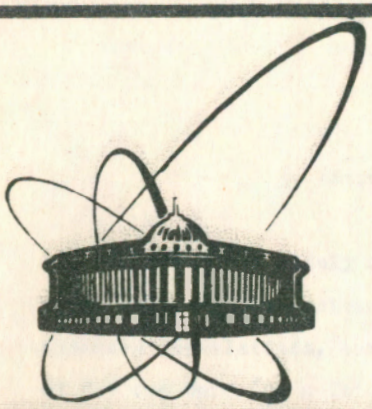

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ON SUPERCONDUCTING PAIRING IN THE TWO-BAND HUBBARD MODEL

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I. Introduction

By now it is widely accepted that essential properties of cuprate superconductors, which are systems with strong electron correlations, can be adequately described on the basis of the one-band (or multi-band) Hubbard model /1/. To examine low-lying energy properties of this model one usually projects out states with doubly occupied lattice sites with strong repulsion $\mathcal{U}$ that results in an effective Hamiltonian with an antiferromagnetic exchange term. Pairing caused by the antiferromagnetic exchange interaction /2,3/ is one of the promising mechanisms investigated within the framework of the well-known t-J model in a number of theoretical papers (see the review /4/) describing superconducting properties of the strongly correlated electron system.

At the same time it was pointed out /5/ that for the t-J model in $\mathcal{U}\to\infty$ limit when the exchange interaction $J \to 0$ the superconducting pairing may be caused by the so-called kinematic interaction $\sim t$. However, it was shown in /6/ that due to an exact condition in the lower Hubbard subband (eq. (23) in /6/) the kinematic interaction gives no contribution to the pairing. So it is very important to study superconducting pairing in more realistic many-band Hubbard models by taking into account this exact condition.

In this paper we consider the two-band Hubbard model describing highly hybridized copper $3d_{x^2-y^2}$ and oxygen $2p_{x,y}$ electron orbitals in a CuO_2 plane /7-9/ . After excluding doubly occupied copper sites the effective Hamiltonian is

obtained. It includes an antiferromagnetic copper-oxygen exchange interaction term, and the exchange-mediated hybrid (p-d) pairing in this system seems likely, by analogy with the t-J model. In particular, this possibility has been investigated with Gutzwiller-type approximation in /10,11/ and this kind of pairing has been argued. We develop here a mean-field approach without Gutzwiller approximation violating the statistic of carriers in the lower Hubbard sub-band and obtain, as the main result of the paper, that the exchange-mediated pairing suggested in /10, 11/ is forbidden due to the strong Hubbard repulsion at copper sites.

The paper is organized as follows. In Sec.II the generalized Hubbard model (p-d model) is formulated and a canonical transformation is applied to obtain an effective Hamiltonian to the second order in the hybridization p-d hopping term t^{dp}. We discuss also validity of some approximations in treating this Hamiltonian and justify the use of the Hubbard operators. In Sec.III a matrix two-time Green function is introduced and the projection technique is developed to linearize the equation of motion for the Green function. Solutions of this equation are presented in Sec.IV taking into account the on-site restriction due to the strong Hubbard repulsion. As a consequence, we obtain that anomalous correlations of the superconducting type are forbidden due to this restriction. In Sec.V some concluding remarks are made.

II. Model Hamiltonian and the kinematic restriction

A realistic Hamiltonian describing electronic properties of a CuO_2 plane is of the form /4,7-9/

$$\mathcal{H} = \varepsilon_d \sum_{i\sigma} d^+_{i\sigma} d_{i\sigma} + \sum_{\substack{\langle im\rangle \\ \sigma}} t^{dp}_{im} (d^+_{i\sigma} c_{m\sigma} + c^+_{m\sigma} d_{i\sigma}) + \qquad (I)$$

$$+\sum_{\langle mn\rangle \sigma} t_{mn}^{pp} c_{m\sigma}^{+} c_{n\sigma} + U_d \sum_i n_{i\uparrow} n_{i\downarrow} \ ,$$

which we choose to be presented in the hole notation with the "vacuum" ($3d^{10}$, $2p^6$) configuration; $d_{i\sigma}^{+}$ and $c_{m\sigma}^{+}$ are creation operators for a hole at Cu or O site, respectively; summation in the second and third terms in (I) is taken over the nearest neighbour sites. The parent undoped compounds contain one hole per Cu site. We treat the limit of strong Hubbard repulsion on copper sites, $U_d > \varepsilon_p - \varepsilon_d$, when extra holes go on the oxygen 2p orbital with $\varepsilon_p (= 0)$ energy /7/. Regarding hybridization integrals t_{im}^{dp} and t_{mn}^{pp} , we suggest

$$|t_{mn}^{pp}| < |t_{im}^{dp}| \ll U_d + \varepsilon_d \qquad (2)$$

in accord with representative values of the parameters in (I) discussed in /4,8/.

