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Superconductivity in doped planar CuO_2 systems

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Abstract. We present a model to describe high-T_c superconductivity in doped planar CuO_2 systems. Each doped hole on the oxygen site interacts through strong antiferromagnetic (AF) coupling with two neighbouring copper holes to form Cu–O spin singlet pairs and interacts with a Cu–RVB state to lead to the condensation of O holes in momentum space, which is responsible for the superconductivity. The ground state of this system and the spin correlation of Cu and O holes are also studied. The results are in good agreement with previous works.

1. Introduction

Experiments [1–2] show that strong electron correlation induced magnetism plays an essential role in the newly discovered high-T_c superconductivity. One of the most important problems [3] is: why does small doping (about 5%) destroy the magnetic order thoroughly and drive the material into a superconducting state? Anderson *et al* [4–6] believe that the extra holes make it more difficult to keep the AF order and that the spins are in some sort of spin liquid phase (RVB state). Doped holes mainly occupy Cu sites and form boson solitons, and superconductivity is caused by the boson condensation in the RVB background. However, experiments [7] have shown that doped holes mainly occupy the O sites and Emery [8] has proposed a more general model which takes into account explicitly the oxygen p-orbitals connecting two neighbouring copper sites. Although much work [9–11] has been done in this respect, it is not clear [12] which part and what interactions in the CuO_2 layer are really responsible for the high-T_c superconductivity.

In this paper, a possible superconductive mechanism of this strong correlated system is studied by the Gutzwiller approximation method [13], which treats the single occupation condition by the Gutzwiller projection operator and relates the quantum mechanical expectation values in the correlated system to the corresponding uncorrelated ones by a classical weighting factor. This approach method was used for the heavy fermion problem by Rice and Ueda [14] and for the one-band RVB state superconductivity problem by Zhang *et al* [15], which has been shown to be very reasonable. We describe the correlative motions of O and Cu holes using Emery's two-band Hamiltonian. Since there are strong AF interactions of Cu–O holes and of Cu–Cu holes induced from the Cu–O hopping term in the strong correlation limit, we expect that there must be two kinds of spin singlet pair correlations: Cu–Cu and Cu–O. Then in the uncorrelated

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system (relax the Cu site single occupation condition) there should be two kinds of non-zero order parameters $\langle d_{j\beta}d_{i\alpha}\rangle_0$ and $\langle d_{i\beta}p_{j\alpha}\rangle_0$ and non-zero O pair condensation. In the corresponding strong correlated system only O pair condensation remains and contributes to superconductivity.

In the following sections we perform the mean-field theory of our model, study the ground state wavefunction and conclude with some discussions.

2. Theory

We start from the two-band Hubbard Hamiltonian describing a single CuO_2 layer:

$$\hat{H} = -\sum_{(i,j)\sigma} t(d^+_{i\sigma}p_{j\sigma} + \text{HC}) + \varepsilon_p \sum_{j\sigma} p^+_{j\sigma}p_{j\sigma} + U_d \sum_i d^+_{i\alpha}d_{i\alpha}d^+_{i\beta}d_{i\beta}. \tag{1}$$

For equation (1) the vacuum is defined as a filled Cu d^{10} and O p^6 state. The operator $d^+_{i\sigma}$ creates a $Cu(3d_{x^2-y^2})$ hole at site i, and $p^+_{j\sigma}$ creates an $O(2p_x, 2p_y)$ hole at site j. The summation of (i, j) is taken over the nearest-neighbour Cu and O sites.

