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Spin-fluctuation superconductivity in the Hubbard model

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The theory of the superconductivity mediated by kinematic and exchange interactions in $t-J$ and two-band Hubbard models in a paramagnetic state is formulated. The Dyson equations for the matrix Green functions in terms of the Hubbard operators are obtained in the non-crossing approximation. To calculate superconducting T_c a numerical solution of self-consistent Eliashberg equations is proposed.

Key words: *superconductivity, strong electron correlations, Hubbard model, $t-J$ model, spin fluctuations*

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1. Introduction

Since the discovery of high temperature superconductivity in cuprates it has been believed by many researchers that an electronic mechanism could be responsible for high values of T_c. Recent experimental evidences of a d-wave superconducting pairing in high-T_c cuprates strongly support this idea (see, for example, [1,2]). At present various phenomenological models for the spin-fluctuation pairing mechanism are known (for reference see, e.g., [2,3]). Numerical finite cluster calculations also suggest a d-wave superconducting instability for models with strong electron correlations [4].

Anderson [5] was the first who stressed the importance of strong electron correlations in copper oxides and proposed to take them into account within the framework of a one-band Hubbard model:

$$H = -t \sum_{\langle ij \rangle \sigma} (a^{+}_{i\sigma} a_{j\sigma} + \mathrm{H.}c.) + U \sum_{i} n_{i\uparrow} n_{i\downarrow}, \tag{1}$$

where t is an effective transfer integral for the nearest neighbour sites, $\langle ij \rangle$, and U is the Coulomb single-site energy. He also considered the so-called $t-J$ model which results from the Hubbard model (1) in the strong coupling limit, $U \gg t$, when only singly occupied sites are taken into account, since a doubly occupied site needs a large additional energy U:

$$H_{t-J} = -t \sum_{\langle ij\rangle,\sigma} (\tilde{a}^{+}_{i\sigma}\tilde{a}_{j\sigma} + \mathrm{H}.c.) + J\sum_{\langle ij\rangle}(\boldsymbol{S}_i\boldsymbol{S}_j - \frac{1}{4}n_i n_j). \tag{2}$$

Here electron operators $\tilde{a}^{+}_{i\sigma} = a^{+}_{i\sigma}(1 - n_{i-\sigma})$ act in the subspace without a double occupancy and $n_i = n_{i\uparrow} + n_{i\downarrow}$ is the number operator for electrons. The second term describes the spin-1/2 Heisenberg antiferromagnet (AFM) with the exchange energy $J = 4t^2/U$ for the nearest neighbours.

To allow for the constraint of no double occupancy on a rigorous basis it is convenient to rewrite the $t-J$ model (2) in terms of the Hubbard operators (HO):

$$H_{t-J} = -\sum_{i\neq j,\sigma} t_{ij} X_i^{\sigma 0} X_j^{0\sigma} - \mu \sum_{i\sigma} X_i^{\sigma\sigma} + \frac{1}{2}\sum_{i\neq j,\sigma} J_{ij}\left(X_i^{\sigma\bar{\sigma}} X_j^{\bar{\sigma}\sigma} - X_i^{\sigma\sigma} X_j^{\bar{\sigma}\bar{\sigma}}\right), \tag{3}$$

where $t_{ij} = t, t'$ is the electron hopping energy for the nearest and the second neighbours on the 2D square lattice, respectively, and J_{ij} is the exchange interaction. We have also introduced chemical potential μ and number operator $n_i = \sum_\sigma X_i^{\sigma\sigma}$. The HO are defined as

$$X_i^{\alpha\beta} = |i,\alpha\rangle\langle i,\beta| \tag{4}$$

for three possible states at the lattice site i: $|i,\alpha\rangle = |i,0\rangle, \quad |i,\sigma\rangle$ for an empty site and for a site singly occupied by an electron with the spin $\sigma/2$ ($\sigma = \pm 1,\ \bar{\sigma} = -\sigma$). They obey the completeness relation

$$X_i^{00} + \sum_\sigma X_i^{\sigma\sigma} = 1, \tag{5}$$

which rigorously preserves the constraint of no double occupancy.

