

DYNAMICAL EQUATIONS IN A RVB MODEL OF HIGH- T_c SUPERCONDUCTIVITY

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A model is studied for the high- T_c superconductivity based on the generalized Hubbard Hamiltonian with a two-dimensional lattice containing two interpenetrative sublattices. The origin of the superconducting pairing of the mobile charge carriers is their strong on-site repulsion in the presence of the hopping between nearest-neighbouring sites. The dynamical equations for all order parameters of the model were derived in the self-consistent field approximation.

The investigation has been performed at the Institute of Theoretical Physics, Hanoi, SRV.

Динамические уравнения в одной модели
высокотемпературной сверхпроводимости
с резонирующей валентной связью

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Изучается модель высокотемпературной сверхпроводимости, основанная на обобщенном гамильтониане Хаббарда с двумерной кристаллической решеткой, содержащей две проникающие друг в друга подрешетки. Источником сверхпроводящего спаривания подвижных носителей заряда является сильное отталкивание носителей, находящихся в одном и том же узле, в присутствии перепрыгивания между ближайшими соседними узлами. В приближении самосогласованного поля выводятся динамические уравнения для всех параметров порядка теории.

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1. INTRODUCTION

In the RVB theory of high- T_c superconductivity proposed by Anderson^{/1/} and developed in many subsequent works^{/2-10/} the origin of the effective attractive interaction of the charge carriers is their strong on-site repulsion in the presence of the hopping between nearest-neighbouring sites of the lattice. The system of dynamical equations for the order parameter of the superconducting pairing of holes and other order parameters of the high- T_c superconductors with this RVB mechanism has been derived and studied in the case of the simplest

model with some two-dimensional lattice containing only one type of sites^{/2-10/}, the original Hamiltonian being that of the Hubbard model. However the experimental results have shown that the lattice of newly discovered high- T_c ceramic superconductors must contain two interpenetrative sublattices: sublattice of Cu ions with electrons in d-orbitals and that of O ions with electrons in p-orbitals. The corresponding theoretical model has been also proposed by Emery^{/11/} and was studied by many authors^{/12-16/}. In particular, some physical aspects of the model were discussed qualitatively in a recent paper by Imada^{/16/}. It is the purpose of the present work to give a more complete study of this realistic RVB model of high- T_c superconductivity. The starting point is some extended Hubbard Hamiltonian. The system of dynamical equations for the order parameter of the superconducting pairing and other order parameters of the model will be derived. On the basis of this system of dynamical equations it is possible to study analytically the physical aspects of the model. To the periodic Anderson model^{/17-20/} which is similar to that discussed in the present work the application of our reasonings is also straightforward. For the simplicity we neglect the effect of the antiferromagnetism of the half-filled Cu band. Its role will be studied separately in a subsequent work.

2. EFFECTIVE HAMILTONIAN

The structure of the two-dimensional square lattice of the superconductor is represented in Fig.1. Each Cu site has 4 nearest-neighbouring O sites, and each O site has 2 nearest-neighbouring Cu sites. If the lattice constant of the Cu sublattice equals a , then that of the O sublattice is $a/\sqrt{2}$. Denote the destruction and creation operators for the holes at the Cu and O sites by $d_{i\sigma}$, $d_{i\sigma}^+$ and $p_{j\sigma}$, $p_{j\sigma}^+$, resp., i and j labeling the sites, $\sigma = \uparrow, \downarrow$ being the spin projection. We start from the extended Hubbard Hamiltonian

$$\begin{aligned}
 H = & \epsilon_p \sum_{p_j} p_{j\sigma}^+ p_{j\sigma} + \epsilon_d \sum_i d_{i\sigma}^+ d_{i\sigma} + \\
 & + t \sum_{\langle ij \rangle} (d_{i\sigma}^+ p_{j\sigma} + p_{j\sigma}^+ d_{i\sigma}) + \\
 & + U_d \sum_i n_{i\uparrow}^d n_{i\downarrow}^d + U_p \sum_j n_{j\uparrow}^p n_{j\downarrow}^p, \quad (1) \\
 n_{i\sigma}^d = & d_{i\sigma}^+ d_{i\sigma}, \quad n_{j\sigma}^p = p_{j\sigma}^+ p_{j\sigma}, \quad \epsilon_p > \epsilon_d.
 \end{aligned}$$