The phases of the wave functions in the CuO_2 plane are chosen so that $t_{im}^{dp} = t^{dp}(-1)^{l_{im}}$ with $l_{im} = 2$ if $\vec{m} = \vec{i} + \vec{x}, \vec{i} - \vec{y}$ and $l_{im} = 1$ if $\vec{m} = \vec{i} - \vec{x}$, $\vec{m} = \vec{i} + \vec{y}$, where the vectors $\pm\vec{x}$ and $\pm\vec{y}$ connect each copper site i with the four nearest oxygen sites. Now it is worth noting that Hamiltonian (I) can be formulated in terms of appropriate linear combinations of four oxygen p-orbitals surrounding a given copper site /12,13/. These combinations reflect the symmetry of the CuO_2 plane and transform like (x^2-y^2)-, (x^2+y^2)-, x- and y- orbitals under the operations of the point group of a site $\vec{i}$. Only the (x^2-y^2)-oxygen orbital is hybridized with the copper d-orbital through the t_{im}^{dp} term in (I). Therefore, other three combinations may be excluded from the consideration provided, in accord with (2), that the direct p-p hopping term ($\sim t_{mn}^{pp}$) which mixes different oxygen orbitals, is the

smallest in (I). This circumstance will allow us to avoid some complications of minor importance by modifying the three-band into a two-band model that allow us to obtain straightforwardly the main result of this paper in an analytical form.

As in the case of the single-band Hubbard model with large U_d /1-4/, we are interested in low-energy properties of the model (I) excluding doubly occupied copper sites by canonical Schrieffer - Wolf transformation /14/. To do this, it is natural, first, to introduce the Hubbard operators $X_i^{pq} \equiv |i;p\rangle\langle i;q|$ instead of the operators $d_{i\sigma}^{+}(d_{i\sigma})$ by means of the equations

$$d_{i\uparrow}^{+} = X_i^{\uparrow 0} + X_i^{2\downarrow}, \qquad d_{i\downarrow}^{+} = X_i^{\downarrow 0} - X_i^{2\uparrow} \tag{3}$$

with the usual notation /15/.

Making the Schrieffer - Wolf transformation $e^{S}\mathcal{H}e^{-S} \to \tilde{\mathcal{H}}$ with

$$S = \frac{1}{U_d + \varepsilon_d} \sum_{\substack{\langle im\rangle \\ \sigma\sigma'}} t_{im}^{dp} \varepsilon_{\sigma\sigma'} \left(X_i^{2\sigma'} c_{m\sigma} - h.c. \right), \tag{4}$$

where $\varepsilon_{\sigma\sigma'}$ is the antisymmetric tensor with nonzero elements $\varepsilon_{\uparrow\downarrow} = -\varepsilon_{\downarrow\uparrow} = 1$, we restrict our consideration to the second order in $|t_{im}^{dp}|/(U_d + \varepsilon_d) \ll 1$. Then, the effective transformed Hamiltonian $\mathcal{H}_{eff}$ has the form

$$\begin{aligned}
\mathcal{H}_{eff} = {} & \varepsilon_d \sum_{i\sigma} X_i^{\sigma\sigma} + \sum_{\substack{\langle im\rangle \\ \sigma}} t_{im}^{dp} \left(X_i^{\sigma 0} c_{m\sigma} + h.c. \right) + \\
& + 2\mathcal{J} \sum_{\langle im\rangle} \left[S_i s_m - \frac{1}{4} \left(\sum_{\sigma} X_i^{\sigma\sigma} \right) n_m \right] + \\
& + \sum_{\substack{\langle m \neq n\rangle \\ \sigma}} \left(t_{mn}^{pp} - \sum_i \frac{t_{im}^{dp} t_{in}^{dp}}{U_d + \varepsilon_d} X_i^{\bar{\sigma}\bar{\sigma}} \right) c_{m\sigma}^{+} c_{n\sigma} + \\
& + \sum_{\substack{\langle m \neq n\rangle \\ \sigma}} \frac{t_{im}^{dp} t_{in}^{dp}}{U_d + \varepsilon_d} X_i^{\sigma\bar{\sigma}} c_{m\bar{\sigma}}^{+} c_{n\sigma},
\end{aligned} \tag{5}$$

with $\mathcal{J} = |t_{im}^{dp}|^2/(\mathcal{U}_d + \varepsilon_d)$ and $n_m = n_{m\uparrow} + n_{m\downarrow}$ is the number operator for oxygen sites $\vec{m}$; $\bar{\sigma} \equiv -\sigma$.

