Pairing superconductivity in two-dimensional CuO₂

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The strongly correlated two-dimensional CuO₂ layer is studied to identify the mechanism of possible pairing superconductivity. The correlative motions of O and Cu holes are treated by a reasonable mean-field theory, and we find that holes on oxygen sites couple strongly to Cu holes to form Cu-O spin singlet pairs, which in turn interact strongly with the Cu resonating-valence-bond state and lead to an effective attraction between O holes, which is responsible for superconductivity.

I. INTRODUCTION

Since the discovery of high- T_c superconductors¹⁻³ much progress has been made and it is clear that the high- T_c superconductivity is mainly induced by strongly correlated spin interactions.^{4,5} Anderson *et al.*⁶⁻⁸ first pointed out that the high- T_c superconductive state can be described as a doped resonating-valence-bond (RVB) state. Doped holes occupy Cu sites and couple to the original spinon solitons to form boson solitons,⁹ then the system shows boson condensation on the RVB background, which is responsible for superconductivity. However, experiments have shown that doped holes mainly occupy the O sites¹⁰ and Emery has proposed a

more general model which explicitly takes into account the oxygen p orbitals connecting two neighboring copper sites.¹¹ This has also been taken up by some authors¹²⁻¹⁴ in connection with high- T_c superconductivity, but it is not clear which part and what interactions in the CuO₂ layer are really responsible for the high- T_c superconductivity.

In this paper we study a possible pairing superconductive mechanism¹⁵ by a reasonable mean-field theory. Following Emery, we describe the correlative motions of O holes and of Cu holes by the two-band Hubbard Hamiltonian. We find that when a doped hole occupies an O site, the hole and its two neighboring Cu holes form Cu-O spin singlet pairs

$$(2|\alpha_1\beta_0\alpha_2\rangle - |\alpha_1\alpha_0\beta_2\rangle - |\beta_1\alpha_0\alpha_2\rangle) = (|\alpha_1\beta_0\rangle - |\beta_1\alpha_0\rangle)(|\alpha_2\rangle - |\alpha_1\rangle)(|\alpha_0\beta_2\rangle - |\beta_0\alpha_2\rangle)$$

(here the subindexes 1,0,2 represent the spins of neighboring Cu, O, and Cu holes, respectively) by breaking the original Cu-Cu singlet pairs due to the strong antiferromagnetic (AF) coupling between Cu and O spins. The effective motion of O holes becomes Cu-O singlet pairs moving in the RVB background, and the Cu-Cu singlet pair will be restored when the O hole hops away with the Cu-Cu spin flip term

$$J_1 S_{i\alpha}^\dagger S_{i\beta} S_{j\beta}^\dagger S_{j\alpha}.$$

These two kinds of singlet pairs interact with each other and lead to superconductivity.

In the following sections we study the mean-field theory of our model, give some numerical results, and conclude with some discussion.

II. THEORY

We consider the Hamiltonian describing a single CuO₂ layer:

$$\hat{H} = - \sum_{(i,j)\sigma} t_0 (C_{i\sigma}^\dagger p_{j\sigma} + \text{H.c.}) + \epsilon_p \sum_{j\sigma} p_{j\sigma}^\dagger p_{j\sigma} + U_d \sum_i C_{i\alpha}^\dagger C_{i\alpha} C_{i\beta}^\dagger C_{i\beta} + U_p \sum_j p_{j\alpha}^\dagger p_{j\alpha} p_{j\beta}^\dagger p_{j\beta}. \quad (1)$$

for Eq. (1), the vacuum is defined as filled Cu d^{10} and O p^6 states. The operator $C_{i\sigma}^\dagger$ creates a Cu ($3d_{x^2-y^2}$) hole at site i , and $p_{j\sigma}^\dagger$ creates a O($2p_x, 2p_y$) hole at site j . The summation of (i,j) is taken over the nearest-neighboring Cu and O sites.