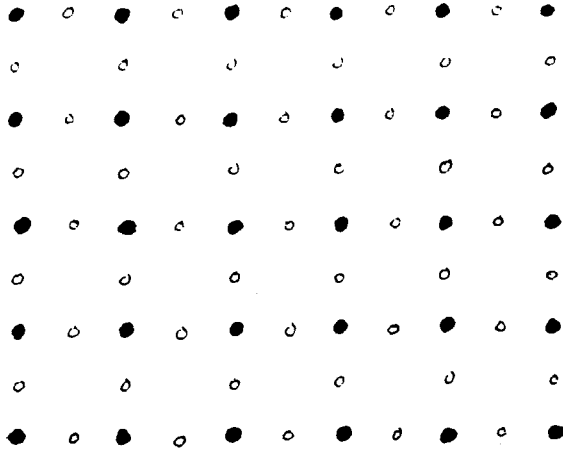


Fig.1. ● - Cu ion, ○ - O ion.

Here ϵ_d and ϵ_p denote the energies of the free holes at the sites of the Cu and O sublattices, resp., t is the hopping constant, U_d and U_p are the repulsion potential energies of two holes with opposite spin projections at the same site of the Cu and O lattices, resp., $\sum_{\langle ij \rangle}$ denotes the sum over all pairs of nearest-neighbouring sites.

We consider the limit of very strong on-site repulsions:

$$U_p, U_d \gg |t|, |\epsilon_p|, |\epsilon_d|.$$

In this case the holes at non-doubly occupied sites belong to narrow lower energy bands while those at doubly occupied sites have very high energies. By means of a suitable Schrieffer-Wolf transformation

$$\tilde{H} = e^{-iS} H e^{iS}$$

$$\begin{aligned} S = it \sum_{\langle ij \rangle} \left\{ \frac{1}{U_d} n_{i-\sigma}^d d_{i\sigma}^+ p_{j\sigma} (1 - n_{j-\sigma}^p) + \right. \\ \left. + \frac{1}{U_p} n_{j-\sigma}^p p_{j\sigma}^+ d_{i\sigma} (1 - n_{i-\sigma}^d) \right\} + \text{h.c.} \end{aligned} \quad (2)$$

we rewrite Hamiltonian in such a convenient form that the terms corresponding to the real transitions of the holes from a lower energy band to a higher one and vice versa are those of the second order of the

small constants $|t|/U_p$, $|t|/U_d$ and may be neglected. By applying the projection operator

$$P = \prod_i \prod_j (1 - n_{i\uparrow}^d n_{i\downarrow}^d) (1 - n_{j\uparrow}^p n_{j\downarrow}^p) \quad (3)$$

we can project out the high energy states containing doubly occupying holes and obtained the effective Hamiltonian for the system of interacting lower energy holes (non-doubly occupying):

$$\begin{aligned} H_{\text{eff}} = P \tilde{H} P = P \{ & \epsilon_d \sum_i d_{i\sigma}^+ d_{i\sigma} + \epsilon_p \sum_j p_{j\sigma}^+ p_{j\sigma} + \\ & + t \sum_{\langle ij \rangle} (d_{i\sigma}^+ p_{j\sigma} + p_{j\sigma}^+ d_{i\sigma}) - J_p \sum_{\langle ij \rangle} \sum_{\langle kj \rangle} B_{ji}^+ B_{jk} - \\ & - J_d \sum_{\langle ij \rangle} \sum_{\langle il \rangle} B_{ji}^+ B_{li} \} P, \end{aligned} \quad (4)$$

$$J_p = \frac{t^2}{U_p}, \quad J_d = \frac{t^2}{U_d}, \quad B_{jk} = p_{j\downarrow} d_{k\uparrow} - p_{j\uparrow} d_{k\downarrow}.$$

The four-hole interaction terms in above Hamiltonian (4) are the contributions of the virtual transitions to the intermediate states containing doubly occupying holes.