For the sake of simplicity, we have neglected the on-site Coulomb correlation (U_p) of O holes and the intersite Coulomb correlation (V) between neighbouring Cu and O holes because of the low density of O holes and the smallness of V. We set the site energy of Cu holes $\varepsilon_d = 0$, and consider the case $\varepsilon_p > 0$. In the small t [16] limit, the first term in equation (1) can be treated as a perturbation term. Keeping one hole per Cu site, and by projecting out virtual states in which the copper site is doubly occupied or empty, we obtain the effective Hamiltonian [12]:

$$\begin{aligned}\hat{H}_{\text{eff}} = &-(4t^2/\varepsilon_p)\sum_{i\sigma} d^+_{i\sigma}d_{i\sigma} + (\varepsilon_p + 2t^2/\varepsilon_p)\sum_{j\sigma} p^+_{j\sigma}p_{j\sigma} \\ &+ J_2 \sum_{(i,j)\sigma} (d^+_{i\sigma}d_{i\bar{\sigma}}p^+_{j\bar{\sigma}}p_{j\sigma} - d^+_{i\bar{\sigma}}d_{i\bar{\sigma}}p^+_{j\sigma}p_{j\sigma}) \\ &+ \sum_{\substack{(i,l)(i,j)\sigma \\ l\neq j}} \tfrac{1}{2}\{J_2 d^+_{i\sigma}d_{i\bar{\sigma}}p^+_{l\bar{\sigma}}p_{j\sigma} - [J'_2 d^+_{i\bar{\sigma}}d_{i\bar{\sigma}} - (t^2/\varepsilon_p)d^+_{i\sigma}d_{i\sigma}]p^+_{l\sigma}p_{j\sigma}\} \\ &+ J_1 \sum_{(i,j)} d^+_{i\alpha}d^+_{j\beta}(d_{j\alpha}d_{i\beta} + d_{i\alpha}d_{j\beta})\end{aligned} \tag{2}$$

where $J_1 = 4t^2(1/\varepsilon_p^3 + 1/\varepsilon_p^2 U_d)(1 - \delta/2)$, $J_2 = t^2[1/\varepsilon_p + 1/(U_d - \varepsilon_p)]$, $J'_2 = t^2/(U_d - \varepsilon_p)$. δ is the doping concentration of O holes and N is the number of the Cu site.

In fourth order we only preserve the Cu–Cu AF interaction which determines the background spin state of Cu holes. This interaction mainly occurs when the intermediate O site is empty. When O site is occupied it will be reduced to almost zero. For the same reason the O–O super-exchange interaction has been neglected in the Cu site's single-occupation case. In equation (2) both the third and the fourth terms are responsible for the forming of the Cu–O spin singlet pair and its correlative motion in the background of the Cu–Cu RVB state.

The effective Hamiltonian contains the strict local constraint of Cu single occupation. This may be treated by the Gutzwiller approximation method: that is, first we relax the Cu site single occupation condition and get the corresponding uncorrelated wavefunction $|\varphi\rangle$. The strong correlated wavefunction $|\Psi\rangle$ could be obtained by imposing a projection operator $\hat{P}_N$ on $|\varphi\rangle$ which projects out the configurations in which the site is

doubly occupied and fix the Cu hole number as N. And the effect of the projection operator on the double occupied sites is taken into account by a classical statistical weighting factor which multiplies the quantum coherent result calculated with $|\varphi\rangle$ in this approximation.

First we relax the local single occupation condition and study the uncorrelated system. Using the Hartree–Fock self-consistent field approximation for $\hat{H}_{\text{eff}}$ and transforming to Bloch representation, we obtain

$$\hat{H}_{\text{eff}} = \sum_{k\sigma} \varepsilon_{1k} d^+_{k\sigma} d_{k\sigma} + \sum_{k\sigma} \varepsilon_{2k} p^+_{k\sigma} p_{k\sigma} - \sum_k (\lambda^*_{1k} d_{k\beta} d_{k\alpha} + \lambda^*_{2k} \sum \sigma p_{k\bar{\sigma}} d_{k\sigma}$$