For the sake of simplicity, we have neglected the inter-

site correlation between neighboring Cu and O holes. We set the site energy of the Cu holes $\varepsilon_d=0$ and consider the case $\varepsilon_p > 0$. In the small t_0 (Ref. 16) limit, the first term in Eq. (1) can be treated as a perturbation term. We treat the strongly correlated Cu hole by the “slave-boson” field technique and treat the O hole within the ordinary Hartree-Fock (HF) approximation because the correlation term (U_p term) of the O hole is not important in the case of low-density of O holes. We express the true Cu-hole operator as

$$C_{i\sigma}^\dagger = e_i S_{i\sigma}^\dagger + \sigma d_i^\dagger S_{i\bar{\sigma}}, \quad (2)$$

where the boson operators $e_i^\dagger$ and $d_i^\dagger$ create empty and doubly occupied Cu sites, respectively, and the fermion operator $S_{i\sigma}^\dagger$ creates singly occupied Cu sites. The strong correlation term of the Cu hole becomes the single-particle energy of the d boson ($U_d d_i^\dagger d_i$ term) and the fermion operator $S_{i\sigma}^\dagger$ ($S_{i\sigma}$) can be treated by an ordinary mean-field approximation.¹⁷ Then the state space is enlarged to include unphysical states by containing a set of bosons, and the physical states can be obtained by imposing the constraint of the completeness relation for each Cu site¹⁷

$$e_i^\dagger e_i + d_i^\dagger d_i + \sum_\sigma S_{i\sigma}^\dagger S_{i\sigma} = 1. \quad (3)$$

$C_{i\sigma}^\dagger$ still satisfies the anticommutation relations in this case.⁸ Substituting Eq. (2) into Eq. (1), we obtain

$$\hat{H} = \hat{H}_0 + \hat{H}',$$

$$\begin{aligned} \hat{H}_0 = & \varepsilon_p \sum_{j\sigma} p_{j\sigma}^\dagger p_{j\sigma} + U_d \sum_i d_i^\dagger d_i + U_p \sum_{j\sigma} p_{j\alpha}^\dagger p_{j\alpha} p_{j\beta}^\dagger p_{j\beta} \\ & + \mu_1 \sum_i \left[e_i^\dagger e_i + d_i^\dagger d_i + \sum_\sigma S_{i\sigma}^\dagger S_{i\sigma} - 1 \right] \\ & + \mu_2 \left[\sum_{j\sigma} p_{j\sigma}^\dagger p_{j\sigma} + \sum_i (d_i^\dagger d_i - e_i^\dagger e_i) - \delta N \right], \quad (4) \\ \hat{H}' = & -t_0 \left[\sum_{(i,j)\sigma} (e_i S_{i\sigma}^\dagger + \sigma d_i^\dagger S_{i\bar{\sigma}}) p_{j\sigma} + \text{H.c.} \right], \end{aligned}$$

where, μ_1 and μ_2 are Lagrange multipliers which are introduced to enforce the completeness condition of Cu site and the occupation-number condition of holes. δ is the doping concentration, and N is the number of Cu sites. In the large U_d and ε_p case, the Cu site remains singly occupied, $e_i^\dagger e_i = d_i^\dagger d_i = 0$. We believe that the most important interaction is between the spin of a singly occupied Cu hole and that of a doped O hole, which is induced by the virtual processes in which the Cu site is empty or doubly occupied. We accomplish a canonical transformation to eliminate the virtual processes

$$\hat{H}' + [\hat{H}_0, \hat{S}] = 0, \quad (5)$$

$$\hat{S} = - \sum_{n,m} \frac{|n\rangle \langle n| H' |m\rangle \langle m|}{E_n - E_m}, \quad (6)$$

where $|n\rangle$ and $|m\rangle$ are eigenstates of H_0 with eigenvalues E_n and E_m , respectively. By considering the single-occupation condition of the Cu site, we obtain