3. SELF-CONSISTENT FIELD METHOD

In this section we apply the well-known self-consistent field method of Bogolubov²¹ and substitute each four-fermion interaction term in the effective Hamiltonian (4) by a bilinear combination of the fermion operators in which the coefficient of each product of two operators is the vacuum expectation value of the product of two remaining ones. Because the vacuum is the ground state of the system of non-doubly occupying holes the expressions of the vacuum expectation value always contain explicitly the projection operator (3). In such a substitution procedure there arise six expectation values which are the order parameters of the model and may be chosen to be real:

$$\begin{aligned} \frac{1}{2} n_d &= \langle P (d_{i\uparrow}^+ d_{i\uparrow}) P \rangle = \langle P (d_{i\downarrow}^+ d_{i\downarrow}) P \rangle, \\ \frac{1}{2} n_p &= \langle P (p_{j\uparrow}^+ p_{j\uparrow}) P \rangle = \langle P (p_{j\downarrow}^+ p_{j\downarrow}) P \rangle, \end{aligned}$$

$$\begin{aligned}
\frac{1}{2} \tilde{n}_d &= \sum_{i,k \in D_j} \langle P(d_{i\uparrow}^+ d_{k\uparrow}) P \rangle = \sum_{i,k \in D_j} \langle P(d_{i\downarrow}^+ d_{k\downarrow}) P \rangle \\
\frac{1}{2} \tilde{n}_p &= \sum_{j,\ell \in D_i} \langle P(p_{j\uparrow}^+ p_{\ell\uparrow}) P \rangle = \sum_{j,\ell \in D_i} \langle P(p_{j\downarrow}^+ p_{\ell\downarrow}) P \rangle, \\
h &= \sum_{i \in D_j} \langle P(d_{i\uparrow}^+ p_{j\uparrow}) P \rangle = \sum_{i \in D_j} \langle P(d_{i\downarrow}^+ p_{j\downarrow}) P \rangle = \\
&= \frac{1}{2} \sum_{j \in D_i} \langle P(p_{j\uparrow}^+ d_{i\uparrow}) P \rangle = \frac{1}{2} \sum_{j \in D_i} \langle P(p_{j\downarrow}^+ d_{i\downarrow}) P \rangle \quad (5) \\
\Delta &= \frac{1}{2} \sum_{i \in D_j} \langle P(d_{i\uparrow}^+ p_{j\downarrow}^+ - d_{i\downarrow}^+ p_{j\uparrow}^+) P \rangle = \\
&= \frac{1}{4} \sum_{j \in D_i} \langle P(p_{j\uparrow}^+ d_{i\downarrow}^+ - p_{j\downarrow}^+ d_{i\uparrow}^+) P \rangle.
\end{aligned}$$

Here D_i and D_j denote the set of all neighbouring sites of the sites i and j . We obtain following bilinear Hamiltonian in the self-consistent field approximation

$$\begin{aligned}
H_0 &= P \{ (\epsilon_d - \frac{1}{2} \tilde{n}_p J_d - \epsilon_F) \sum_i d_{i\sigma}^+ d_{i\sigma} - \\
&- \frac{1}{2} n_p J_p \sum_j \sum_{i,k \in D_j} d_{i\sigma}^+ d_{k\sigma} + \\
&+ (\epsilon_p - \frac{1}{2} \tilde{n}_d J_p - \epsilon_F) \sum_j p_{j\sigma}^+ p_{j\sigma} - \\
&- \frac{1}{2} n_d J_d \sum_i \sum_{j,\ell \in D_i} p_{j\sigma}^+ p_{\ell\sigma} + \\
&+ [t - h(J_p + 2J_d)] \sum_{\langle ij \rangle} (d_{i\sigma}^+ p_{j\sigma} + p_{j\sigma}^+ d_{i\sigma}) - \\
&- 2\Delta(J_p + 2J_d) \sum_{\langle ij \rangle} [(p_{j\uparrow}^+ d_{i\downarrow}^+ - p_{j\downarrow}^+ d_{i\uparrow}^+) + \\
&+ (d_{i\downarrow} p_{j\uparrow} - d_{i\uparrow} p_{j\downarrow})] | P, \quad (6)
\end{aligned}$$

where ϵ_F is the Fermi energy.