$$+ \text{HC}) + \text{const. term} \tag{3}$$

where

$$\lambda^*_{1k} = \tfrac{3}{2} J_1 \Delta^*_1 \nu_{1k} \qquad \lambda^*_{2k} = \tfrac{3}{2} J_{2\text{eff}} \Delta^*_2 \gamma_{2k}$$

$$\varepsilon_{1k} = -\tfrac{3}{2} J_1 \langle d^+_{i\sigma} d_{j\sigma} \rangle_0 \nu_{1k} - \mu_1 \qquad \varepsilon_{2k} = \tfrac{1}{4}(t^2/\varepsilon_p - J'_2)\nu_{0k} - \mu_2$$

$$\Delta^*_1 = \langle d^+_{i\alpha} d^+_{j\beta} \rangle_0 \qquad \Delta^*_2 = \langle p^+_{i\alpha} d^+_{j\beta} \rangle_0$$

$$J_{2\text{eff}} = 2J_2 + J'_2/2 \qquad \nu_{0k} = 4\, cos(k_x/2) \cos(k_y/2)$$

$$\nu_{1k} = 2[\cos(k_x) + \cos(k_y)] \qquad \nu_{2k} = 2[\cos(k_x/2) + \cos(k_y/2)].$$

Here, i and j represent nearest neighbours.

The chemical potentials μ_1 and μ_2 are determined by the conditions $\Sigma_\sigma \langle d^+_{i\sigma} d_{i\sigma} \rangle = 1$ and $\Sigma_\sigma \langle p^+_{j\sigma} p_{j\sigma} \rangle = \delta/2$.

Although there is no direct interaction between O holes, the non-zero order parameters Δ_1 and Δ_2 will lead to O pair condensation. This can be easily confirmed by investigating the equations of motion for Green functions. We find that it is necessary to introduce the anomalous Green function of the O hole into the equations in order to make them closed.

We diagonalise the Hamiltonian $\hat{H}_{\text{eff}}$ by the quasiparticle operators $\hat{O}_m$ (we have omitted the detailed form of them [17]):

$$\hat{O}_m = \sum_{n=1}^{4} a_{nm} \hat{h}_n \qquad (m = 1 \ldots 4) \tag{4}$$

where $\hat{h}_1 = d_{k\alpha}, \hat{h}_2 = d^+_{-k\beta}, \hat{h}_3 = p_{k\alpha}, \hat{h}_4 = p^+_{-k\beta}$. The corresponding eigenvalues are (here we have omitted the index k of the quantities appearing above for simplicity):

$$\omega_l(\boldsymbol{k}) = \pm[U(\boldsymbol{k}) \pm (U^2(\boldsymbol{k}) - V(\boldsymbol{k}))^{1/2}]^{1/2}$$

$$U(\boldsymbol{k}) = \tfrac{1}{2}[\varepsilon^2_{1k} + \varepsilon^2_{2k} + |\lambda_{1k}|^2 + 2|\lambda_{2k}|^2] \tag{5}$$

$$V(\boldsymbol{k}) = \varepsilon^2_{1k}\varepsilon^2_{2k} + 2\varepsilon_{1k}\varepsilon_{2k}|\lambda_{2k}|^2 + \varepsilon^2_{2k}|\lambda_{1k}|^2 + |\lambda_{2k}|^4.$$

We then define the single-particle Green functions (including anomalous ones) as follows:

$$G_{mn}(\boldsymbol{k}, \tau) = \langle T_\tau(\hat{h}_m(\boldsymbol{k}, \tau)\hat{h}_n^+(\boldsymbol{k}, 0))\rangle \qquad (m, n = 1 \ldots 4) \tag{6}$$

where τ is an imaginary time and T_τ is the imaginary time ordering operator. Transforming to Matsubara frequencies, we find that

$$G_{mn}(\boldsymbol{k}, \mathrm{i}\omega_q) = \sum_l a_{ml}(\boldsymbol{k})a_{nl}^*(\boldsymbol{k})/\mathrm{i}\omega_q - \omega_l(\boldsymbol{k}).$$