Hamiltonian (5) acts in the subspace with projected out doubly occupied copper sites. The second term in (5) gives the residual hybridization which mixes oxygen states with hole states only on the lower copper level. This term cannot be removed by a canonical perturbation transformation because the charge-transfer gap $|\varepsilon_d|$ is not large as compared to $\mathcal{U}_d + \varepsilon_d$. The third term in (5) provides antiferromagnetic coupling of a copper hole spin S_i with neighbouring oxygen ones S_m. The next term in (5) now includes a renormalized p-p hopping integral, while the last gives a new spin-flip p-p hopping for oxygen holes.

According to /2,3/, one may suggest that the second order (in $t^{dp}/(\mathcal{U}_d + \varepsilon_d)$) interactions in (5) provide in the system not only antiferromagnetic correlations but superconducting pairing as well. This is hydrid pairing which includes a singlet state of copper d- and oxygen p - holes at neighbouring sites.

We investigate this problem by two-time Green function method in a mean-field approximation. Our approach based on a projection technique, is a convenient way to linearize the equation of motion for Green functions and obtain excitation spectrum renormalized due to various correlations in the system. The approach was first employed in /16/ to investigate normal state properties of the single-band Hubbard model and then developed in our paper /6/ to examine superconducting pairing in this model. A similar projection technique in terms of the Hubbard operators has recently been used in the case of the Anderson model as $\mathcal{U} \to \infty$ /17/.

In the recent papers /10/, Spalek has investigated singlet pairing mediated by antiferromagnetic exchange interaction

between conduction and f-electrons in a heavy-fermion two-band system. He showed that this hybrid pairing provides a superconducting gap in the electron spectrum of this system. Two points of the mean-field approach have been used in /10/, the first is the Gutzwiller-type renormalization of the residual hybridization term

$$t_{im}^{df} X_i^{\sigma 0} c_{m\sigma} \equiv t_{im}^{df}(1-n_{i-\sigma}) d_{i\sigma}^{+} c_{m\sigma} \to q^{1/2} t_{im}^{df} d_{i\sigma}^{+} c_{m\sigma}, \quad (6)$$

where $q = (1-n)/(1-n/2)$ and $n(\leq 1)$ is an average occupation of the f-level; the second point is the Hartree-Fock approximation of the second order term in (5) that includes real space hybrid pairing.

Taking Hamiltonian (5) as a starting point to investigate high-T_c superconductors we note that the simple ansatz (6) with subsequent substitution of the Hubbard operators $X_i^{\sigma 0}(X_i^{0\sigma})$ by the usual fermion ones $d_{i\sigma}^{+}(d_{i\sigma})$, as it was done in /10,11/, does not properly take into account the local constraint (no double-site occupation):

$$\langle \sum_{\sigma} d_{i\sigma}^{+} d_{i\sigma} \rangle \equiv \langle n_i \rangle \leq 1. \quad (7)$$

This should be considered as a sort of kinematic condition that restricts the phase space for electron (or hole) motion. The constraint (7) arises in each case when one deals with extremely strong correlation limit $U \to \infty$ for the Hubbard model of for the periodic Anderson model /18/ and it is not a trivial problem to incorporate (7) into consideration consistently. In the slave - boson representation, for instance, it is usually taken into account on the average by substituting this local constraint by a global one /19/, and one needs to make strong efforts to improve this approximation /20/. The other convenient

way is the variational Gutzwiller method which deals with a manifold of projected wave functions obeying the condition (7) /21/.

We treat the problems in terms of the Hubbard operators which act in the lower Hubbard subband and hence conserve the necessary kinematic condition (7). Employing the Hubbard operators gives us also a natural way to investigate a role of kinematic restrictions in superconducting pairing and show that the hybrid p-d exchange-mediated pairing does not provide to the second order in $t^{dp}/(U_d+\varepsilon_d)$ a gap in a hole excitation spectrum of the doped system.