Note that n_d and n_p are the mean values of the numbers of holes at each site of the sublattices Cu and O, resp., Δ is the order parameter of the superconducting pairing of holes. The fermion operators at the sites can be expanded in the form

$$d_{i\sigma} = \frac{1}{\sqrt{N_d}} \sum_{\vec{\nu} \in B_d} e^{i\vec{\nu} \cdot \vec{R}_i} d_{\sigma}(\vec{\nu}), \quad (7)$$

$$p_{j\sigma} = \frac{1}{\sqrt{N_p}} \sum_{\vec{\lambda} \in B_p} e^{i\vec{\lambda} \cdot \vec{R}_j} p_{\sigma}(\vec{\lambda}),$$

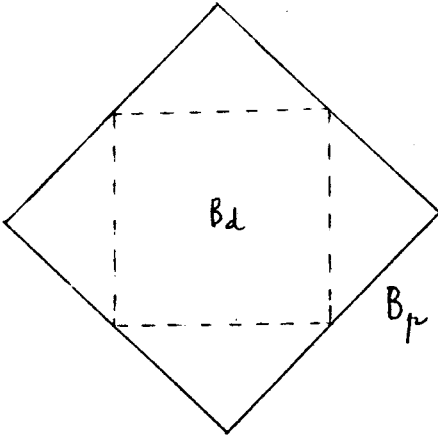


Fig.2. Brillouin zones B_p (large square) and B_d (small square).

where R_i and R_j are the coordinate vectors of the sites i and j , N_d and N_p are the numbers of the elementary cells in the sublattices of Cu and O, B_d and B_p denote their Brillouin zones and are represented in Fig.2. For some wave vector $\vec{\lambda}$ of B_p not belonging to B_d there always exists a unite vector \vec{K} of the reciprocal lattice B_d such that $\vec{\lambda} + \vec{K} \in B_d$. For such a pair $\vec{\lambda} \notin B_d$ and $\vec{\lambda} + \vec{K} \in B_d$ we set $p_{\sigma}(\vec{\lambda}) = q_{\sigma}(\vec{\lambda} + \vec{K})$. Inserting the expansion (7) into Eq.(6), we obtain

$$\begin{aligned} H_0 = & P \sum_{\vec{\nu} \in B_d} \{ E_d(\vec{\nu}) d_{\sigma}(\vec{\nu}) d_{\sigma}(\vec{\nu}) + E_r(\vec{\nu}) r_{\sigma}^+(\vec{\nu}) r_{\sigma}(\vec{\nu}) + \\ & + E_s(\vec{\nu}) s_{\sigma}^+(\vec{\nu}) s_{\sigma}(\vec{\nu}) + g(\vec{\nu}) [d_{\sigma}^+(\vec{\nu}) r_{\sigma}(\vec{\nu}) + r_{\sigma}^+(\vec{\nu}) d_{\sigma}(\vec{\nu})] + \\ & + \delta(\vec{\nu}) [(d_{\uparrow}^+(\vec{\nu}) r_{\downarrow}^+(-\vec{\nu}) - d_{\downarrow}^+(-\vec{\nu}) r_{\uparrow}^+(\vec{\nu})) + (r_{\downarrow}(-\vec{\nu}) d_{\uparrow}(\vec{\nu}) - r_{\uparrow}(\vec{\nu}) d_{\downarrow}(-\vec{\nu}))] \} P, \end{aligned} \quad (8)$$

where

$$r_{\sigma}(\vec{\nu}) = \frac{p_{\sigma}(\vec{\nu}) + q_{\sigma}(\vec{\nu})}{\sqrt{2}}, \quad s_{\sigma}(\vec{\nu}) = \frac{p_{\sigma}(\vec{\nu}) - q_{\sigma}(\vec{\nu})}{\sqrt{2}} \quad (9)$$

$$E_d(\vec{\nu}) = \epsilon_d - \frac{1}{2} \tilde{n}_p J_d - \frac{1}{2} n_p J_p [\phi_d(\nu_x)^2 + \phi_d(\nu_y)^2] - \epsilon_F$$

$$E_s(\vec{\nu}) = \epsilon_p - \frac{1}{2} \tilde{n}_d J_p - \epsilon_F, \quad (10)$$