Below we consider a more realistic for copper-oxide compounds two-band $p-d$ model. It can be reduced to the asymmetric Hubbard model with the lower Hubard sub-band (LHB) occupied by one-hole Cu-d like states and the upper Hubbard sub-band (UHB) occupied by two-hole $p-d$ singlet states [6]. In terms of the Hubbard operators the asymmetric Hubbard model reads:

$$H = H_0 + H_t = E_1 \sum_{i\sigma} X_i^{\sigma\sigma} + E_2 \sum_i X_i^{22}$$

$$- \sum_{i\neq j\sigma} \{t_{ij}^{11} X_i^{\sigma 0} X_j^{0\sigma} + t_{ij}^{22} X_i^{2\sigma} X_j^{\sigma 2} + \sigma t_{ij}^{12}(X_i^{2\bar{\sigma}} X_j^{0\sigma} + X_i^{\sigma 0} X_j^{\bar{\sigma} 2})\}. \tag{6}$$

Here the energy levels $E_1 = E_0 - \mu$ and $E_2 = 2E_0 - 2\mu + \Delta$ are introduced for singly and doubly occupied sites, respectively, where E_0 is a reference energy. In the singlet-hole model (6) the Coulomb repulsion energy U in the standard Hubbard model (1) is substituted by the charge transfer energy $\Delta = \epsilon_p - \epsilon_d$ between p- and d-levels in the CuO_2 plane. The hopping integrals have different values for the LHB (t_{ij}^{11}), the UHB (t_{ij}^{22}) and the inter-band transitions (t_{ij}^{12}). They can be written in the form $t_{ij}^{\alpha\beta} = -K_{\alpha\beta} 2t\nu_{ij}$ where $t = t_{pd}$ is the $p-d$ hybridization integral and

ν_{ij} are the overlapping parameters for the Wannier oxygen states which are equal to: $\nu_1 = \nu_{j\ j\pm a_{x/y}} \simeq -0.14$ for the nearest neighbours and $\nu_2 = \nu_{j\ j\pm a_x \pm a_y} \simeq -0.02$ for the second neighbours, where $a_{x/y}$ are lattice constants. The coefficients $K_{\alpha\beta}$ depend on the dimensionless parameter t/Δ and for a realistic value of $\Delta = 2t$ they are of the order $0.5 - 0.9$ [6] (also see [7]).

The Hubbard operators (4) for a two-band model (6) are defined for 4 possible states at lattice site i: $|i, \alpha\rangle = |i, 0\rangle$, $|i, \sigma\rangle$, $|i, \uparrow\downarrow\rangle$ for an empty site, a site singly occupied by an electron with the spin σ and for a doubly-occupied site, respectively. For these states the completeness relation for the Hubbard operators reads:

$$X_i^{00} + \sum_\sigma X_i^{\sigma\sigma} + X_i^{22} = 1 \, . \tag{7}$$

A number of attempts have been made to obtain a superconducting pairing within the microscopical theory for the Hubbard models discussed above. It should be pointed out that the superconducting pairing due to the kinematic interaction in the Hubbard model (1) in the limit of strong electron correlations ($U \to \infty$) was first proposed by Zaitsev and Ivanov [8]. Close results were obtained by Plakida and Stasyuk [9] by applying an equation of the motion method to two-time Green functions (GF) [10]. However, in these papers only the mean field approximation was considered which results in the s-wave pairing irrelevant to strongly correlated systems (for the discussion see [11]). Later on the theory in the mean field approximation was considered for the $t - J$ model within the GF approach in [11,12] where the d-wave spin-fluctuation superconducting pairing due to the exchange interaction J was studied.

Superconductivity in the original Hubbard model (1) was discussed in [13,14] in the mean field type approximation within the projection technique for the GF. Local superconducting pairings of the s- and d-symmetry were obtained which, however, should disappear in the limit of strong correlations, $U \to \infty$. Unfortunately, in this approximation the self-energy operator caused by kinematic and exchange interactions is ignored, though it results in finite life-time effects and gives a substantial contribution to the renormalization of the quasiparticle (QP) spectrum in the normal state. The self-energy of the anomalous GF is also responsible for the non-local spin-fluctuation d-wave superconducting pairing.

Recently it was demonstrated for the spin-polaron representation of the $t - J$ model in [15]. A self-consistent numerical treatment of the strong coupling Eliashberg equations revealed a strong renormalization of the QP hole spectrum due to spin-fluctuations and proved the d- wave pairing. The maximum $T_c \simeq 0.01t$ was obtained at the optimal concentration of doped holes $\delta \simeq 0.2$. However, a two-sublattice representation used in [15] can be rigorously proved only for a small doping with a long-range AFM order. At a moderate doping one has to consider a paramagnetic (spin-rotationally invariant) state in the $t - J$ model.