$$\begin{aligned} \hat{H}_{\text{eff}} = & -\frac{4t_0^2}{\varepsilon_p} \sum_{i\sigma} S_{i\sigma}^\dagger S_{i\sigma} + [\varepsilon_p + 2t_0^2/(\varepsilon_p + U_p)] \sum_{j\sigma} p_{j\sigma}^\dagger p_{j\sigma} + J_2 \sum_{(i,j)\sigma} (S_{i\sigma}^\dagger S_{i\bar{\sigma}} p_{j\bar{\sigma}}^\dagger p_{j\sigma} - S_{i\bar{\sigma}}^\dagger S_{i\sigma} p_{j\sigma}^\dagger p_{j\bar{\sigma}}) \\ & + \sum_{\substack{(i,L)(i,j)\sigma \\ l \neq j}} \frac{1}{2} [J_3 (S_{i\sigma}^\dagger S_{i\bar{\sigma}} p_{l\bar{\sigma}}^\dagger p_{l\sigma}) - (J'_3 S_{i\bar{\sigma}}^\dagger S_{i\sigma} - t_0^2/\varepsilon_p S_{i\sigma}^\dagger S_{i\sigma}) p_{l\sigma}^\dagger p_{l\sigma}] \\ & + J_1 \sum_{\substack{(i,l)(l,j) \\ i \neq j}} S_{i\alpha}^\dagger S_{j\beta}^\dagger (S_{j\alpha} S_{i\beta} + S_{i\alpha} S_{j\beta}) \left[1 - \sum_\sigma p_{l\sigma}^\dagger p_{l\sigma} \right] \\ & + U_p \sum_{j\sigma} p_{j\alpha}^\dagger p_{j\alpha} p_{j\beta}^\dagger p_{j\beta} + \mu_1 \sum_i \left[\sum_\sigma S_{i\sigma}^\dagger S_{i\sigma} - 1 \right] + \mu_2 \left[\sum_{j\sigma} p_{j\sigma}^\dagger p_{j\sigma} - \delta N \right], \quad (7) \end{aligned}$$

where

$$J_1 = 4t_0^4 [1/(\varepsilon_p + U_{p/2}) + 1/U_d] / \varepsilon_p^2,$$

$$J_2 = t_0^2 [1/(\varepsilon_p + U_p) + 1/(U_d - \varepsilon_p)],$$

$$J_3 = t_0^2 [1/\varepsilon_p + 1/(U_d - \varepsilon_p)],$$

and

$$J'_3 = t_0^2 / (U_d - \varepsilon_p).$$

In fourth-order we only preserve the Cu-Cu superexchange interaction which determines the background spin state of the Cu hole. This Cu-Cu interaction mainly occurs when the intermediate O site is empty ($J_1 \sim 0.12$

eV); otherwise this interaction will be reduced to almost zero

$$[J'_1 = 4t_0^4 / U_d (\varepsilon_p + U_p)^2 \sim 0.004 \text{ eV}].$$

For the same reason, the O-O superexchange interaction has been neglected in the intermediate Cu-site single-occupation case. In Eq. (7) the third term represents the antiferromagnetic (AF) interaction between neighboring Cu and O sites. (The motion of O holes is mainly reflected in the fourth term, $J_3 S_{i\sigma}^\dagger S_{i\bar{\sigma}} p_{l\bar{\sigma}}^\dagger p_{l\sigma}$, i.e., a Cu-O singlet pair transfer from one pair of sites to another through the spin flip of a Cu hole. We believe that the motion should destroy the Cu-Cu AF long-range order because it causes the Cu spin flip, but the Cu-Cu spin

correlation remains due to the Cu-Cu AF interaction.) Both of these terms are responsible for the forming of Cu-O spin-singlet pairs and their correlative motion in the Cu-Cu RVB background.

Going over to momentum space and applying a Hartree-Fock factorization by retaining all the possible nonzero pairing condensations (order parameters) $\langle S_{i\sigma}^\dagger S_{j\bar{\sigma}}^\dagger \rangle$ and $\langle p_{i\sigma}^\dagger S_{j\bar{\sigma}}^\dagger \rangle$, etc., we obtain

$$\begin{aligned} \hat{H}_{\text{eff}} = & \sum_{\mathbf{k}\sigma} \xi_{1\mathbf{k}} S_{\mathbf{k}\sigma}^\dagger S_{\mathbf{k}\sigma} + \sum_{\mathbf{k}\sigma} \xi_{2\mathbf{k}} p_{\mathbf{k}\sigma}^\dagger p_{\mathbf{k}\sigma} \\ & - \sum_{\mathbf{k}} \left[\lambda_{1\mathbf{k}}^* S_{-\mathbf{k}\beta} S_{\mathbf{k}\alpha} + \lambda_{2\mathbf{k}}^* \sum_{\sigma} \sigma p_{-\mathbf{k}\bar{\sigma}} S_{\mathbf{k}\sigma} + \text{H.c.} \right] \\ & + \text{const}, \end{aligned} \quad (8)$$