$$E_r(\vec{\nu}) = \epsilon_p - \frac{1}{2} \tilde{n}_d J_p - \frac{1}{2} n_d J_d \phi_p(\vec{\nu})^2 - \epsilon_F,$$

$$g(\vec{\nu}) = [t - h(J_p + 2J_d)] \phi_p(\vec{\nu}),$$

$$\delta(\vec{\nu}) = -2\Delta(J_p + 2J_d) \phi_p(\vec{\nu}),$$

$$\phi_p(\vec{\nu}) = 2[\cos \nu_x a + \cos \nu_y a], \quad (11)$$

$$\phi_d(\nu_{x,y}) = 2 \cos \nu_{x,y} a.$$

4. BOGOLUBOV TRANSFORMATIONS

In order to establish the system of dynamical equations for six order parameters n_d , n_p , \tilde{n}_d , \tilde{n}_p , h and Δ from the bilinear Hamiltonian (8) now we diagonalize this Hamiltonian by means of the Bogolubov transformations. For abbreviating the formulæ we introduce two four-element columns

$$C(\vec{\nu}) = \begin{pmatrix} r_{\uparrow}(\vec{\nu}) \\ d_{\uparrow}(\vec{\nu}) \\ r_{\downarrow}^{\dagger}(-\vec{\nu}) \\ d_{\downarrow}^{\dagger}(-\vec{\nu}) \end{pmatrix}, \quad \Gamma(\vec{\nu}) = \begin{pmatrix} a_{\uparrow}(\vec{\nu}) \\ \beta_{\uparrow}(\vec{\nu}) \\ a_{\downarrow}^{\dagger}(-\vec{\nu}) \\ \beta_{\downarrow}^{\dagger}(-\vec{\nu}) \end{pmatrix} \quad (12)$$

and write the Bogolubov transformations in the matrix form

$$C(\vec{\nu}) = X(\vec{\nu})\Gamma(\vec{\nu}). \quad (13)$$

We can choose the phases of the operators in such a way that all matrix elements $X_{ij}(\vec{\nu})$, $ij = 1,2,3,4$ of $X(\vec{\nu})$ are real functions of $\vec{\nu}$. Since

the fermion operators $r_\sigma(\vec{\nu})$, $d_\sigma(\vec{\nu})$ as well as $a_\sigma(\vec{\nu})$, $\beta_\sigma(\vec{\nu})$ satisfy the canonical anticommutation relations, the matrix $X(\vec{\nu})$ must be orthogonal. Standard calculations give following results:

$$X(\vec{\nu}) = \begin{pmatrix} Y(\vec{\nu}) & Z(\vec{\nu}) \\ Z(\vec{\nu}) & -Y(\vec{\nu}) \end{pmatrix} \quad (14)$$

$$Y(\vec{\nu}) = \begin{pmatrix} X_{11}(\vec{\nu}) & X_{12}(\vec{\nu}) \\ X_{21}(\vec{\nu}) & X_{22}(\vec{\nu}) \end{pmatrix}, \quad Z(\vec{\nu}) = \begin{pmatrix} X_{13}(\vec{\nu}) & X_{14}(\vec{\nu}) \\ X_{23}(\vec{\nu}) & X_{24}(\vec{\nu}) \end{pmatrix}$$

$$X_{ij}(\vec{\nu}) = \frac{M_{ij}(\vec{\nu})}{M_i(\vec{\nu})} \quad (15)$$

$$M_i(\vec{\nu}) = [M_{i1}(\vec{\nu})^2 + M_{i2}(\vec{\nu})^2 + M_{i3}(\vec{\nu})^2 + M_{i4}(\vec{\nu})^2]^{1/2} \quad (16)$$

$$M_{11} = \delta [(E_d - \xi_\alpha)(E_r + \xi_\alpha) + \delta^2 + g^2],$$

$$M_{12} = -2\delta g E_r,$$

$$M_{13} = g[(E_r - \xi_\alpha)(E_d - \xi_\alpha) - \delta^2 - g^2],$$

$$M_{14} = (E_r + \xi_\alpha)[g^2 - (E_r - \xi_\alpha)(E_d - \xi_\alpha)] - (E_r - \xi_\alpha)\delta^2, \quad (17)$$

