Enhancement of maximum superconducting temperature by applying pressure and reducing the charge transfer gap

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Abstract

Recent Scanning Tunneling Spectra (STS) measurement on underdoped cuprate discovers the increase of the maximum superconducting transition temperature $T_c$ when the size of charge transfer gap (CTG) is reduced. Applying pressure is another well known method to increase maximum $T_c$. However, these pressure experiments also found another puzzle that $T_c$ is enhanced in underdoped and optimal doped samples but suppressed in overdoped. Here we present a possible mechanism based on the charge fluctuation to explain both these two effects simultaneously. Starting from 3-band Hubbard model, we retrieve the charge fluctuation (CF) between oxygen $p$-band and copper $d$-band which is ignored in the $t$–$J$ model. This model is studied via variational Monte Carlo method (VMC).

Keywords: cuprate, high-temperature superconductor, t-J model, t-J-U model, VMC

1. Introduction

About 30 years ago, right after the discovery of high temperature superconductor [1–5] (HTS), Anderson [6] has proposed that this system is a Mott insulator at half filling. Either the strong coupling one-band Hubbard model or its equivalent low-energy $t$–$J$ model is a good starting Hamiltonian to understand the physics. Later, it was shown by Emery [7] that the half-filled cuprate with both copper and oxygens considered is actually a charge transfer insulator to be described by a three-band Hubbard model. Not long after, Zhang and Rice [8, 9] showed that the large charge transfer gap could help to form a singlet state, known as Zhang-Rice singlet (ZRS), representing the doped hole. Therefore, the system could still be considered as an effective one-band model. In this case, the oxygen charge degrees of freedom are effectively frozen. Also, there are a number of experiments to support the presence of ZRS [10–12].

Many works tried to search for the dominant factors to enhance the superconducting transition temperature $T_c$, for example, the number of layers, the distance of apical oxygen, the magnetism, the hole density of Cu and O and the charge transfer gaps, etc. Few years ago, Weber et.al [13, 14] have shown that the maximum $T_c$ or $T_{c\text{max}}$ becomes larger with the decreasing charge transfer energy, increasing nearest hopping $|t'|$ and apical oxygen distance. Recently several experiments have provided evidences to reexamine this idea of one-band model beyond optimal doping [15–17]. The charge transfer gap (CTG) was directly measured by using the scanning tunneling microscopy (STM) for one and two layers $Bi_2(Sr,La)_2CuO_{6+δ}$ (Bi-2201) and $Ca_2CuO_2Cl_2$ (CCOC) [18]. Not only the gap size is surprisingly small of the order of 1 – 2 eV, but the maximum superconducting temperature $T_{c\text{max}}$ is higher for the smaller gap. The result is also confirmed by angle-resolved photoemission spectroscopy (ARPES) [19]. Thus the magnitude of the CTG is about same order of magnitude as the hopping energy between oxygen p orbital and copper d orbital, clearly we need to have a re-examination of the CF effect.
The effect of charge transfer between Cu$d^{10}$ and O$2p^6$, which shall be denoted as CF hopping in this paper, is also examined by a number of other experiments. For example, applying hydrostatic [20, 21] and uniaxial pressure[22], will enhance $T_c^{\max}$. However, a puzzling phenomena [23] is the reduction of $T_c$ with pressure in the overdoped (OD) regime but enhancement of $T_c$ in the underdoped (UD) and optimal doping regimes, it leads to the shift of the $T_c$ dome to lower dopant density and with enhancement of $T_c^{\max}$. This unusual behavior for $T_c$ under pressure cannot be simply attributed to the change of lattice constant or carrier density. A theoretical understanding is still lacking. We will show below that proper consideration of CF hopping provides a simple explanation of enhancement of $T_c^{\max}$ and the oppositie behavior in the UD and OD regimes.

Before we start to present the details on our model and calculations, we note that the model without explicitly including oxygen has successfully explained a number of experiments. However, to study the CF effect, we will have to bring back the oxygen degrees of freedom. Instead of taking into account of the full degree of freedom of oxygen which will require extensive numerical works, in this paper we will present an effective model that keeps the ZRS but includes the CF effect to reveal the physics.