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

$$\langle d_{i\alpha}^+ d_{i\alpha}\rangle_0 = \tfrac{1}{2} = \frac{1}{N}\sum_{k,l} f(\omega_l(\boldsymbol{k}))a_{1l}^*(\boldsymbol{k})a_{1l}(\boldsymbol{k}) \tag{7}$$

$$\langle p_{j\alpha}^+ p_{j\alpha}\rangle_0 = \delta/4 = (1/2N)\sum_{k,l} f(\omega_l(\boldsymbol{k}))a_{3l}^*(\boldsymbol{k})a_{3l}(\boldsymbol{k}) \tag{8}$$

$$\langle d_{i\alpha}^+ d_{j\beta}^+\rangle_0 = (1/4N)\sum_{k,l} f(\omega_l(\boldsymbol{k}))\nu_{1k}a_{1l}^*(\boldsymbol{k})a_{2l}(\boldsymbol{k}) \tag{9}$$

$$\langle p_{i\alpha}^+ d_{j\beta}^+\rangle_0 = (1/4N\sqrt{2})^{-1}\sum_{k,l} f(\omega_l(\boldsymbol{k}))\nu_{2k}a_{3l}^*(\boldsymbol{k})a_{2l}(\boldsymbol{k}) \tag{10}$$

$$\langle d_{i\alpha}^+ d_{j\alpha}\rangle_0 = (1/4N)\sum_{k,l} f(\omega_l(\boldsymbol{k}))\nu_{1k}a_{1l}^*(\boldsymbol{k})a_{1l}(\boldsymbol{k}) \tag{11}$$

where $f(\omega)$ is the Fermi distribution function

$$f(\omega) = [\exp(\beta\omega) + 1]^{-1}.$$

When both Δ_1 and Δ_2 are non-zero, the O pair condensation is not zero and is given by:

$$\langle p_{k\alpha}^+ p_{-k\beta}^+\rangle = \sum_l f(\omega_l(\boldsymbol{k}))a_{3l}^*(\boldsymbol{k})a_{4l}(\boldsymbol{k}). \tag{12}$$

(We prefer the RVB-like Cu spin state to the antiferromagnetic state as a result of strong Cu–O AF coupling $J_{2\mathrm{eff}}$ (about 1 eV). This interaction should induce effective ferromagnetic correlation in neighbouring Cu sites and may flip the Cu spin when the O hole is hopping away. So this interaction should frustrate and destroy the Cu AF long-range order and prefer spin liquid phase. A similar problem has been studied by Andrei and Coleman [18], and they suggested the possibility of novel ground states (spin liquid state), and that the formation of the novel ground state might pre-empt the formation of an antiferromagnet because of the local AF exchange interaction between Cu and O holes even in the case of neglecting the p band dispersion.)

Now we restore the Cu site single-occupation condition by imposing the Gutzwiller projection operator on the uncorrelated ground state $|\varphi\rangle$, and treat this operator by the Gutzwiller approximation to study the correlated system. Then the quantum mechanical expectation values are related as follows:

$$\langle A\rangle = g\langle A\rangle_0 \tag{13}$$

where $\langle A\rangle$ and $\langle A\rangle_0$ are the expectation values in the states $|\Psi\rangle$ and $|\varphi\rangle$ respectively. The renormalisation factor g is determined by the ratios of the probabilities of the corresponding physical processes in the states $|\Psi\rangle$ and $|\varphi\rangle$. Although there are non-zero

order parameters Δ_1 and Δ_2 in the uncorrelated system, they do not represent the superconductivity order parameters of the correlated system [15]. The condensation of Cu–Cu pairs and Cu–O pairs are really zero in the correlated system because the corresponding physical processes could not take place in the Cu site single-occupation case (zero probability). But the spin singlet pair correlations of Cu–Cu and Cu–O remain (similar to Anderson's half-filled RVB state) and are renormalised by a factor [15]:

$$\langle \boldsymbol{S}_i \cdot \boldsymbol{S}_j \rangle = g_s \langle s_i \cdot s_j \rangle_0 \tag{14}$$

$$g_s = \frac{(n_{j\sigma} n_{i\bar{\sigma}} n_{j\sigma}, n_{i\bar{\sigma}'})^{1/2}}{[n_{j\sigma}(1-n_{j\bar{\sigma}}) n_{i\bar{\sigma}}(1-n_{i\sigma}) n_{j\sigma'}(1-n_{j\bar{\sigma}'}) n_{i\bar{\sigma}'}(1-n_{i\sigma})]^{1/2}} = 4$$

or

$$g_s = \frac{(n_{i\sigma} n_{i\sigma'})^{1/2}}{[n_{i\sigma}(1-n_{i\bar{\sigma}}) n_{i\sigma'}(1-n_{i\bar{\sigma}'})]^{1/2}} = 2$$

for Cu–Cu or Cu–O respectively. And $n_{i\sigma} = \langle d^+_{i\sigma} d_{i\sigma} \rangle$. In the correlated system only O pair condensation remains unchanged because this condensation does not change the Cu hole configuration, and the probability of the corresponding physical processes in the states $|\Psi\rangle$ and $|\varphi\rangle$ remains unchanged:

$$\langle p^+_{i\alpha} p^+_{j\beta} \rangle = \langle p^+_{i\alpha} p^+_{j\beta} \rangle_0. \tag{15}$$

Superconductivity is caused by this O pair condensation.

3. Superconducting ground state

In this section we want to study the ground state of the system by a reasonable approximation. We choose the parameters as follows: $t = 1.0\,\text{eV}$, $\varepsilon_p = 3.0\,\text{eV}$, $U_d = 8.0\,\text{eV}$. Then we have $J_1 = 0.20\,\text{eV}$, $J_{2_{\text{eff}}} = 1.16\,\text{eV}$. Because the effective Cu–O coupling $J_{2_{\text{eff}}}$ is much larger than that of Cu–Cu, we first diagonalise the Cu–O interacting term of the Hamiltonian (3) by the quasiparticle operators $\xi_{k\sigma}$ and $\eta_{k\sigma}$:

$$\xi_{k\sigma} = u_k d_{k\sigma} + \sigma v_k p^+_{\bar{k}\bar{\sigma}}$$

$$\eta_{k\sigma} = -\sigma v_k d_{k\sigma} + u_k p^+_{\bar{k}\sigma}$$

$$u_k = \frac{\lambda_{2k}}{[|\lambda_{2k}|^2 + (\varepsilon_{1k} - E_{1k})^2]^{1/2}}$$

$$v_k = \frac{\varepsilon_{1k} - E_{1k}}{[|\lambda_{2k}|^2 + (\varepsilon_{1k} - E_{1k})^2]^{1/2}}$$

$$E_{ik} = (\varepsilon_{1k} - \varepsilon_{2k})/2 \pm \tfrac{1}{2}[(\varepsilon_{1k} + \varepsilon_{2k})^2 + 4|\lambda_{2k}|^2]^{1/2} \qquad (i = 1, 2). \tag{16}$$

The Hamiltonian becomes

$$\hat{H}_{\text{eff}} = \sum_{k\sigma} E_{lk} \xi^+_{k\sigma} \xi_{k\sigma} + \sum_{k\sigma} E_{2k} \eta^+_{k\sigma} \eta_{k\sigma}$$

$$- \left\{ \sum_k \lambda^*_{1k} [u_k^2 \xi_{-k\beta} \xi_{k\alpha} - v_k^2 \eta_{-k\beta} \eta_{k\alpha} - u_k v_k (\xi_{k\alpha} \eta_{-k\beta} + \xi_{-k\beta} \eta_{k\alpha})] + \text{HC} \right\}$$