$$M_{21} = -2\delta g E_d,$$

$$M_{22} = \delta[(E_r - \xi_\beta)(E_d + \xi_\beta) + \delta^2 + g^2],$$

$$M_{23} = (E_d + \xi_\beta)[g^2 - (E_r - \xi_\beta)(E_d - \xi_\beta)] - (E_d - \xi_\beta)\delta^2,$$

$$M_{24} = g[(E_d - \xi_\beta)(E_r - \xi_\beta) - \delta^2 - g^2],$$

where $\xi_\alpha(\vec{\nu})$ and $\xi_\beta(\vec{\nu})$ are the eigenvalues of the Hamiltonian (8) corresponding to the quasiparticles with the destruction operators $a_\sigma(\vec{\nu})$ and $\beta_\sigma(\vec{\nu})$,

$$\xi_\alpha^2 = \frac{(E_r^2 + E_d^2) + 2(\delta^2 + g^2) + (E_r^2 - E_d^2)\theta}{2} \quad (18)$$

$$\xi_\beta^2 = \frac{(E_r^2 + E_d^2) + 2(\delta^2 + g^2) + (E_r^2 - E_d^2)\theta}{2}$$

$$\theta = \left[1 + 4 \left(\frac{\delta^2}{(E_r + E_d)^2} + \frac{g^2}{(E_r - E_d)^2} \right) \right]^{1/2}. \quad (19)$$

The Hamiltonian (8) becomes

$$\begin{aligned} H_0 = & P \sum_{\vec{\nu} \in B_d} \{ \xi_\alpha(\vec{\nu}) a_\sigma^+(\vec{\nu}) a_\sigma(\vec{\nu}) + \xi_\beta(\vec{\nu}) \beta_\sigma^+(\vec{\nu}) \beta_\sigma(\vec{\nu}) + \\ & + E_s(\vec{\nu}) s_\sigma^+(\vec{\nu}) s_\sigma(\vec{\nu}) \} P. \end{aligned} \quad (20)$$

5. EQUATIONS FOR ORDER PARAMETERS

From the results of preceding sections it is straight-forward to derive the self-consistency conditions of the theory which form the system of six equations for six order parameters n_d , n_p , \tilde{n}_d , \tilde{n}_p , h and Δ . Denote by $f_T(\xi)$ the Fermi distribution function at temperature T

$$f_T(\xi) = \frac{1}{1 + \exp \xi/T}. \quad (21)$$

The dynamical equations are:

$$\begin{aligned} n_p = & \frac{a^2}{8\pi^2} \iint_{B_d} d^2\nu \{ X_{12}^2 f_T(\xi_\beta) + X_{14}^2 [1 - f_T(\xi_\beta)] + \\ & + X_{11}^2 f_T(\xi_\alpha) + X_{13}^2 [1 - f_T(\xi_\alpha)] + f_T(E_s) \} \\ n_d = & \frac{a^2}{4\pi^2} \iint_{B_d} d^2\nu \{ X_{22}^2 f_T(\xi_\beta) + X_{24}^2 [1 - f_T(\xi_\beta)] + \\ & + X_{21}^2 f_T(\xi_\alpha) + X_{23}^2 [1 - f_T(\xi_\alpha)] \} \\ \tilde{n}_p = & \frac{a^2}{8\pi^2} \iint_{B_d} d^2\nu \{ X_{12}^2 f_T(\xi_\beta) + X_{14}^2 [1 - f_T(\xi_\beta)] + \\ & + X_{11}^2 f_T(\xi_\alpha) + X_{13}^2 [1 - f_T(\xi_\alpha)] + f_T(E_s) \} \phi_p(\vec{\nu})^2 \end{aligned} \quad (22)$$