where

$$\begin{aligned} \lambda_{1\mathbf{k}}^* &= \frac{3}{2} J_1 \Delta_1^* v_{1\mathbf{k}} (1 - \delta/2), \quad \lambda_{2\mathbf{k}}^* = \frac{3}{2} J_{2\text{eff}} \Delta_2^* v_{2\mathbf{k}}, \\ \xi_{1\mathbf{k}} &= -\frac{3}{2} J_1 \langle S_{i\sigma}^\dagger S_{j\sigma} \rangle v_{1\mathbf{k}} (1 - \delta/2) - \bar{\mu}_1, \\ \xi_{2\mathbf{k}} &= \frac{1}{2} (J_2 - J_3') v_{0\mathbf{k}} - \bar{\mu}_2, \\ \Delta_1^* &= \langle S_{i\alpha}^\dagger S_{j\beta}^\dagger \rangle, \quad \Delta_2^* = \langle p_{i\alpha}^\dagger S_{j\beta}^\dagger \rangle, \\ J_{2\text{eff}} &= J_2 + J_3 + J_{3'/2}, \quad v_{0\mathbf{k}} = 4 \cos(k_x/2) \cos(k_y/2), \\ v_{1\mathbf{k}} &= 2[\cos(k_x) + \cos(k_y)], \\ v_{2\mathbf{k}} &= 2[\cos(k_x/2) + \cos(k_y/2)]. \end{aligned}$$

Here, i and j represent the nearest neighbors.

The renormalized chemical potentials $\bar{\mu}_1$ and $\bar{\mu}_2$ are determined by the conditions $\sum_{\sigma} \langle S_{i\sigma}^\dagger S_{i\sigma} \rangle = 1$ and $\sum_{\sigma} \langle p_{j\sigma}^\dagger p_{j\sigma} \rangle = \delta/2$.

Because there is no direct interaction between O holes the order parameter $\langle p_{i\sigma}^\dagger p_{j\bar{\sigma}}^\dagger \rangle$ does not appear in the Hamiltonian. But the pairing condensations of $\langle S_{j\beta} S_{i\alpha} \rangle$ and $\langle S_{j\beta} p_{i\alpha} \rangle$ lead to a nonzero O-hole pairing condensation. This can be easily confirmed by investigating the equations of motion for the Green's functions. We find that it is necessary to introduce the anomalous Green's function of the O hole into the motion equations in order to make them closed as shown below.

It is convenient first to diagonalize the Hamiltonian $\hat{H}_{\text{eff}}$ by the quasiparticle operators $\hat{O}_m$:

$$\begin{aligned} \hat{O}_m &= \sum_{n=1}^4 a_{nm} \hat{f}_n, \quad m=1, \dots, 4, \\ a_{1m} &= -A_m \{ [\xi_{1\mathbf{k}} + \hbar w_m(\mathbf{k})] [\xi_{2\mathbf{k}}^2 - \hbar w_m^2(\mathbf{k})] \\ &\quad + |\lambda_{2\mathbf{k}}|^2 [\xi_{2\mathbf{k}} + \hbar w_m(\mathbf{k})] \}, \\ a_{2m} &= A_m \lambda_{1\mathbf{k}}^* [\xi_{2\mathbf{k}}^2 - \hbar w_m^2(\mathbf{k})], \\ a_{3m} &= A_m \lambda_{1\mathbf{k}}^* \lambda_{2\mathbf{k}} [\xi_{2\mathbf{k}} + \hbar w_m(\mathbf{k})], \\ a_{4m} &= A_m \{ \lambda_{2\mathbf{k}}^* [\xi_{1\mathbf{k}} + \hbar w_m(\mathbf{k})] [\xi_{2\mathbf{k}} - \hbar w_m(\mathbf{k})] \\ &\quad + |\lambda_{2\mathbf{k}}|^2 \lambda_{2\mathbf{k}}^* \}, \end{aligned} \quad (9)$$