We will start with the Emery’s 3-band mode [7]:

\[ \hat{H}_U = \sum_{l,\sigma} \epsilon_p \hat{p}_{l,\sigma}^\dagger \hat{p}_{l,\sigma} + \sum_{l,\sigma} \epsilon_d \hat{d}_{l,\sigma}^\dagger \hat{d}_{l,\sigma} + \sum_{l,\sigma} U_d \hat{n}_{d_{l,\sigma}}^\dagger \hat{n}_{d_{l,\sigma}} \]

\[ \hat{H}_{pd} = -\sum_{l,\sigma} \sum_{l' \subset \{1,4\}} t_{pd} \hat{v}_{p} \hat{d}_{l,\sigma}^\dagger \hat{p}_{l',\sigma} + \text{h.c.} \]

where $l$ runs over the four oxygen around a copper, and $V_d = 1$ for $l = i + \frac{1}{2}x$ and $i + \frac{1}{2}y$, while $V_d = -1$ for $l = i - \frac{1}{2}x$ and $i - \frac{1}{2}y$. $d_{l,\sigma}$ creates a d-hole with spin $\sigma$ in the Cu$(d_{x^2-y^2})$ at site $l$. $p_{l',\sigma}$ creates a p-hole with spin $\sigma$ in the O(p$_x$ and p$_y$) orbitals at site $j$. $\epsilon_d$ and $\epsilon_p$ correspond to the energy of the local Cu$(d_{x^2-y^2})$ and O(p$_x$ and p$_y$) orbital, respectively. $U_d$ is on-site Coulomb repulsion, of copper. The vacuum is defined as Cu $d^{10}$ and O $p^6$.

At half-filling, i.e., before a hole or an electron is doped into the system, every Cu will be at $d^9$ state with a single hole and all oxygens are at $p^6$ without holes and the system is a Mott insulator and a spin-1/2 quantum Heisenberg system [6]. To consider the effect of doping, Zhang and Rice[8, 9] have derived an effective single-band model from Emery’s 3-band model. In their argument, when a hole is doped into a cuprate, it will reside on oxygen. However, the superexchange coupling between this hole’s spin and the spin at the nearest neighbor Cu $d^9$ site will form a ZRS spin singlet. All the other triplet and nonbonding state have much higher energies and could be neglected from the low energy Hamiltonian. In this picture, the hole’s energy on oxygen site is actually the ZRS state with energy $\tilde{\epsilon}_H$, where the tilde means a renormalized energy of $\epsilon_p$. If the only charge degrees of freedom considered is from the doped holes that forming ZRS, then the degrees of freedom left are the original spin -1/2 on the Cu $d^9$ site and doped holes or ZRSs and then we obtain the well-known $t - J$ Hamiltonian[9].

\[ \hat{H}_{t-J} = -t \sum_{\langle i,j \rangle} P_G c_{i}^\dagger c_{j} P_G + J \sum_{\langle i,j \rangle} (\hat{S}_{i} \cdot \hat{S}_{j} - \frac{1}{4} \hat{n}_{i} \hat{n}_{j}) \]

where $P_G = \prod_{i,j} (1 - \hat{n}_{i} \hat{n}_{j})$, $t$ is the effective hopping amplitude of ZRS, and $J$ is the superexchange interaction between nearest neighbor Cu $d^9$ holes.

However, in principle several other charge degrees of freedom could be important. One possibility is that instead of being at the oxygen, the hole could sit at the Cu site to form Cu $d^{10}$ which has energy $2\epsilon_d + U_d$ according to Eq. (1). This could be neglected at large $U_d$. The other possibility is to have the hole hopping from the Cu $d^{10}$ site to the nearest oxygen site to form a ZRS with the adjacent Cu while leaving a Cu $d^{10}$ behind. This is schematically shown in Fig.1a. The energy difference between the initial and final configurations of this process is $\tilde{\epsilon}_p - \epsilon_d$, which is exactly the charge transfer gap, $\Delta_{CT}$, discussed before. If only this process is to be considered besides $t$ and $J$, we could completely eliminate the oxygen and denote the two configurations as in Fig.1b, where the Cu $d^{10}$ is now represented by a doublon. The rate of this
process switching from a pair of nearest-neighbor holes to a holon-doublon pair is denoted as $\bar{t}$. Once we have Cu$^{d_{10}}$ as a doublon, then it can also exchange with a Cu$^{d_{9}}$ through the middle oxygen as shown in Fig. 1c. This is equivalent to the hopping of a doublon, as shown in Fig. 1d. Finally, we have an effective one-band charge transfer model