$$+ \text{const. term.} \tag{17}$$

In the no Cu–Cu interaction case, the self-consistent equations for chemical potentials and order parameter Δ_2 are

$$\langle d_{i\sigma}^{+} d_{i\sigma} \rangle = \tfrac{1}{2} = (1/N) \sum_k \{u_k^2 f(E_{1k}) + v_k^2 f(E_{2k})\} \tag{18}$$

$$\langle p_{j\sigma}^{+} p_{j\sigma} \rangle = (\delta/4) = (1/2N) \sum_k \{1 - u_k^2 f(E_{2k}) - v_k^2 f(E_{1k})\} \tag{19}$$

$$\langle p_{i\alpha}^{+} d_{j\beta}^{+} \rangle = (4N\sqrt{2})^{-1} \sum_k \{\nu_{2k} u_k v_k [f(E_{2k}) - f(E_{1k})]\} \tag{20}$$

$$\langle d_{i\sigma}^{+} d_{j\sigma} \rangle = (1/N) \sum_k \nu_k \{u_k^2 f(E_{1k}) + v_k^2 f(E_{2k})\}. \tag{21}$$

In this case of $J_{2_{\text{eff}}}$ large and δ small, we can self-consistently obtain the following result:

$$\mu_2 \approx -0.95 J_{2_{\text{eff}}}$$

$$\Delta_2 \approx 0.26 \delta^{1/2}$$

$$v_k^2 \approx \delta \nu_{2k}^2 / \langle \nu_{2k}^2 \rangle$$

$$u_k^2 = 1 - v_k^2$$

and two reduced quasiparticle energy bands:

$$E_{1k} \approx \varepsilon_{1k} - \lambda_{2k}^2 / \mu_2$$

$$E_{2k} \approx -\varepsilon_{2k} + \lambda_{2k}^2 / \mu_2 < 0.$$

The former is approaching half-filled, the latter is completely filled at zero temperature.

In this Cu–O strong-coupling limit the O hole occupies a large momentum state in order to form a bound Cu–O pair, the chemical potential μ_2 corresponding to the Cu–O pair bound energy $-J_{2_{\text{eff}}}$. We believe that taking into account the influence of the J_1 term should not change the results much. Then we always have the relation $u_k^2 \gg v_k^2$. In the Hamiltonian (17), the interaction between the ξ quasiparticles is much larger than that of others, and also, because the single-particle energy E_{1k} is much smaller than that of $|E_{2k}| (\approx -\mu_2)$, the most important interaction is between the ξ particles; the others could be neglected reasonably (the pairing condensation easily takes place for small single-particle energy). Now the effective Hamiltonian is reduced to

$$\hat{H}_{\text{eff}} = \sum_{k\sigma} E_{1k} \xi_{k\sigma}^{+} \xi_{k\sigma} + \sum_{k\sigma} E_{2k} \eta_{k\sigma}^{+} \eta_{k\sigma} - \left\{ \sum_k \lambda_{1k}^{*} u_k^2 \xi_{-k\beta} \xi_{k\alpha} + \text{HC} \right\}$$

$$+ \text{const. term.} \tag{22}$$

We introduce another quasiparticle $q_{k\sigma}$ which could diagonalise this Hamiltonian (22):

$$q_{k\sigma} = \tilde{u}_k \xi_{k\sigma} + \sigma \tilde{v}_k \xi_{-k\bar{\sigma}}^{+}$$

$$\tilde{u}_k = \frac{\lambda_k u_k^2}{[u_k^4 \lambda_{1k}^2 + (E_k - E_{1k})^2]^{1/2}}$$

$$\tilde{v}_k = \frac{E_{1k} - E_k}{[u_k^4 \lambda_{1k}^2 + (E_k - E_{1k})^2]^{1/2}}$$

$$E_k = (E_{1k}^2 + u_k^4 \lambda_{1k}^2)^{1/2} > 0$$

$$\tilde{H}_{\text{eff}} = \sum_{k\sigma} E_k q_{k\sigma}^+ q_{k\sigma} + \sum_{k\sigma} E_{2k} \eta_{k\sigma}^+ \eta_{k\sigma} + \text{const. term.} \tag{23}$$

