{k} \int_{-\infty}^{+\infty} d\omega_{1} K^{(+)}(\omega, \omega_{1}|k, \omega_{1})$$

$$\Phi_{\sigma}(q, \omega) = \frac{1}{N} \sum_{k} \int_{-\infty}^{+\infty} d\omega_{1} K^{(+)}(\omega, \omega_{1}|k, \omega_{1})$$
The diagonal matrix elements \( M^{22}(\mathbf{q}, \omega) \), \( M^{11}(\mathbf{q}, \omega) \), for the singlet subband are given by Eqs. (46), (47), while for the one-hole subband, \( M^{12}(\mathbf{q}, \omega), \hat{\Phi}_{12}(\mathbf{q}, \omega) \), can be easily obtained from the matrices (B6), (B7).

\[
\hat{\Phi}_{12}(\mathbf{q}, \omega) = \frac{1}{N} \sum_{\mathbf{k}} \int_{-\infty}^{+\infty} \, d\omega_1 K^{(-)}(\omega, \omega_1 | \mathbf{k}, \mathbf{q} - \mathbf{k})
\]

\[
\left\{ -\frac{1}{\pi} \text{Im} \left[ \hat{P}^{(+) \dagger}_2 G^{22}_\sigma(\mathbf{k}, \omega_1) + \hat{P}^{(+) \dagger}_1 G^{11}_\sigma(\mathbf{k}, \omega_1) \right] \right\}, \quad (B6)
\]

\[
\left\{ -\frac{1}{\pi} \text{Im} \left[ \hat{P}^{(-) \dagger}_2 F^{22}_\sigma(\mathbf{k}, \omega_1) - \hat{P}^{(-) \dagger}_1 F^{11}_\sigma(\mathbf{k}, \omega_1) \right] \right\}, \quad (B7)
\]

where

\[
\hat{P}^{(+)}_2 = \left( \begin{array}{cc} K_{22}^2 & \pm 2\sigma K_{21} K_{22} \\ 2\sigma K_{21} K_{22} & \pm K_{21}^2 \end{array} \right), \quad (B8)
\]

\[
\hat{P}^{(+)}_1 = \left( \begin{array}{cc} K_{21}^2 & \pm 2\sigma K_{21} K_{11} \\ 2\sigma K_{21} K_{11} & \pm K_{11}^2 \end{array} \right). \quad (B9)
\]

The diagonal matrix elements \( M^{22}(\mathbf{q}, \omega) \), \( M^{11}(\mathbf{q}, \omega) \), can be easily obtained from the matrices (B6), (B7).

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