$$\hat{H}_{CT} = \hat{H}_{t-J} + \hat{H}_{CF}$$

$$\hat{H}_{CF} = -\bar{t} \sum_{\langle i,j \rangle} (1 - \hat{n}_{i,\sigma}) c^\dagger_{i\sigma} c_{j,\sigma} \hat{n}_{j,\sigma} + \hat{n}_{i,\sigma} c^\dagger_{i\sigma} c_{j,\sigma} (1 - \hat{n}_{j,\sigma}) + h.c$$

where $\langle i,j \rangle$ denotes nearest neighboring sites. There are three kinds of nearest neighboring hoppings as shown schematically in Table.1. First, $t$ is the hopping of ZRS or hole in the $t-J$ model. Second, $\bar{t}$ controls the creation and annihilation of a holon-doublon pair. Finally, $t_d$ describes doublon hopping. We notice that the process of creation and annihilation of a holon-doublon pair is actually one of the many intermediates states considered in the derivation of the superexchange $J$[6, 8, 9]. Thus in principle $J$ should be reduced from the values used in the pure $t-J$ model by a small amount. Thus in this work we consider a small $J/t = 0.33$. The generic parameter $J$ ranges from 0.1 $eV$ to 0.13 $eV$ among various cuprates, which has been determined systematically by Raman scattering[24, 25] and neutron scattering[26, 27].

By setting $t = \bar{t} = t_d$, the model is equivalent to the $t-J-U$ model where $\Delta_{CT}$ is the effective Hubbard $U$. The model[28-33] has been studied via various method like variational Monte Carlo (VMC) method [34–37], slave-particle method[38, 39]. Gutzwiller renormalized mean field theory(RMFT) [40–46], diagrammatic expansion of the Gutzwiller wave function (DE-GWF)[47–49], and density matrix renormalization group(DMRG)[28, 50]. To examine CF effect more carefully, we will consider more general cases where the three hopping amplitudes, $t$, $\bar{t}$, and $t_d$, are different. Their difference will become apparent when we discuss the effect of pressure in Sec.3.3. The derivation of these parameters from the 3-band model of Eqs. (1) and (2) are quite tedious[51]. They depend on CTG, hybridization $t_{pd}$ and $d-d$ Coulomb repulsion $U_d$. In this work, we will just treat these as parameters of our model.

| $t$ | $\uparrow \uparrow$ | $0 \uparrow$ | $0 \uparrow$ |
| $\bar{t}$ | $\uparrow \downarrow$ | $0 \uparrow \downarrow$ | $0 \uparrow \downarrow$ |
| $t_d$ | $\uparrow \downarrow \downarrow$ | $\downarrow \uparrow \downarrow$ | $\downarrow \uparrow \downarrow$ |

Table 1: Classification of hopping

This paper is organized as follows. In Section 2 the wave function used in the VMC method is presented. The effect of the three CF parameters: $t$, $\bar{t}$, and $\Delta_{CT}$ are analyzed in Section 3.1. In Section 3.2 we discuss the relation between CTG and pairing magnitude. In Section 3.3, we discuss the effect of pressure on pairing. Finally, the conclusion is given in Section 4.

2. Formalism and Method

For the variational ground state ansatz in the VMC calculation, we use the correlated $d$-wave BCS wave function [52–56]

$$|\Psi\rangle = \hat{P}_d \hat{P}_{dh} \hat{P}_{Ne} |\Psi_{d-BCS}\rangle$$

where $\hat{P}_{Ne}$ is the projection operator to fix the total number of particles to be $N_e$ and the $d$-wave BCS trial wave function[52, 53] is

$$|\Psi_{d-BCS}\rangle = \prod_{k \in BZ} (u_k + v_k c_{-k\uparrow}^\dagger c_{-k\downarrow}) |0\rangle$$
Figure 1: Mapping the CF hopping processes in three bands into our effective one-band model with schematic illustrations.

(a) Three band picture of CF hopping. 
(b) CF hopping in one band representation. 
(c) Three band picture of doublon hopping. 
(d) Doublon hopping in one band representation.