where $\hat{f}_1 = S_{\mathbf{k}\alpha}$, $\hat{f}_2 = S_{-\mathbf{k}\beta}^\dagger$, $\hat{f}_3 = p_{\mathbf{k}\alpha}$, $\hat{f}_4 = p_{-\mathbf{k}\beta}^\dagger$, and A_m are defined by the condition: $\sum_{n=1}^4 a_{nm}^* a_{nm} = 1$. The corresponding eigenvalues are (here we have omitted the in-

dex k of the preceding quantities appearing for simplicity)

$$\hbar w_l(\mathbf{k}) = \pm \{ U(\mathbf{k}) \pm [U^2(\mathbf{k}) - V(\mathbf{k})]^{1/2} \}^{1/2}, \quad l=1, \dots, 4,$$

$$U(\mathbf{k}) = \frac{1}{2} (\xi_{1\mathbf{k}}^2 + \xi_{2\mathbf{k}}^2 + |\lambda_{1\mathbf{k}}|^2 + 2|\lambda_{2\mathbf{k}}|^2), \quad (10)$$

$$V(\mathbf{k}) = \xi_{1\mathbf{k}}^2 \xi_{2\mathbf{k}}^2 + 2\xi_{1\mathbf{k}} \xi_{2\mathbf{k}} |\lambda_{2\mathbf{k}}|^2 + \xi_{2\mathbf{k}}^2 |\lambda_{1\mathbf{k}}|^2 + |\lambda_{2\mathbf{k}}|^4.$$

Then we define the single-particle Green's functions (including anomalous ones) as follows:

$$G_{mn}(\mathbf{k}, \tau) = \langle T_\tau \hat{f}_m(\mathbf{k}, \tau) \hat{f}_n^+(\mathbf{k}, 0) \rangle, \quad m, n=1, \dots, 4. \quad (11)$$

τ is an imaginary time, T_τ is the imaginary time-ordering operator and $\langle \rangle$ denotes an expectation value in the system described by $\hat{H}_{\text{eff}}$. Transforming to Matsubara frequencies, we find that

$$G_{mn}(\mathbf{k}, i\omega_q) = \sum_l \frac{a_{ml}(\mathbf{k}) a_{nl}^*(\mathbf{k})}{i\omega_q - \hbar w_l(\mathbf{k})}. \quad (12)$$

The self-consistent equations for the order parameters and chemical potentials are obtained as follows:

$$\langle S_{i\alpha}^\dagger S_{i\alpha} \rangle = \frac{1}{2} = \frac{1}{N} \sum_{\mathbf{k}, l} g(l, \mathbf{k}) a_{il}^*(\mathbf{k}) a_{il}(\mathbf{k}), \quad (13)$$

$$\langle p_{j\alpha}^\dagger p_{j\alpha} \rangle = \frac{\delta}{4} = \frac{1}{2N} \sum_{\mathbf{k}, l} g(l, \mathbf{k}) a_{3l}^*(\mathbf{k}) a_{3l}(\mathbf{k}), \quad (14)$$

$$\langle S_{i\alpha}^\dagger S_{j\beta}^\dagger \rangle = \frac{1}{4N} \sum_{\mathbf{k}, l} g(l, \mathbf{k}) v_{1\mathbf{k}} a_{il}^*(\mathbf{k}) a_{2l}(\mathbf{k}), \quad (15)$$

$$\langle p_{i\alpha}^\dagger S_{j\beta}^\dagger \rangle = \frac{1}{4\sqrt{2}N} \sum_{\mathbf{k}, l} g(l, \mathbf{k}) v_{2\mathbf{k}} a_{3l}^*(\mathbf{k}) a_{2l}(\mathbf{k}), \quad (16)$$

$$\langle S_{i\alpha}^\dagger S_{j\alpha} \rangle = \frac{1}{4N} \sum_{\mathbf{k}, l} g(l, \mathbf{k}) v_{1\mathbf{k}} a_{1l}^*(\mathbf{k}) a_{1l}(\mathbf{k}), \quad (17)$$

where, $g(l, \mathbf{k})$ is the fermion distribution function,

$$g(l, \mathbf{k}) = \frac{1}{\exp[\beta \hbar w_l(\mathbf{k}) + 1]}. \quad (18)$$