III. Green functions and projection technique

A minimal set of one-particle hole operators associated with a site $\vec{i}$ includes an operator $X_i^{\sigma 0}$ for a copper site and two $c^{+}_{i+x\sigma}$, $c^{+}_{i+y\sigma}$ for oxygen sites in accord with the elementary cell structure in the CuO_2 plane. This gives us the column-operator

$$\psi_{i\sigma} \equiv \begin{pmatrix} X_i^{0\sigma} \\ c_{i+x\sigma} \\ c_{i+y\sigma} \end{pmatrix}, \tag{8a}$$

and the hermitian conjugate row-operator

$$\psi^{+}_{i\sigma} = \left(X_i^{\sigma 0}, \; c^{+}_{i+x\sigma}, \; c^{+}_{i+y\sigma} \right). \tag{8b}$$

To study a superconducting pairing in the system, it is convenient to introduce the Nambu operators.

$$\Psi_{i\sigma} = \begin{pmatrix} \psi_{i\sigma} \\ (\psi^{+}_{i\bar{\sigma}})^{T} \end{pmatrix}, \quad \Psi^{+}_{i\sigma} = \left(\psi^{+}_{i\sigma}, \; \psi^{T}_{i\bar{\sigma}} \right), \tag{9}$$

where $\psi_{i\sigma}^{T}$ is transposed to $\psi_{i\sigma}$; and the (6x6) matrix two-time Green function $\langle\langle \Psi_{i\sigma}(t) / \Psi_{j\sigma}^{+}(t') \rangle\rangle = -i\,\theta(t-t') \times$

$\times \langle \{ \Psi_{i\sigma}(t), \Psi_{j\sigma}^{+}(t') \} \rangle$.

Now let us define the inner product $(A|B^{+})$ of two fermion-like operators A and B as a thermodynamic average of their anticommutator

$$(A|B^{+}) \equiv \langle \{A, B^{+}\} \rangle \quad . \tag{10}$$

This allows one to project the equation of motion for any of the operators $\Psi_{i\sigma}(t)$ onto the initial set of these operators as

$$\frac{\partial}{\partial t} \Psi_{i\sigma}(t) = i \left[\mathcal{H}_{eff}, \Psi_{i\sigma}(t) \right] \simeq$$

$$\simeq \sum_{j} \left(\dot{\Psi}_{i\sigma} / \Psi_{j\sigma}^{+} \right) \left(\Psi_{j\sigma} / \Psi_{j\sigma}^{+} \right)^{-1} \Psi_{j\sigma}(t) \,. \tag{11}$$

Based on this projection, the equation of motion for the Green function $\langle\langle \Psi_{i\sigma}(t) / \Psi_{j\sigma}^{+}(t') \rangle\rangle$ may be written after the Fourier transformation in the linearized form

$$\omega \langle\langle \Psi_{i\sigma} / \Psi_{j\sigma}^{+} \rangle\rangle_{\omega} + \sum_{\ell} \hat{A}_{i\ell} \langle\langle \Psi_{\ell\sigma} / \Psi_{j\sigma}^{+} \rangle\rangle_{\omega} = \left(\Psi_{i\sigma} / \Psi_{i\sigma}^{+} \right) \delta_{ij} \,, \tag{12}$$

where the (6x6) matrix $\hat{A}_{i\ell}$ is presented as

$$\hat{A}_{i\ell} = \left(\left[\mathcal{H}_{eff}, \Psi_{i\sigma} \right] / \Psi_{\ell\sigma}^{+} \right) \left(\Psi_{\ell\sigma} / \Psi_{\ell\sigma}^{+} \right)^{-1} . \tag{13}$$

The validity of this approximation and some details of the projection technique are discussed in /6,16,17/.

After employing (13), the matrix elements of $\hat{A}_{i\ell}$ can be written in terms of three types of pair correlation functions. Two of them, K_{i}^{σ} and L_{i}^{σ} are of the normal type

$$K_i^{\sigma} = \frac{1}{\langle Q_i^{\bar{\sigma}} \rangle} \sum_{m(i)} (-1)^{L_{im}} \langle X_i^{\bar{\sigma}0} c_{m\sigma} \rangle ,$$

$$L_i^{\sigma} = \sum_{m(i)} \sum_{n(i)} (-1)^{L_{im}+L_{in}} \langle c_{m\bar{\sigma}}^{+} c_{n\sigma} \rangle , \qquad (14)$$

$$\langle Q_i^{\sigma} \rangle \equiv 1 - \langle X_i^{\sigma\sigma} \rangle$$

and the third, Δ_i^{σ}, is the hybrid correlation function of the anomalous type corresponding to a real-space singlet pairing of neighbouring oxygen and copper holes

$$\Delta_i^{\uparrow} = t^{dp} \sum_{m(i)} (-1)^{L_{im}} \left(\langle X_i^{\uparrow 0} c_{m\downarrow}^{+} \rangle - \langle X_i^{\downarrow 0} c_{m\uparrow}^{+} \rangle \right). \qquad (15)$$