The self-consistent equations for this Hamiltonian become

$$\tfrac{1}{2} = (1/N) \sum_k \{u_k^2[\tilde{u}_k^2 f(E_k) + \tilde{v}_k^2(1 - f(E_k))] + v_k^2 f(E_{2k})\} \tag{24}$$

$$\delta/2 = (1/N) \sum_k \{1 - u_k^2 f(E_{2k}) - v_k^2[\tilde{u}_k^2 f(E_k) + \tilde{v}_k^2(1 - f(E_k))]\} \tag{25}$$

$$\langle d_{i\alpha}^+ d_{j\beta}^+ \rangle_0 = (1/4N) \sum_k \{\nu_{1k} u_k^2 \tilde{u}_k \tilde{v}_k [2f(E_k) - 1]\} \tag{26}$$

$$\langle p_{i\alpha}^+ d_{j\beta}^+ \rangle_0 = (4N\sqrt{2})^{-1} \sum_k u_k v_k \nu_{1k} \{f(E_{2k}) - [\tilde{u}_k^2 f(E_k) + \tilde{v}_k^2(1 - f(E_k))]\} \tag{27}$$

$$\langle d_{i\alpha}^+ d_{j\alpha} \rangle_0 = (1/4N) \sum_k \nu_k \{u_k^2[u_k^2 f(E_k) + \tilde{v}_k^2(1 - f(E_k))] + v_k^2 f(E_{2k})\}. \tag{28}$$

We have compared these equations with equations (7)–(11) in § 2. We have found that if we take large $J_{2_{\text{eff}}}$ and the small δ limit, equations (7)–(11) will be reduced to equations (24)–(28) correspondingly.

We have solved these equations (24)–(28) self-consistently and obtained non-zero order parameters Δ_1 and Δ_2 in the doping concentration region $\delta \leqslant 30\%$. Then the O pair condensation is also non-zero and is given by

$$\langle p_{k\alpha}^+ p_{-k\beta}^+ \rangle = -v_k^2 \langle \xi_{k\alpha}^+ \xi_{-k\beta}^+ \rangle = v_k^2 \tilde{u}_k \tilde{v}_k [1 - 2f(E_k)]. \tag{29}$$

When δ exceeds about 30%, Δ_1 goes to zero ($\tilde{v}_k = 0$), and the O pair condensation also goes to zero. The results are in quantitative agreement with that obtained from solving equations (7)–(11) [17].

We now study the ground state wavefunction. By considering that the vacuum state $|0\rangle$ is not the eigenstate of quasiparticle operators such as $\xi_{k\sigma}^+ \xi_{k\sigma}$, $\eta_{k\sigma}^+ \eta_{k\sigma}$, $q_{k\sigma}^+ q_{k\sigma}$, and the BCS-like ground state at zero temperature must satisfy the conditions

$$\langle q_{k\sigma}^+ q_{k\sigma} \rangle = 0$$

$$\langle \eta_{k\sigma}^+ \eta_{k\sigma} \rangle = 1$$

we can obtain the wavefunction as follows:

$$|\Psi\rangle = \hat{p}_N |\varphi\rangle \tag{30}$$

$$|\varphi\rangle = \Big(\prod_k q_{k\alpha} q_{-k\beta} \eta_{k\alpha}^+ \eta_{-k\beta}^+ |0\rangle\Big) \Big/ \Big(\prod_k v_k^2 \tilde{u}_k\Big)$$

$$= \prod_k [u_k^2 \tilde{u}_k - d_{k\alpha}^+ d_{-k\beta}^+ (\tilde{v}_k + \tilde{u}_k v_k^2 p_{k\alpha}^+ p_{-k\beta}^+)$$

$$- \tilde{u}_k u_k v_k (d_{k\alpha}^+ p_{-k\beta}^+ + p_{k\beta}^+ d_{-k\beta}^+)] |0\rangle. \tag{31}$$