The opposite limit of low electron densities in the $t - J$ model was studied by M. Kagan and Rice [16]. They observed various forms of electron pairing at low temperatures including the d-wave instability at the values $J/t > 1$. A special diagram technique for the Hubbard operators was also applied by Izyumov et al. [17] to consider spin fluctuations and a superconducting pairing in the $t-J$ model. However, no numerical results were presented.

In the given paper we consider a paramagnetic state with only short-range dynamic spin fluctuations at a moderate doping. We develop the theory of superconductivity for the $t-J$ model (3) and the asymmetric Hubbard model (6) by applying the projection technique to the GF [10] in terms of the Hubbard operators. Contrary to the above mentioned papers, the self-energy operators due to kinematic and exchange interactions are explicitly calculated in the non-crossing approximation. The QP spectrum in the normal state of the $t-J$ model within the GF approach at $T=0$ was also studied recently by Prelovśek [18].

Below, the Dyson equations for the matrix Green function are presented for the $t-J$ model in section 2 and for the Hubbard model in section 3, which are a direct generalization of the theory developed earlier in collaboration with Professor I.V.Stasyuk [9,11].

2. Dyson equation for the $t-J$ model

To discuss the superconducting pairing within model (3) we consider the matrix Green function (GF)

$$\hat{G}_{ij,\sigma}(t-t') = \langle\langle \Psi_{i\sigma}(t) | \Psi^{+}_{j\sigma}(t') \rangle\rangle \tag{8}$$

in terms of the Nambu operators:

$$\Psi_{i\sigma} = \begin{pmatrix} X_i^{0\sigma} \\ X_i^{\bar\sigma 0} \end{pmatrix}, \qquad \Psi^{+}_{i\sigma} = \begin{pmatrix} X_i^{\sigma 0} \; X_i^{0\bar\sigma} \end{pmatrix}, \tag{9}$$

where Zubarev notation [10] for the anticommutator Green function (8) is used.

To calculate the GF (8) we use the equation of motion for the HO:

$$\left(i\frac{d}{dt} + \mu\right) X_i^{0\sigma} = -\sum_l t_{il} B_{i\sigma\sigma'} X_l^{0\sigma'} + \sum_l J_{il}(B_{l\sigma\sigma'} - \delta_{\sigma\sigma'}) X_i^{0\sigma'}, \tag{10}$$

where

$$B_{i\sigma\sigma'} = (X_i^{00} + X_i^{\sigma\sigma})\delta_{\sigma'\sigma} + X_i^{\bar\sigma\sigma}\delta_{\sigma'\bar\sigma} = (1 - \frac{1}{2}n_i + \sigma S_i^{\sigma})\delta_{\sigma'\sigma} + S_i^{\bar\sigma\sigma}\delta_{\sigma'\bar\sigma} \; . \tag{11}$$

The boson-like operator $B_{i\sigma\sigma'}$ describes electron scattering on spin and charge fluctuations caused by the nonfermionic commutation relations for the HO's (the first term in (10) – the so-called kinematical interaction) and by the exchange spin-spin interaction (the second term in (10)).

By differentiating the GF (8) with respect to time t and t' and employing the projection technique (see, e.g., [6]) we get the following Dyson equation:

$$\hat{G}_{ij\sigma}(\omega) = \hat{G}^0_{ij\sigma}(\omega) + \sum_{kl} \hat{G}^0_{ik\sigma}(\omega) \; \hat{\Sigma}_{kl\sigma}(\omega) \; \hat{G}_{lj\sigma}(\omega) \tag{12}$$

for the Fourier component. Here the zero–order GF is calculated in the mean-field approximation

$$\hat{G}^{0}_{ij\sigma}(\omega) = Q\,\{\omega\hat{\tau}_0\delta_{ij} - \hat{E}_{ij\sigma}\}^{-1} \tag{13}$$

with the frequency matrix $\hat{E}_{ij\sigma} = \langle\{[\Psi_{i\sigma}, H], \Psi^{+}_{j\sigma}\}\rangle\, Q^{-1}$ and the correlation function $Q = \langle X^{00}_{i} + X^{\sigma\sigma}_{i}\rangle = 1 - n/2$. In a paramagnetic state it depends only on the average number of electrons $n = \langle n_i\rangle = \sum_\sigma\langle X^{\sigma\sigma}_{i}\rangle$. The self-energy operator $\hat{\Sigma}_{kl\sigma}(\omega)$ is defined by the equation:

$$\hat{\Sigma}_{ij\sigma}(\omega) = Q^{-1}\,\tilde{\Sigma}_{ij\sigma}(\omega) = Q^{-1}\,\langle\!\langle\hat{Z}^{(irr)}_{i\sigma} \mid \hat{Z}^{(irr)+}_{j\sigma}\rangle\!\rangle^{(irr)}_{\omega}\, Q^{-1} \tag{14}$$