The summations in (14) and (15) run over oxygen m and n sites nearest to the $\vec{i}$ site;

Assuming space homogeneity and a non-magnetic state in the system, we omit below in K_i^{σ} and L_i^{σ} the indices $\vec{i}$ and σ. The pair correlation functions K and L define renormalized parameters of an excitation spectrum in the normal state. These parameters are given by

$$\begin{aligned} \tilde{\varepsilon}_d &= \varepsilon_d - t^{dp} K - \mathcal{J} L , \\ \tilde{t}^{dp} &= t^{dp} - \mathcal{J} K , \\ \tilde{t}^{pp} &= t^{pp} - \mathcal{J}(1 - \langle Q \rangle) . \end{aligned} \qquad (16)$$

After transformaing into the momentum $\vec{q}$-space, the matrix $\hat{A}_q$ can be written as

$$\hat{A}_q = \begin{pmatrix} -\hat{\Omega}_q & \hat{\Delta}_q \\ \hat{\Delta}_q^{+} & \hat{\Omega}_q \end{pmatrix}, \qquad (17)$$

where two (3x3) matrices $\hat{\Omega}_q$ and $\hat{\Delta}_q$ are presented as

$$\hat{\Omega}_q = \begin{pmatrix} \tilde{\varepsilon}_d & -\langle Q\rangle \tilde{t}^{d_p} \lambda(q_x) & \langle Q\rangle \tilde{t}^{d_p} \lambda(q_y) \\ -\tilde{t}^{d_p} \lambda^*(q_x) & -\mathcal{J}(1-\langle Q\rangle)|\lambda(q_x)|^2 & \tilde{t}^{pp} \lambda^*(q_x)\lambda(q_y) \\ \tilde{t}^{pp} \lambda^*(q_y) & \tilde{t}^{pp} \lambda(q_x)\lambda^*(q_y) & -\mathcal{J}(1-\langle Q\rangle)|\lambda(q_y)|^2 \end{pmatrix} \tag{18}$$

$$\hat{\Delta}_q = \frac{\Delta}{\tilde{t}^{d_p}} \begin{pmatrix} \langle Q\rangle^{-1} \tilde{t}^{d_p} & -\mathcal{J}\langle Q\rangle \lambda(q_x) & \mathcal{J}\langle Q\rangle \lambda(q_y) \\ -\mathcal{J}\lambda^*(q_x) & 0 & 0 \\ \mathcal{J}\lambda^*(q_y) & 0 & 0 \end{pmatrix},$$

where $\lambda(q_{x,y}) = 2i \sin(q_{x,y}/2)$. Note, the Fourier transform for the operators $\psi_{j\sigma}$ from (8) is given by

$$\begin{aligned} \psi^+_{q\sigma} &= \left(X^{+\sigma}_q , c^{+(x)}_{q\sigma} , c^{+(y)}_{q\sigma} \right), \\ X^{+\sigma}_q &= \frac{1}{\sqrt{N}} \sum_j X^{+\sigma}_j e^{-iqj} , \\ c^{+(\alpha)}_{q\sigma} &= \frac{1}{\sqrt{N}} \sum_j c^+_{j+\alpha\sigma} e^{-iq(j+\alpha)} , \quad \alpha = x, y . \end{aligned} \tag{19}$$

Before deriving solutions of the linearized equation (12), it is worth simplifying our consideration in the way discussed in Sec.II. Namely, taking into account the point symmetry in the CuO_2 plane, we choose a new oxygen orbital basis by means of the canonical transformation $\psi_{q\sigma} \to \tilde{\psi}_{q\sigma} = \hat{u}^+_q \psi_{q\sigma}$ with

$$\hat{u}_q = \begin{pmatrix} 1 & 0 \\ 0 & \hat{S}_q \end{pmatrix}, \quad \hat{S}_q = i \begin{pmatrix} \cos\theta_q & \sin\theta_q \\ \sin\theta_q & -\cos\theta_q \end{pmatrix}. \qquad (20)$$

Putting the rotation parameter θ_q to be $tg\,\theta_q = -\,d(q_y)/d(q_x)$ one may check that the matrix elements $(\widetilde{\hat{\Omega}}_q)_{13}$, $(\widetilde{\hat{\Omega}}_q)_{31}$ and $(\widetilde{\hat{\Delta}}_q)_{13}$, $(\widetilde{\hat{\Delta}}_q)_{31}$ for the transformed matrices $\widetilde{\hat{\Omega}}_q = \hat{u}_q^+ \hat{\Omega}_q \hat{u}_q$ and $\widetilde{\hat{\Delta}}_q = \hat{u}_q^+ \hat{\Delta}_q \hat{u}_q$ vanish, i.e., $(\widetilde{\hat{\Omega}}_q)_{13} = (\widetilde{\hat{\Omega}}_q)_{31} = 0$ and $(\widetilde{\hat{\Delta}}_q)_{13} = (\widetilde{\hat{\Delta}}_q)_{31} = 0$.