When both orders Δ_1 and Δ_2 are nonzero, the O-hole pairing condensation is also not zero and is given by

$$\langle p_{i\alpha}^\dagger p_{-k\beta}^\dagger \rangle = \sum_l g(l, \mathbf{k}) a_{3l}^*(\mathbf{k}) a_{4l}(\mathbf{k}). \quad (19)$$

It is important to note that the orders $\langle S_{i\beta} S_{j\alpha} \rangle$ and $\langle S_{i\beta} p_{j\alpha} \rangle$ do not give rise to superconductivity themselves, because in real physical space the condensations of Cu-Cu pairs and Cu-O pairs correspond to $\langle C_{i\beta} C_{j\alpha} \rangle$ and $\langle C_{i\beta} p_{j\alpha} \rangle$, respectively, which are really zero because of the single occupation conditions of the Cu site: $\langle e_i^\dagger e_i \rangle = 0$ and $\langle d_i^\dagger d_i \rangle = 0$.

$$\langle C_{i\beta} C_{j\alpha} \rangle = \langle (e_i^\dagger S_{i\beta} - d_i S_{i\alpha}^\dagger) (e_j^\dagger S_{j\alpha} + d_j S_{j\beta}^\dagger) \rangle = 0, \quad (20)$$

$$\langle C_{i\beta} p_{j\alpha} \rangle = \langle (e_i^\dagger S_{i\beta} - d_i S_{i\alpha}^\dagger) p_{j\alpha} \rangle = 0. \quad (21)$$

These two nonzero order parameters Δ_1 and Δ_2 can only exhibit spin-singlet pairs of Cu-Cu holes (similar to Anderson's half-filled RVB state⁸) and Cu-O holes. This kind of strong correlation between Cu-Cu and Cu-O spins should result in some correlation between two O holes, i.e., the pairing condensation $\langle p_{i\beta} p_{j\alpha} \rangle$ will be nonzero. Physically doped O holes, couple strongly with neighboring Cu spins and break down the surrounding Cu-Cu spin-singlet pairs, and the system loses Cu-Cu exchange energy. Two doped O holes attract each other so as to decrease the energy loss by surrounding Cu holes, gaining some Cu-Cu exchange energy. This kind of attraction could lead to O-hole singlet pairing condensation. But the O pair condensation is not an *s*-wave one and our numerical results have shown that the next-nearest neighbors have the largest pairing condensation as shown in the following section.

III. RESULTS AND DISCUSSIONS

In our calculation, we choose the values of parameters^{16,18} as follows: $t_0 = 1$ eV, $\epsilon_p = 3$ eV, and $U_\alpha = U_p = 8$ eV. Then we get that $J_1 = 0.12$ eV, $J_{2\text{eff}} = 0.91$ eV. The AF coupling between the Cu-O neighboring holes $J_{2\text{eff}}$ is much larger than the other energy scales (ξ_{1k}, ξ_{2k}, J_1). In this strong Cu-O coupling limit meanfield theory could also provide a reasonable description.¹⁹ The Cu and O holes must form bound spin-singlet pairs. At zero temperature these bound pairs condense into the lowest-energy state with total momentum $q=0$. The chemical potential should correspond to the binding energy $-J_{2\text{eff}}$, and not change much with the doping concentration δ . In the small doping case, the order parameter should be approximately proportional to $\delta^{1/2}$. Our numerical results have proved all these points.

We have solved Eqs. (13)–(17) self-consistently at zero temperature. In Figs. 1 and 2 the order parameters Δ_1 and Δ_2 are shown as functions of the doping concentration δ , respectively. As shown in Fig. 1, when δ exceeds about 20%, the order parameter will go to zero, so the

FIG. 1. The order parameter $\langle S_{i\beta} S_{j\alpha} \rangle$ as a function of the doping concentration δ ; the parameters are chosen as $t_0 = 1$ eV, $\epsilon_p = 3$ eV, $U_d = U_p = 8$ eV.