The initial state has an $\text{O}^2_{p6}$ in between two neighboring $\text{Cu}^3_{d9}$ holes with opposite spin. In the three-band model, one of these two holes on Cu site could hop to the middle O site to form a ZRS with the hole on the other Cu and leaving a Cu $3d^{10}$ or the doublon state. Hence this is equivalent to the formation of a holon-doublon pair in our one-band representation as shown in (b). (c) In the three-band model, the initial configuration of $\text{Cu}^3_{d10}$, $\text{O}^2_{p6}$ and $\text{Cu}^3_{d9}$ could change to the intermediate configuration with $\text{Cu}^3_{d10}$, $\text{O}^2_{p5}$ and $\text{Cu}^3_{d10}$, before it reaches the final configuration with $\text{Cu}^3_{d9}$, $\text{O}^2_{p6}$ and $\text{Cu}^3_{d10}$, but this process is equivalent to the exchange between $\text{Cu}^3_{d10}$ and neighboring $\text{Cu}^3_{d9}$ which could be easily seen as the hopping of doublon in our representation shown in (d).

\[ u_k = \frac{1}{2}(1 + \frac{\xi_k}{\sqrt{\xi_k^2 + \Delta_k^2}}), \quad u_k^2 + v_k^2 = 1, \xi_k = -2(\cos k_x + \cos k_y) - 4t'_v \cos k_x \cos k_y - \mu_v, \quad \Delta_k = \Delta_v(\cos k_x - \cos k_y), \quad t'_v, \mu_v \quad \text{and} \quad \Delta_v \quad \text{are variational parameters.} \]

\[ \hat{P}_G = \prod_i (1 - (1 - g)\hat{n}_{\uparrow i} \hat{n}_{\downarrow i}) \]  

(8)

which controls the doublon density. For $g = 0$, there is no doublon and we have the strongest correlation in the large $\Delta_{CT}$ limit and this is used for the pure $t - J$ model. On the contrary, there is no correlation for $g = 1$. The Jastrow-type factor \([58]\) $\hat{P}_{dh}$ is introduced to provide an attractive interaction between doublon and hole\([59–61]\) to make sure at half-filling we recover the Mott insulator without free carrier, it is of the form

\[ \hat{P}_{dh} = \prod_i (1 - Q_{dh} \hat{B}_i) \]  

(9)

where $\hat{B}_i = \prod_{r} \hat{d}_i(1 - \hat{h}_{i+r})$, $\tau = \hat{x}, \hat{y}$ represents a nearest neighbor holon-doublon binding state, $\hat{d}_i$ is the doublon creation operator $\hat{d}_i = c_{\uparrow i}^\dagger c_{\downarrow i}^\dagger c_{\uparrow i} c_{\downarrow i}$ and $\hat{h}_i$ is the hole creation operator $\hat{h}_i = (1 - c_{\uparrow i}^\dagger c_{\downarrow i})(1 - c_{\uparrow i}^\dagger c_{\downarrow i})$. For $Q_{dh} = 0$, doublon and hole are free, while for $Q_{dh} = 1$ doublon cannot be separated from a hole. For $Q_{dh} < 0$ doublon and hole are repulsive to each other. In our case, for large $\Delta_{CT}$, $Q_{dh}$ is always positive.

In order to find the ground state we optimize the trial wavefunction by implementing the stochastic reconfiguration(SR) method described in detail in Ref.\([62]\).

The superconductivity is characterized by the d-wave pairing order parameter

\[ \Delta_{SC} = \sum_i <c_{\uparrow i}^\dagger c_{\uparrow i+x\downarrow}^\dagger> - (x \leftrightarrow y) \]
However, in canonical VMC, what we can measure is the pair-pair correlation function
\[ P(\vec{r}) = \frac{1}{N_s} \sum_i \Delta(\vec{R}_i) \Delta(\vec{R}_i + \vec{r}) \]
where \( N_s \) is the number of the sites and
\[ \Delta(\vec{R}_i) = \frac{1}{\sqrt{2}} (c_{i\uparrow} c_{i+x\downarrow} - c_{i\downarrow} c_{i+x\uparrow}) - (x \leftrightarrow y) \]
By taking the square root of the pair-pair correlation at the maximum distance, \( r_{max} \), we can estimate the magnitude of pairing order parameter.
\[ \Delta_{SC} \approx \sqrt{P(\vec{r}_{max})} \]

3. Results

As mentioned above, the three hopping amplitudes in Table 1 are not necessarily the same. In this section, we investigate the effect of varying \( t, t_d \) and \( \Delta_{CT} \) with fixed \( t = 1 \) and \( J = 0.33 \). Throughout this work, the lattice size considered is \( 20 \times 20 \). In the main text we will show the result of having only the nearest neighboring hopping terms. A very similar result is obtained by including the second nearest neighboring hopping terms where we set \( t'/t = t'/t = t_d/t_d = -0.3 \) which is presented in the Supplementary Material.