The symmetric (x^2-y^2)-combination of oxygen orbitals, extracted explicitly in this way, with the corresponding creation operator $\tilde{c}^+_{q\sigma} = -i\left[c^{+(x)}_{q\sigma}\cos\theta_q + c^{+(y)}_{q\sigma}\sin\theta_q\right]$, is strongly hybridized with the d-level through mixing parameters $(\widetilde{\hat{\Omega}}_q)_{12} \sim (\widetilde{\hat{\Omega}}_q)_{21} \sim \tilde{t}^{dp}$ and weakly with other oxygen orbitals through $(\widetilde{\hat{\Omega}}_q)_{32} \sim (\widetilde{\hat{\Omega}}_q)_{23} \sim \tilde{t}^{pp}$. Further, ignoring the latter we come to the matrices $\widetilde{\hat{\Omega}}_q$ and $\widetilde{\hat{\Delta}}_q$ of less (2x2) dimension

$$\widetilde{\hat{\Omega}}_q = \begin{pmatrix} \tilde{\varepsilon}_d - \mu & -\langle Q\rangle \tilde{t}^{dp}\gamma_q \\ -\tilde{t}^{dp}\gamma_q & \xi_q - \mu \end{pmatrix}; \quad \widetilde{\hat{\Delta}}_q = \frac{\Delta}{\tilde{t}^{dp}} \begin{pmatrix} \langle Q\rangle^{-1}\tilde{t}^{dp} & -\langle Q\rangle\gamma\gamma_q \\ -\gamma\gamma_q & 0 \end{pmatrix}, \qquad (21)$$

which act in the space of reduced operators

$$\tilde{\psi}^+_{q\sigma} \equiv \left(X^{\sigma o}_q, \tilde{c}^+_{q\sigma}\right), \quad \psi_{q\sigma} \equiv \begin{pmatrix} X^{o\sigma}_q \\ \tilde{c}_{q\sigma} \end{pmatrix}$$

and describe an effective two-band model Here,

$$\gamma_q = \sqrt{|d(q_x)|^2 + |d(q_y)|^2}, \quad \xi_q = 2\tilde{t}^{pp}\frac{|d(q_x)d(q_y)|^2}{\gamma_q^2} - (1-\langle Q\rangle)\gamma\gamma_q^2 \qquad (22)$$

and we introduce the chemical potential μ in $\widetilde{\hat{\Omega}}_q$ in a usual way.

The transformed matrix $\widetilde{\hat{A}}_q$ of reduced (4x4) dimension preserves its general from (17) with the substitution $\hat{\Omega}_q \to \widetilde{\hat{\Omega}}_q$, $\hat{\Delta}_q \to \widetilde{\hat{\Delta}}_q$ and the resulting matrix equation for the Green function $\langle\langle \widetilde{\Psi}_{q\sigma} | \widetilde{\Psi}^+_{q\sigma} \rangle\rangle_\omega$ becomes

$$\left(\omega + \widetilde{\hat{A}}_q\right) \langle\langle \widetilde{\Psi}_{q\sigma} | \widetilde{\Psi}^+_{q\sigma} \rangle\rangle_\omega = \widetilde{\hat{B}} , \qquad (23)$$

where the diagonal matrix $\widetilde{\hat{B}} = diag\left(\langle Q\rangle, 1, \langle Q\rangle, 1\right)$.