$$\begin{aligned}
\tilde{n}_d &= \frac{a^2}{4\pi^2} \iint_{B_d} d^2\nu \{ X_{22}^2 f_T(\xi_\beta) + X_{24}^2 [1 - f_T(\xi_\beta)] + X_{21}^2 f_T(\xi_\alpha) + \\
&+ X_{23}^2 [1 - f_T(\xi_\alpha)] \} [\phi_d(\nu_x)^2 + \phi_d(\nu_y)^2] \\
h &= \frac{a^2}{16\pi^2} \iint_{B_d} d^2\nu \{ X_{22} X_{12} f_T(\xi_\beta) + X_{24} X_{14} [1 - f_T(\xi_\beta)] + \\
&+ X_{21} X_{11} f_T(\xi_\alpha) + X_{23} X_{13} [1 - f_T(\xi_\alpha)] \} \phi_p(\vec{\nu}) \\
\Delta &= \frac{a^2}{16\pi^2} \iint_{B_d} d^2\nu \{ X_{22} X_{14} f_T(\xi_\beta) - X_{24} X_{12} [1 - f_T(\xi_\beta)] + \\
&+ X_{21} X_{13} f_T(\xi_\alpha) - X_{23} X_{11} [1 - f_T(\xi_\alpha)] \} \phi_p(\vec{\nu})
\end{aligned} \tag{22}$$

6. DISCUSSION

On the basis of the system of dynamical equations (22) it is not easy to make obvious conclusions on the physical consequences of the model. The numerical solution of these lengthy equations must be studied in a separate work. Here we draw the attention to some immediate physical consequences which might be deduced easily from the equations (22) in some special case. For this purpose let us assume a simplifying approximation by setting $g(\vec{\nu})=0$. In this special case the expressions (18) and (19) for the energies of the quasiparticles become

$$\xi_\alpha(\vec{\nu}) = \frac{E_r(\vec{\nu}) - E_d(\vec{\nu})}{2} + [E(\vec{\nu})^2 + \delta(\vec{\nu})^2]^{1/2} \tag{23}$$

$$\xi_\beta(\vec{\nu}) = \frac{E_d(\vec{\nu}) - E_r(\vec{\nu})}{2} + [E(\vec{\nu})^2 + \delta(\vec{\nu})^2]^{1/2},$$

where

$$E(\vec{\nu}) = \frac{E_r(\vec{\nu}) + E_d(\vec{\nu})}{2}. \tag{24}$$

The dynamical equations are:

$$\begin{aligned}
 n_p &= \frac{a^2}{8\pi^2} \iint_{B_d} d^2\nu \{ u^2 f_T(\xi_\alpha) + v^2 (1 - f_T(\xi_\beta)) + f_T(E_s) \} \\
 n_d &= \frac{a^2}{4\pi^2} \iint_{B_d} d^2\nu \{ u^2 f_T(\xi_\beta) + v^2 [1 - f_T(\xi_\alpha)] \} \\
 \bar{n}_p &= \frac{a^2}{8\pi^2} \iint_{B_d} d^2\nu |\phi_p(\vec{\nu})|^2 \{ u^2 f_T(\xi_\alpha) + v^2 [1 - f_T(\xi_\beta)] + f_T(E_s) \} \\
 \bar{n}_d &= \frac{a^2}{4\pi^2} \iint_{B_d} d^2\nu \{ \phi_d(\nu_x)^2 + \phi_d(\nu_y)^2 \} \{ u^2 f_T(\xi_\beta) + v^2 [1 - f_T(\xi_\alpha)] \} \\
 \Delta &= \frac{a}{16\pi^2} \iint_{B_d} d^2\nu \phi_p(\vec{\nu}) 2uv [1 - f_T(\xi_\alpha) - f_T(\xi_\beta)], \quad h = 0,
 \end{aligned} \tag{25}$$

where

$$\begin{aligned}
 u(\vec{\nu}) &= \frac{1}{\sqrt{2}} \left[1 + \frac{E(\vec{\nu})}{\sqrt{E(\vec{\nu})^2 + \delta(\vec{\nu})^2}} \right]^{1/2} \\
 v(\vec{\nu}) &= -\frac{1}{\sqrt{2}} \left[1 - \frac{E(\vec{\nu})}{\sqrt{E(\vec{\nu})^2 + \delta(\vec{\nu})^2}} \right]^{1/2}.
 \end{aligned} \tag{26}$$