where the irreducible part of the operator $\hat{Z}_{i\sigma} = [\Psi_{i\sigma}, H]$ is defined by the projection equation

$$\hat{Z}^{(irr)}_{i\sigma} = \hat{Z}_{i\sigma} - \sum_{l}\hat{E}_{il\sigma}\Psi_{l\sigma}\,, \quad \langle\{\hat{Z}^{(irr)}_{i\sigma}, \Psi^{+}_{j\sigma}\}\rangle = 0\,. \tag{15}$$

Equations (12) - (14) give an exact representation for the one-electron GF (8). To calculate it, however, one has to apply approximations to many-particle GF in the self-energy matrix (14) which describes inelastic scattering of electrons on a spin and charge fluctuations. Here we employ a non-crossing approximation (or a self-consistent Born approximation) for the irreducible part of many-particle Green functions in (14). It neglects vertex corrections and is given by the following two-time decoupling for the correlation functions:

$$\langle X^{\sigma'0}_{j'} B^{+}_{j\sigma\sigma'} X^{0\sigma'}_{i'}(t) B_{i\sigma\sigma'}(t)\rangle_{(j\neq j',\, i\neq i')} \simeq \langle X^{\sigma'0}_{j'} X^{0\sigma'}_{i'}(t)\rangle\langle B^{+}_{j\sigma\sigma'} B_{i\sigma\sigma'}(t)\rangle\,. \tag{16}$$

Using a spectral representation for the GF we obtain the following results for self-energy matrix elements in the $\boldsymbol{k}$-representation:

$$\tilde{\Sigma}^{\sigma}_{11(12)}(k,\omega) = \frac{1}{N}\sum_{q}\iint\limits_{-\infty}^{+\infty} \mathrm{d}z\mathrm{d}\Omega N(\omega,z,\Omega)\lambda_{11(12)}(q,k-q\mid\Omega)A^{\sigma}_{11(12)}(q,z), \tag{17}$$

with

$$N(\omega,z,\Omega) = \frac{1}{2}\frac{\tanh(z/2T) + \coth(\Omega/2T)}{\omega - z - \Omega}\,. \tag{18}$$

Here we introduce a spectral density for the normal (G_{11}) and anomalous (G_{12}) GF:

$$A^{\sigma}_{11}(q,z) = -\frac{1}{Q\pi}\mathrm{Im}\,\langle\langle X^{0\sigma}_{q} \mid X^{\sigma 0}_{q}\rangle\rangle_{z+i\delta}\,, \tag{19}$$

$$A^{\sigma}_{12}(q,z) = -\frac{1}{Q\pi}\mathrm{Im}\,\langle\langle X^{0\sigma}_{q} \mid X^{0\bar{\sigma}}_{-q}\rangle\rangle_{z+i\delta} \tag{20}$$

and the electron - electron interaction functions caused by spin and charge fluctuations

$$\lambda_{11(12)}(q,k-q\mid\Omega) = g^{2}(q,k-q)\; D^{+(-)}(k-q,\Omega), \tag{21}$$

where $g(q,k-q) = t(q) - J(k-q)$ and the spectral density of bosonic excitations are given by the imaginary part of the spin and charge susceptibilities:

$$D^{\pm}(q,\Omega) = -\frac{1}{\pi}\mathrm{Im}\ \left\{\langle\langle \boldsymbol{S}_q \mid \boldsymbol{S}_{-q}\rangle\rangle_{\Omega+i\delta} \pm (1/4)\langle\langle n_q \mid n_q^{+}\rangle\rangle_{\Omega+i\delta}\right\}. \tag{22}$$

A linearized system of Eliashberg equations close to T_c can be written as self-consistent equations for the normal GF and its self-energy operator

$$\tilde{G}_{11}^{\sigma}(k,i\omega_n) = \{i\omega_n - E_k + \tilde{\mu} - \tilde{\Sigma}_{11}^{\sigma}(k,i\omega_n)\}^{-1},$$

$$\tilde{\Sigma}_{11}^{\sigma}(k,i\omega_n) = -\frac{T}{N}\sum_q\sum_m \tilde{G}_{11}^{\sigma}(q,i\omega_m)\lambda_{11}(q,k-q \mid i\omega_n - i\omega_m) \tag{23}$$

and for the gap equation:

$$\Phi^{\sigma}(k,i\omega_n) = \Delta_k^{\sigma} + \tilde{\Sigma}_{12}^{\sigma}(k,i\omega_n) = \frac{T}{N}\sum_q\sum_m\{2J(k-q)+$$

$$+\lambda_{12}(q,k-q \mid i\omega_n - i\omega_m)\}\tilde{G}_{11}^{\sigma}(q,i\omega_m)\tilde{G}_{11}^{\bar{\sigma}}(q,-i\omega_m)\Phi^{\sigma}(q,i\omega_m). \tag{24}$$