FIG. 2. The order parameter $\langle S_{i\beta} p_{j\alpha} \rangle$ as a function of the doping concentration δ , with the same parameters as in Fig. 1.

superconductivity should be destroyed completely.

The O-pair condensation is the spin-singlet one

$$\langle p_{i\alpha}^\dagger p_{j\beta}^\dagger \rangle = \frac{1}{2N} \sum_{\mathbf{k}} e^{i\mathbf{k} \cdot (\mathbf{R}_i - \mathbf{R}_j)} \langle p_{\mathbf{k}\alpha}^\dagger p_{-\mathbf{k}\beta}^\dagger \rangle. \quad (22)$$

In Fig. 3 the pairing condensation of the next-nearest neighbors of O holes is shown as a function δ , which is the largest one among all the O-pair condensations. And in the mean-field approximation, two such neighbors have equal values of the condensation. But taking into account the strong Cu-O singlet pair correlation, the condensation of the pairs which are connected by a middle Cu site is suppressed and only the other remains large. The nearest-neighbor pair is suppressed because the intermediate Cu hole interacting with two neighboring O holes through a strong Cu-O AF coupling should result in an effective O-O nearest-neighbor ferromagnetic correlation. It can be seen from Fig. 3 that in the region of doping concentration δ less than 20% of this condensation is nonzero. The system shows superconductivity in this region.

Now we discuss the thermodynamic properties of the system. As seen from Eq. (10), the system consists of two

FIG. 3. The O-pair condensation of next-nearest-neighbor $\langle p_{i\beta} p_{j\alpha} \rangle$ as a function of the doping concentration δ , with the same parameters as in Fig. 1.

kinds of excitations. Because $\bar{\mu}_2 \sim -J_{2\text{eff}}$ is much larger than the other energy values, we can approximately get that

$$\begin{aligned} \hbar W_1(\mathbf{k}) &= \{U(\mathbf{k}) + [U^2(\mathbf{k}) - V(\mathbf{k})]^{1/2}\}^{1/2} \\ &\approx (\xi_{2\mathbf{k}}^2 + 2|\lambda_{2\mathbf{k}}|^2 - 2\xi_{1\mathbf{k}}|\lambda_{2\mathbf{k}}|^2/\xi_{2\mathbf{k}})^{1/2}, \end{aligned} \quad (23)$$

$$\begin{aligned} \hbar W_2(\mathbf{k}) &= \{U(\mathbf{k}) - [U(\mathbf{k}) - V(\mathbf{k})]^{1/2}\}^{1/2} \\ &\approx [(\xi_{1\mathbf{k}} - |\lambda_{2\mathbf{k}}|^2/\xi_{2\mathbf{k}})^2 + |\lambda_{1\mathbf{k}}|^2]^{1/2}. \end{aligned} \quad (24)$$

Then we can see that the former is the excitation breaking of the Cu-O pair, which is not important in the low-temperature case because of the large Cu-O bonding energy. The latter is the RVB-like one (in the small doping case) breaking the Cu-Cu pair, which is gapless [in the two-dimensional Brillouin zone there are eight points which have zero values of $V(\mathbf{k})$, so also zero values of $\hbar W_2(\mathbf{k})$]. From the approximate formula (24), we can see that this excitation is very like the single band one of Anderson *et al.*⁶⁻⁸ $[(\xi_{1\mathbf{k}}^2 + \lambda_{1\mathbf{k}}^2)^{1/2}]$. The energy $\xi_{1\mathbf{k}}$ is

changed by a term $U_{2\mathbf{k}}|\xi_{2\mathbf{k}}|^2$ proportional to $\delta J_{2\text{eff}}$ which is due to the Cu-O spin interaction. This gapless excitation contributes a nonexponential term to the low-temperature specific heat and spin susceptibility which is consistent with experiments.

In conclusion, we have given a mean-field description of the two-dimensional planar CuO_2 system. Because of the strong AF coupling between the nearest-neighbor Cu-Cu and Cu-O holes, the system consists of two kinds of spin-singlet pairs. They interact with each other and lead to O-hole pairing condensation which is responsible for superconductivity. We also study the excitation properties of the system, the RVB-like excitation still proves gapless which leads to a nonexponential term in the low-temperature specific heat and spin susceptibility.

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