IV. Normal state spectrum and analysis of the gap function

The spectrum of the system in a normal state, when $\widetilde{\hat{\Delta}} \sim \Delta = 0$, consists of two hybridized bands

$$E_{q\pm} = \frac{1}{2}\left(\tilde{\varepsilon}_d + \xi_q\right) \pm \frac{1}{2}\sqrt{\left(\tilde{\varepsilon}_d - \xi_q\right)^2 + 4\langle Q\rangle\left(\tilde{t}^{dp}\gamma_q\right)^2} \qquad (24)$$

and quasiparticle correlations are described by the following Green functions:

$$\langle\langle X^{0\sigma}_q | X^{\sigma 0}_q \rangle\rangle_\omega = \langle Q\rangle \frac{\omega - \xi_q + \mu}{det\left[\omega - \widetilde{\hat{\Omega}}_q\right]}, \quad \langle\langle \tilde{C}_{q\sigma} | \tilde{C}^+_{q\sigma} \rangle\rangle_\omega = \frac{\omega - \tilde{\varepsilon}_d + \mu}{det\left[\omega - \widetilde{\hat{\Omega}}_q\right]}, \qquad (25)$$

$$\langle\langle \tilde{C}_{q\sigma} | X^{\sigma 0}_q \rangle\rangle_\omega = \langle\langle X^{0\sigma}_q | \tilde{C}^+_{q\sigma} \rangle\rangle = -\langle Q\rangle \frac{\tilde{t}^{dp}\gamma_q}{det\left[\omega - \widetilde{\hat{\Omega}}_q\right]},$$

where $det\left[\omega - \widetilde{\hat{\Omega}}_q\right] = \left(\omega - E_{q+} + \mu\right)\left(\omega - E_{q-} + \mu\right)$.

In particular, we obtain self-consistent equations to determine the filling both for the copper d-level, n_d, and the symmetric oxygen p-level, n_p, and the chemical potential μ as well, respectively

$$\frac{n_d}{1-n_d/2} = \frac{1}{N}\sum_{q\sigma}\frac{(E_{q-}-\xi_q)f(E_{q-}-\mu)-(E_{q+}-\xi_q)f(E_{q+}-\mu)}{E_{q-}-E_{q+}}, \quad (26a)$$

$$n_p = \frac{1}{N}\sum_{q\sigma}\frac{(E_{q-}-\hat{\varepsilon}_d)f(E_{q-}-\mu)-(E_{q+}-\hat{\varepsilon}_d)f(E_{q+}-\mu)}{E_{q-}-E_{q+}}, \quad (26b)$$

$$n = n_d + n_p, \quad (27)$$

where f is the Fermi factor. As values of the right hand sides in (26a) and (26b) do not exceed two, the maximal filling of the p-level is two, while a filling of the d-level is always less or equal to one, i.e., $0 \leq n_d \leq 1$. This is due to the proper account (through the Hubbard operators) of the statistics for carriers in the d-level.

If $\Delta \neq 0$, the spectrum becomes

$$\omega^2_{q\pm} = \frac{1}{2}\Big\{(E_{q+}-\mu)^2+(E_{q-}-\mu)^2+\Delta^2 \pm \quad (28)$$

$$\pm\sqrt{\left[(E_{q+}-\mu)^2-(E_{q-}-\mu)^2\right]^2+2\Delta^2\left[(E_{q+}-\mu)^2+(E_{q-}-\mu)^2\right]-4\Delta^2\left[\xi_q-\mu+2\langle Q\rangle J\gamma_q\right]^2}$$

and the equation for the gap Δ is written as

$$1=\frac{1}{N}\sum_q{}'\frac{\gamma_q^2}{\omega^2_{q-}-\omega^2_{q+}}\left[\frac{J(\omega^2_{q+}-c_q)-(\tilde{t}^{dp})^2(\xi_q-\mu)}{\omega_{q+}}\,th\,\frac{\omega_{q+}}{2T}-\right. \quad (29)$$

$$\left.-\frac{J(\omega^2_{q-}-c_q)-(\tilde{t}^{dp})^2(\xi_q-\mu)}{\omega_{q-}}\,th\,\frac{\omega_{q-}}{2T}\right]$$

where $c_q \equiv (\tilde{t}^{dp})^2\langle Q\rangle\gamma_q^2 - \tilde{\varepsilon}_d\langle Q\rangle(\xi_q-\mu)$.

There are two effective constants in this equation: the first $\sim \mathcal{J} \sim (\tilde{t}^{dp})^2/(\mathcal{U}_d + \varepsilon_d)$ is due to our mean-field approximation of the exchange term in Hamiltonian (5), while the second term $\sim (\tilde{t}^{dp})^2$ is a sort of kinematic contribution /22/ due to the nonfermionic character of the Hubbard operators $X_i^{0\sigma}(X_i^{\bar{\sigma}0})$. This type of contribution to a gap equation in the one-band Hubbard model was proposed in /5/ and compared with the exchange one in some details in /6/.