In equation (24) we omit the $\boldsymbol{k}$-independent part of the gap function Δ_k^{σ} in the MFA (13) which is caused by the kinematic interaction [8], since it gives no contribution to the d-wave pairing ([11]). Here we use the imaginary frequency representation, $\omega = i\omega_n = i\pi T(2n+1)$.

The energy of quasiparticles E_k^{σ} and the renormalized chemical potential $\tilde{\mu} = \mu - \delta\mu$ in the MFA (13) is given by

$$E_k^{\sigma} = -\epsilon(k)Q - \epsilon_s(k)/Q - \frac{4J}{N}\sum_q \gamma(k-q)N_{q\sigma}, \tag{25}$$

where $\epsilon(k) = t(k) = 4t\gamma(k) + 4t'\gamma'(k)$, $\epsilon_s(k) = 4t\gamma(k)\chi_{1s} + 4t'\gamma'(k)\chi_{2s}$ with $\gamma(k) = (1/2)(\cos a_x q_x + \cos a_y q_y)$, $\gamma'(k) = \cos a_x q_x \cos a_y q_y$.

$$\delta\mu = \frac{1}{N}\sum_q \epsilon(q)N_{q\sigma} - 4J(n/2 - \chi_{1s}/Q)\ . \tag{26}$$

The average number of electrons in the $\boldsymbol{k}$-representation is written in the form:

$$n = \frac{1}{N}\sum_{k,\sigma}\langle X_k^{\sigma 0}X_k^{0\sigma}\rangle = \frac{Q}{N}\sum_{k,\sigma} N_{k\sigma}, \tag{27}$$

where

$$N_{k\sigma} = \{1 + \frac{2T}{N}\sum_k\sum_{n=-\infty}^{\infty}\tilde{G}_{11}^{\sigma}(k,i\omega_n)\}, \tag{28}$$

which defines function $N_{q\sigma}$ in equations (25), (26). When calculating the normal part of the frequency matrix (25) we neglect charge fluctuations and introduce spin correlation functions for the nearest, $a_1 = (\pm a_x, \pm a_y)$, and the second, $a_2 = \pm(a_x \pm a_y)$, neighbour lattice sites :

$$\chi_{1s} = \langle \boldsymbol{S}_i \boldsymbol{S}_{i+a_1} \rangle \ , \quad \chi_{2s} = \langle \boldsymbol{S}_i \boldsymbol{S}_{i+a_2} \rangle \ . \tag{29}$$

In the present calculations we take into account only the spin-fluctuation contribution modelled by the spin-fluctuation susceptibility (see, e. g., [18,19]):

$$\chi_s^{''}(q,\omega) = \chi_s(q)\ \chi_s^{''}(\omega) = \frac{\chi_0}{1+\xi^2(\boldsymbol{q}-\boldsymbol{Q}_{AF})^2}\ \tanh\frac{\omega}{2T}\frac{1}{1+(\omega/\omega_s)^2} \tag{30}$$

with the characteristic AFM correlation length ξ and spin-fluctuation energy $\omega_s \simeq J$. To fix constant χ_0 in (30) we use the following normalization condition:

$$\frac{1}{N}\sum_i \langle \boldsymbol{S}_i \boldsymbol{S}_i \rangle = \frac{1}{N}\sum_q \chi_s(q) \int\limits_{-\infty}^{+\infty} \frac{\mathrm{d}z}{\exp\frac{z}{T}-1}\chi_s^{''}(z) = \frac{\pi\omega_s}{2N}\sum_q \chi_s(q) = \frac{3}{4}n\ . \tag{31}$$

In this approximation we get for the interaction functions (21)

$$\lambda_{11}(q, k-q \mid i\omega_\nu) = \lambda_{12}(q, k-q \mid i\omega_\nu)$$

$$= -g^2(q,k-q)\chi_s(k-q) \int\limits_0^{+\infty} \frac{2z\mathrm{d}z}{z^2+\omega_\nu^2}\ \frac{\tanh(z/2T)}{1+(z/\omega_s)^2}. \tag{32}$$