In particular, the critical temperature T_c is determined by equation

$$\frac{1}{J_p + 2J_d} = \frac{a^2}{16\pi^2} \iint_{B_d} \frac{d^2\nu \phi_p(\vec{\nu})^2}{|E(\vec{\nu})|} [1 - f_{T_c}(\xi_\alpha) - f_{T_c}(\xi_\beta)]. \tag{27}$$

Now we deduce some physical conclusions from above results. First we consider the expressions (23) of the energies of quasiparticles. In the limit $\delta(\vec{\nu}) \rightarrow 0$ we have

$$\begin{aligned}
 \xi_\alpha(\vec{\nu}) &\rightarrow E_r(\vec{\nu}), \quad \xi_\beta(\vec{\nu}) \rightarrow E_d(\vec{\nu}) \quad E_r(\vec{\nu}) + E_d(\vec{\nu}) > 0 \\
 \xi_\alpha(\vec{\nu}) &\rightarrow -E_d(\vec{\nu}), \quad \xi_\beta(\vec{\nu}) \rightarrow -E_r(\vec{\nu}) \quad E_r(\vec{\nu}) + E_d(\vec{\nu}) < 0.
 \end{aligned} \tag{28}$$

Thus in the limit $\delta(\vec{\nu}) \rightarrow 0$ $\xi_{\beta}(\vec{\nu})$ is always smaller than $\xi_{\alpha}(\vec{\nu})$

$$\xi_{\beta}(\vec{\nu}) < \xi_{\alpha}(\vec{\nu}). \quad (29)$$

Therefore in Eq.(27) we can neglect $f_T(\xi_{\alpha})$ in comparison with $f_T(\xi_{\beta})$. This means that the critical temperature T_c depends mainly on the distribution of the quasiparticles β . There are two alternatives:

a) If the Fermi energy is nearer to the energy band of the Cu holes than that of the 0 holes ($E_d + E_r > 0$), then T_c depends mainly on the distribution of the Cu holes.

b) If the Fermi energy is nearer to the energy band of the 0 holes ($E_d + E_r < 0$), then T_c is determined mainly by the distribution of the 0 holes.

From Eqs. (10) it is very easy to calculate the width of the energy bands of the Cu and 0 holes, in the approximation with $g(\vec{\nu}) = \delta(\vec{\nu})=0$,

$$W_d = \max E_d(\vec{\nu}) - \min E_d(\vec{\nu}) \quad (30)$$

$$W_r = \max E_r(\vec{\nu}) - \min E_r(\vec{\nu}).$$

We have

$$W_d = 4n_p J_p, \quad (31)$$

$$W_r = 8n_d J_d.$$

Since we have usually $n_p \ll 1$, $n_d \approx 1$, the energy band for the 0 holes is much larger than that of the Cu holes.

In conclusion we discuss a necessary condition for the existence of the solution of Eq.(27). We neglect $f_{T_c}(\xi_{\alpha})$ in comparison with $f_{T_c}(\xi_{\beta})$ and write

$$\frac{1}{J_p + 2J_d} = \frac{a^2}{16\pi^2} \iint_{B_d} \frac{d\nu \phi_p(\vec{\nu})^2}{|E(\vec{\nu})|} [1 - f_{T_c}(\xi_{\beta})]. \quad (32)$$

It follows that there exist some average values $\overline{|E|}$ and $\overline{\xi_{\beta}}$ of the energies $|E(\vec{\nu})|$ and $\xi_{\beta}(\vec{\nu})$ such that

$$\frac{\overline{|E|}}{J_p + 2J_d} = 1 - f_{T_c}(\overline{\xi_{\beta}}). \quad (33)$$

Since

$$0 < f_{T_c}(\bar{\xi}_\beta) < 1$$

the solution of Eq. (33) exists only if the average value $\overline{|E|}$ satisfies the necessary condition

$$\overline{|E|} < J_p + 2J_d. \quad (34)$$

This relation means that the superconducting pairing takes place only in the case when the Fermi energy ϵ_F is not very far from the mean value of the renormalized energies of the Cu and O holes: either the energy band of the Cu holes is nearly half-filled or the concentration of the O holes is low enough. For the quantitative investigation of this problem it is necessary to find approximate solutions of Eq. (32). This will be done in a subsequent work.

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