An important point of our consideration is the appearance due to the p-d hybridization in (5) of the anomalous Green functions describing d-d and p-p pairing:

$$\ll X_q^{\sigma 0} / X_{-q}^{\bar{\sigma} 0} \gg = -\Delta \frac{\omega^2 - [\xi_q + \langle Q \rangle \mathcal{J} \gamma_q^2 - \mu]^2}{(\omega^2 - \omega_{q+}^2)(\omega^2 - \omega_{q-}^2)} , \qquad (30)$$

$$\ll \tilde{c}_{q\sigma}^{+} / \tilde{c}_{-q\bar{\sigma}}^{+} \gg = \Delta \gamma_q^2 \frac{(t^{dp})^2 - 2\langle Q \rangle \mathcal{J}(\tilde{\varepsilon}_d - \mu)}{(\omega^2 - \omega_{q+}^2)(\omega^2 - \omega_{q-}^2)} . \qquad (31)$$

Therefore these d-d and p-p pairing are possible if the gap function Δ (15) is non-zero.

Some properties of anomalous correlations of carriers in the lower Hubbard subband in the one-band model are investigated in /6/. The essence is that the strong repulsion at each copper site imposes some restrictions on a symmetry of the correlation function $\langle X_q^{\sigma 0} X_{-q}^{\bar{\sigma} 0} \rangle$. Specifically, there is an exact obvious condition on the one-point function $\langle X_i^{\sigma 0} X_i^{\bar{\sigma} 0} \rangle \equiv 0$ that can be written, by using the result (30), in the form

$$\langle X_i^{\sigma 0} X_i^{\bar{\sigma} 0} \rangle \equiv 0 = \Delta \cdot \sum(\mu, T) , \qquad (32)$$

where

$$\Sigma(\mu,T)=\frac{1}{2N}\sum_q \frac{1}{\omega_{q-}+\omega_{q+}}\left\{\frac{\omega_{q-}\,th\,\frac{\omega_{q-}}{2T}-\omega_{q+}\,th\,\frac{\omega_{q+}}{2T}}{\omega_{q-}-\omega_{q+}}+\right.$$

$$\left.+\frac{(\xi_q+\langle Q\rangle\gamma_q-\mu)^2}{\omega_{q+}\omega_{q-}}\cdot\frac{\omega_{q+}\,th\,\frac{\omega_{q-}}{2T}-\omega_{q-}\,th\,\frac{\omega_{q+}}{2T}}{\omega_{q+}-\omega_{q-}}\right\}> \qquad (33)$$

$$>\frac{1}{2N}\sum_q\frac{1}{\omega_{q-}+\omega_{q+}}>0.$$

Thus, we estimate that $\Sigma(\mu,T)>0$ and the only way to satisfy equation (32) is to conclude that $\Delta=0$, i.e., in the model considered there is no superconducting hybrid pairing of copper d- and oxygen p-holes. We consider the prediction made in /10/ in favour of this pairing to be as a result of the approximation of Hamiltonian (5) by the Gutzwiller procedure (6) which does not properly take into account the condition (32).

Conclusion

We have investigated the model for copper-oxide superconductors to the second order in $t^{dp}/(U_d+\varepsilon_d)$ by two-time Green-functions in a mean-field approximation on the basis of projection technique (11)-(13). A possibility of a particular type of superconducting correlations described by the hybrid function (15) was considered. To take into account strong electron correlations and to preserve the statistics of carriers on d-levels we avoided the Gutzwiller procedure (6) and treated the problem entirely in terms of the Hubbard operators. As an intermediate results, we derived an excitation spectrum (28) with a "gap" Δ governed by equation (29). Further, we demonstrated that also d-d and p-p anomalous correlations, namely,

$\langle X_q^{\sigma 0} X_{-q}^{\bar{\sigma} 0} \rangle \sim \Delta$ and $\langle \tilde{C}_{q\sigma}^{+} \tilde{C}_{-q\bar{\sigma}}^{+} \rangle \sim \Delta$, are generated due to hybridization in the system as well. However, the first of them is forbidden due to a strong kinematic restriction (32) at each copper site, that gives necessarily for the "gap" the only solution $\Delta = 0$. It seems that Hamiltonian (5) including terms to the second order in $t^{dp}/(U_d + \varepsilon_d)$ is insufficient to give superconducting pairing due to strong electron correlations in the system. This result seems to be in accord with our previous study of the t-J model /6/ where it was pointed out that the kinematic interaction $\sim t$, which according to /13/ is of the second order in t^{dp}, gives no contribution to the gap equation. Therefore if any superconducting pairing can be obtained within the p-d model (I) it should be provided only by higher order terms, e.g., fourth order in t^{dp}, as was proposed in /23/.

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