For model (30) we can calculate static spin correlation functions (29) from the equations:

$$\chi_{1s} = \langle \boldsymbol{S}_i \boldsymbol{S}_{i+a_1} \rangle = \frac{1}{N}\sum_q \gamma(q) \langle \boldsymbol{S}_q \boldsymbol{S}_{-q} \rangle, \quad \chi_{2s} = \langle \boldsymbol{S}_i \boldsymbol{S}_{i+a_2} \rangle = \frac{1}{N}\sum_q \gamma'(q) \langle \boldsymbol{S}_q \boldsymbol{S}_{-q} \rangle,$$

where

$$\langle \boldsymbol{S}_q \boldsymbol{S}_{-q} \rangle = \chi_s(q) \int\limits_{-\infty}^{+\infty} \frac{\mathrm{d}z}{\exp(z/T)-1}\chi_s^{''}(z) = \chi_s(q)\frac{\pi}{2}\omega_s. \tag{33}$$

Therefore, we have obtained a closed system of equations which should be solved numerically. Preliminary calculations [20] confirm the existence of narrow QP peaks for the one-electron spectral density (19) near the Fermi surface (FS). The latter has a characteristic behaviour for strongly correlated systems with the occupation numbers $N(k) \geq 0.5$ throughout the whole Brillouin zone which results in the large FS even at a small doping. A direct numerical solution by the fast Fourier transformation of gap equation (24) proves a superconducting pairing (caused by the exchange, J, and kinematic, t^2, interactions in (24)) of the d-wave symmetry that occurs at high $T_c \simeq 0.06t$.

3. Dyson equation for the $p-d$ model

In this section we discuss the results for the two band $p-d$ model (6). To study the two–band problem we have to introduce a matrix Green function concerning the normal state properties

$$\hat{G}_{ij\sigma}(t-t') = \langle\langle \tilde{X}_{i\sigma}(t); \tilde{X}^{+}_{j\sigma}(t')\rangle\rangle, \tag{34}$$

where we use two–component operators

$$\tilde{X}_{i\sigma} = \begin{pmatrix} X_i^{\sigma 2} \\ X_i^{0\bar{\sigma}} \end{pmatrix}, \qquad \tilde{X}^{+}_{j\sigma} = \begin{pmatrix} X_j^{2\sigma} & X_j^{\bar{\sigma}0} \end{pmatrix} . \tag{35}$$

By differentiating the GF (34) with respect to time t and t' and using the projection technique described above, we get the Dyson equation in the form analogous to (12). In [6] only a zero order GF was calculated in the form analogous to the one band GF (13). The two-band spectrum for d-like holes and $p-d$ singlets as well as the density of states were calculated. It was found that hybridization between d-like holes and singlets results in a substantial renormalization of the spectrum. In addition, the dispersion relation depends strongly on antiferromagnetic short-range spin correlations (given by the static spin correlation functions, equations (29)) in the spin-singlet state. For large spin correlations at small doping values one finds a next-nearest neighbour dispersion. With the doping decreasing spin correlations, the dispersion changes to an ordinary nearest neighbour one.

However, to consider the superconducting properties of the two–band model we introduce the 4×4 matrix Green function [21]:

$$\tilde{G}_{ij\sigma}(t-t') = \langle\langle \hat{X}_{i\sigma}(t); \hat{X}^{+}_{j\sigma}(t')\rangle\rangle \tag{36}$$

for the four–component operators. For example, the H.c. one is given by the row-vector:

$$\hat{X}^{+}_{j\sigma} = \begin{pmatrix} X_j^{2\sigma} & X_j^{\bar{\sigma}0} & X_j^{\bar{\sigma}2} & X_j^{0\sigma} \end{pmatrix}. \tag{37}$$

By differentiating the GF (36) with respect to time t and t' and using the projection technique described above, we get the following Dyson equation in (k,ω) space:

$$\tilde{G}_{\sigma}(k,\omega)^{-1} = \tilde{G}^{0}_{\sigma}(k,\omega)^{-1} - \tilde{\Sigma}_{\sigma}(k,\omega) \, . \tag{38}$$