The projecting operator retains all the configurations in which each Cu site is singly occupied. And the Cu–Cu holes and Cu–O holes couple together in spin singlet pairs, or there are pre-existing spin pairs. But the Cu–O and Cu–Cu pairing condensations do not take place because these kinds of condensation will break the single occupation

condition and the projecting operator will make them zero. The strong Cu spin single-pair correlation forms a Cu–RVB background and the O hole couples strongly to Cu spin, leading to a non-zero O pair condensation, which is reflected in the following term:

$$d^+_{k\alpha} d^+_{-k\beta}(\tilde{v}_k + \tilde{u}_k v_k^2 p^+_{k\alpha} p^+_{-k\beta}). \tag{32}$$

We have also calculated the spin correlation of neighbours of Cu and O holes. The results are very interesting. The Cu–Cu nearest neighbours show spin singlet pairing correlation when the intermediate O site is empty, otherwise it will become ferromagnetic correlation due to strong Cu–O singlet pairing correlation. And the O–O nearest neighbours always show a ferromagnetic one because of the Cu site single-occupation condition. The next-nearest neighbours always show a spin singlet one. (The on-site O spin singlet pair condensation is always zero:

$$\langle p^+_{i\alpha} p^+_{i\beta} \rangle = \sum_k \langle p^+_{k\alpha} p^+_{-k\beta} \rangle = 0 \tag{33}$$

although we have neglected the O hole on-site Coulomb interaction. That is because the effective O pair attraction [19] induced by Cu–Cu and Cu–O spin correlation only occurs in next-nearest neighbours, and some further neighbours and nearest neighbours may show effective repulsion interaction. So this kind of O pair condensation may mainly occur between next-nearest neighbours and further neighbours and does not couple to on-site Coulomb repulsion. So taking into account the U_p term could not destroy O pair superconductivity.) All these results are in good agreement with Ogata and Shiba's numerical calculation results [12] for the corresponding two-band model.

(In our model, we have also neglected the direct O–O hopping term which has been estimated to be about 0.5 eV [16]. So in our calculation we have got a small effective hopping term of about 0.3 eV, which may predict somewhat larger values of the specific heat than that of experiments. However, our superconductivity model does not depend on the small value of effective O–O hopping. The numerical calculation has shown that we always have non-zero order parameters Δ_1 and Δ_2 in the small doping case, provided that the conditions $t_{O\text{-}O} \leqslant J_{2_{\text{eff}}}$ and $\delta J_{2_{\text{eff}}} \leqslant J_1$ are satisfied.)

4. Conclusion

In conclusion, we have given the physical picture of O pair superconductivity in the Cu–RVB background. Doped O holes and their neighbouring Cu holes form the Cu–O spin singlet pairs which interact with each other through Cu–Cu spin correlation and lead to the condensation of O holes in momentum space, which is responsible for superconductivity. In physics, two O holes with opposite spins in two Cu–O spin singlet pairs should attract each other in order to lower the Cu–Cu spin correlative energy. Thus in the region of $\delta \leqslant 30\%$ the system should show O pair superconductivity.

By studying the ground state wavefunction of the system, we find that the spins of Cu and O holes are all correlated together, which is most important for the high-T_c superconductors as found by experiment [1, 2]. We have also calculated the Cu–O and Cu–Cu spin correlations and the results are in good agreement with Ogata and Shiba's numerical results [12]. When the superconductivity is destroyed by raising the temperature we believe that some kind of spin correlation must remain, which will be studied in our later work.

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