The zero–order matrix GF is given by the generalized mean–field approximation:

$$\tilde{G}^{0}_{ij,\sigma}(\omega) = \{\omega\delta_{i,j}\tilde{\tau}_0 - \tilde{A}_{ij,\sigma}\}^{-1}\tilde{\chi}, \tag{39}$$

where

$$\tilde{A}_{ij,\sigma} = \langle\{[\hat{X}_{i\sigma}, H] \ , \hat{X}^{+}_{j\sigma}\}\rangle \ \tilde{\chi}^{-1} \tag{40}$$

is a frequency matrix. The self–energy operator is given by the irreducible part of the scattering matrix:

$$\tilde{\Sigma}_{ij,\sigma}(\omega) = \tilde{\chi}^{-1}\langle\langle [\hat{X}_{i\sigma}, H] | [H, \hat{X}^{+}_{j\sigma}]\rangle\rangle^{(irr)}_{\omega}\tilde{\chi}^{-1}. \tag{41}$$

We also introduce unity matrices $\tilde{\tau}_0$ (4×4) and $\hat{\tau}_0$ (2×2) and the matrix $\tilde{\chi} = \hat{\tau}_0 \hat{\chi}$ with

$$\hat{\chi} = \begin{pmatrix} \chi_2 & 0 \\ 0 & \chi_1 \end{pmatrix}, \tag{42}$$

where $\chi_2 = \langle X_i^{22} + X_i^{\sigma\sigma} \rangle = 1 - \chi_1$. To solve the Dyson equation (38) which can be written in the general form as

$$\tilde{G}_\sigma(k,\omega) = \begin{pmatrix} \hat{G}_\sigma(k,\omega) & \hat{F}_\sigma(k,\omega) \\ (\hat{F}_\sigma(k,\omega))^+ & -\hat{G}_{\bar{\sigma}}(k,-\omega) \end{pmatrix} \tag{43}$$

we have to calculate the zero–order GF (39) and the self-energy matrix (41). The anomalous part of the zero–order GF in (39), $\hat{F}^0_\sigma(k,\omega)$, vanishes if one disregards the mean-field, k-independent gap function (due to the kinematic interaction) which violates the restriction $\langle X_i^{\sigma 2} X_i^{\bar{\sigma} 2} \rangle = 0$, see [22]. For the normal part we can use a diagonal approximation

$$\hat{G}^0_\sigma(k,\omega) = \begin{pmatrix} \chi_2/(\omega - \Omega_2(k)) & 0 \\ 0 & \chi_1/(\omega - \Omega_1(k)) \end{pmatrix}, \tag{44}$$

where the mean field spectrum is given by the dispersions $\Omega_1(k)$ and $\Omega_2(k)$ for a singly occupied d-hole-like band and a doubly occupied singlet band, respectively [6].

To calculate the self-energy matrix (41) we use the non-crossing approximation described above (see equation (16)). Writing down the self-energy matrix as

$$\tilde{\Sigma}_\sigma(k,\omega) = \tilde{\chi}^{-1} \begin{pmatrix} \hat{M}_\sigma(k,\omega) & \hat{\Phi}_\sigma(k,\omega) \\ \hat{\Phi}^+_\sigma(k,\omega) & -\hat{M}_{\bar{\sigma}}(k,-\omega) \end{pmatrix} \tilde{\chi}^{-1} \tag{45}$$

we obtain for the normal part of the matrix

$$\hat{M}_\sigma(k,\omega) = \frac{t^2}{N} \sum_q \frac{\gamma^2(q)}{\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \mathrm{d}\nu \mathrm{d}z N(\omega,\nu,z) D^+(k-q,z),$$

$$\times \{ \hat{P}_2[-\mathrm{Im} G^{22}(q,\nu+i\delta)] + \hat{P}_1[-\mathrm{Im} G^{11}(q,\nu+i\delta)] \} \tag{46}$$

where $\gamma(q) = \sum_j \exp(iqj)\nu_{0j}$, $N(\omega,\nu,z)$ is given by (18) and the spin-charge susceptibility $D^+(k-q,z)$ is given by (22). The contributions from the singlet band and from the d-hole band are defined by the matrices $\hat{P}_2$ and $\hat{P}_1$, respectively. Their diagonal terms are:

$$P_2^{11} = (K_{21})^2\ ,\ P_2^{22} = (K_{22})^2\ ,\ P_1^{11} = (K_{11})^2\ ,\ P_1^{22} = (K_{12})^2\ .$$

Here we use a notation for hopping integrals in the two-band model (6): $t_{ij}^{\alpha\beta} = -K_{\alpha\beta} 2t\nu_{ij}$ where $\alpha, \beta = 2$ or 1 for the singlet and the d-hole band, respectively. Matrix equation (46) defines the renormalization of quasiparticle spectra in the two bands due to spin and charge fluctuations, while the analogous equation for matrix $\hat{\Phi}_\sigma(k,\omega)$ gives a gap equation. In the diagonal approximations for the zero-order GF (44) and self-energy (45), (46), the Dyson equation (43) can be solved, which enables one to write an equation for superconducting gaps $\phi_\sigma^{\alpha\alpha}(k,\omega) = \Phi_\sigma^{\alpha\alpha}(k,\omega)/\chi_\alpha$ in the bands $\alpha = 2, 1$ in the closed form:

$$\phi_\sigma^{\alpha\alpha}(k,\omega) = \frac{t^2}{N}\sum_q \frac{\gamma^2(q)}{\pi}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \mathrm{d}\nu \mathrm{d}z N(\omega,\nu,z) D^-(k-q,z)$$

$$\times\{K_{\alpha\alpha}^2[-\mathrm{Im}\frac{\phi_\sigma^{\alpha\alpha}(q,\nu)}{Q_\alpha(q,\nu)}] - \frac{\chi_\beta K_{12}^2}{\chi_\alpha}[-\mathrm{Im}\frac{\phi_\sigma^{\beta\beta}(q,\nu)}{Q_\beta(q,\nu)}]\}, \qquad (47)$$

where $\alpha \neq \beta$ and the denominator

$$Q_\alpha(q,\omega) = (\omega - \Omega_\alpha(q) - M_\sigma^{\alpha\alpha}(q,\omega)/\chi_\alpha)(\omega + \Omega_\alpha(q) + M_{\bar\sigma}^{\alpha\alpha}(q,-\omega)/\chi_\alpha) - |\phi_\sigma^{\alpha\alpha}|^2 \qquad (48)$$

gives a spectrum of excitation in the superconducting phase.

4. Conclusions

To summarize, we would like to stress that starting from the microscopical $t-J$ (equation (2)) or the two-band $p-d$ (equation (6)) model we obtain a self-consistent system of equations for the Green functions and the corresponding self-energies. The frequency matrices in the zero- order Green functions (equations (13), (39)) and the renormalization of the quasiparticle spectra given by self-energies, (23) for the $t-J$ model and (46) for the two-band model, and the superconducting pairing in gap equations, (24) for the $t-J$ model and (47) for the two-band model, are caused by spin and charge fluctuations which arise from nonfermionic commutation relations for the Hubbard operators in the models (see the equation of motion (11)). Therefore, in our microscopical theory we have no fitting parameters for the electron-spin interaction as in phenomenological approaches. However, the theory is not fully self-consistent in the respect that the phenomenological model for dynamical spin fluctuations (equation (30)), was used. Nevertheless, we believe that numerical results should not depend considerably on the explicit form of the model for spin-charge fluctuations. Being normalized (equation (31)), it cannot change substantially the sum over (q,ω) in the equations for self-energies. The non-crossing approximation for self-energies (equation (16)) also seems to be quite reliable as has explicitly been proved for the spin-polaron $t-J$ model where vertex corrections are small.

It is also interesting to compare the results for the one-band $t-J$ model and the two-band Hubbard model. In the two-band model for the hole (electronically) doped case the chemical potential μ is in the singlet (d-hole) band, $\alpha = 2$ (1), and the main contribution to the integrand in equation (47) comes from the same band (first term), while the contribution from the other band is proportional to t/Δ^2. The latter is analogous to the static spin-exchange contribution of order $J \simeq (t/\Delta^2)$ in the one-band $t-J$ model, i.e. to the first term in equation (24). However, in the two-band model the spin-fluctuation contribution to equation (47) is given by the frequency dependent susceptibility $D^{-}(q,z)$ and the inter-band contributions $\propto K_{12}^2$ cannot be fully allowed for within the framework of the one-band $t-J$ model. It would be interesting to compare the solutions of gap equations in the $t-J$ model, equation (24), and in the two-band model, equation (47). However, it demands rather complicated numerical work and will be considered in future publications.

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Спін-флуктуаційна надпровідність у моделі Хаббарда

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Формулюється теорія надпровідності за посередництвом кінематичної та обмінної взаємодій в $t-J$ моделі та двозонній моделі Хаббарда в парамагнітному стані. Отримано рівняння Дайсона для матричних функцій Гріна в термінах операторів Хаббарда у неперехресному наближенні. Для розрахунку температури переходу в надпровідний стан T_c запрпоновано числовий розв'язок самоузгоджених рівнянь Еліасберга.

Ключові слова: *надпровідність, сильні електронні кореляції, модель Хаббарда, $t-J$ модель, спінові флуктуації*

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