3.1. Tuning parameters \( t, t_d \) and \( \Delta_{CT} \)

In this section, we show the \( d \)-wave pairing order parameter as a function of dopant concentration with varying \( t, t_d \) or \( \Delta_{CT} \) in Figs. 2, 3 and 4 respectively.

First, we consider two cases with \( \Delta_{CT} = 6 \) and \( \Delta_{CT} = 8 \) in Figs 2a and 2b, respectively. By fixing \( t_d = 1 \), the CF process is only related to the formation of holon-doublon pair as shown in Fig. 1b. Three hopping amplitudes \( t = 0.4, 1 \) and 1.5 has been shown in the figure. Note that the label \( t = 0 \) corresponds to the \( t - J \) model, while for \( t = 1 \), it becomes the \( t - J - U \) model. Clearly, pairing is enhanced strongly in the underdoped(UD) regime as \( t \) increases. This enhancement of pairing can be understood by the increase in the effective superexchange interaction arises from the additional \( t \) process. When there is a larger \( \Delta_{CT} \) and a smaller \( t \), the CF is less important and the result is closer to that of the \( t - J \) model. Thus CT is effectively reducing the Hubbard \( U \). We also note that when \( t \) gets larger there is apparent finite superconductivity at very low doping, which is known as the Gossamer superconductivity [30, 31, 40].

In Fig. 3, we study the effect of \( t_d \). The \( d \)-wave pairing order parameter as a function of dopant concentration for \( t_d = 0, 0.5, 1 \) and 1.3 is shown in Fig. 3a and 3b for \( \Delta_{CT} = 6 \) and \( \Delta_{CT} = 8 \), respectively. Notice here we set that \( t = 1 \). By increasing \( t_d \), we found pairing at UD regime is slightly enhanced but suppressed at the OD. Similar to the effect of \( t \), increasing \( t_d \) enhances CF and suppresses strong correlation. The suppression of pairing in the OD regime is due to the lack of singly occupied spin-1/2 particles or spinons, which effectively reduces the number of electrons available for pairing. The controlling parameter of spinon density and how it affects pairing will be elaborated further in the next section.

In Fig 4, we show the \( d \)-wave pairing order parameter as a function of dopant concentration for \( t_d = 1 \) and three different CTG, \( \Delta_{CT} = 6, 8 \) and 10. Fig. 4a is for \( t = 1 \) and 4b for 1.5. Similar to the result of large \( t_d \) or \( t \), smaller \( \Delta_{CT} \) enhances pairing in the UD regime but suppress it in the OD side.

All the results shown in Figs. 2-4 reveal a consistent physical picture. When \( \Delta_{CT} \) becomes smaller or \( t \) or \( t_d \) becomes larger, maximum SC order parameter increases and the pairing dome moves toward the smaller dopant concentration. In addition we found qualitatively similar result with the \( t - J - U \) model for various values of \( t \) and \( t_d \). On the other hand, the “shift” of pairing dome in Fig. 4 is very similar to the high pressure experiment result on Hg1212 [23]. This will be discussed further in Sec.3.3.
Figure 2: Pairing order parameter as a function of dopant concentration for various $\bar{t}$. Here we have $\bar{t}_d = 1$. The CTG is set to (a) $\Delta_{CT} = 6$ and (b) $\Delta_{CT} = 8$. Note that the label $\bar{t} = 0$ stands for $\bar{t} = \bar{t}_d = 0$ which is the same as the $t - J$ model. For the case $\bar{t} = 1$, we have the $t - J - U$ model.

Figure 3: Pairing order parameter correlation as a function of dopant. The CTG is set to (a) $\Delta_{CT} = 6$ and (b) $\Delta_{CT} = 8$. The hopping parameter is $t = \bar{t} = 1$ $J = 0.33$. 
3.2. Relation of CTG and pairing amplitude

Recently, Ruan et al. [18] found anti-correlation between $T_{c,\text{Max}}$ and CTG in both single- and double-layered cuprate via scanning tunneling spectroscopy (STS). To investigate the anti-correlation, we determine the maximum pairing amplitude, $\Delta_{\text{Max}}$, as a function of the CTG by calculating the pairing amplitude as a function of hole density. In Fig. 5, for small $\Delta_{\text{CT}}$ or effective $U$, where Gossamer superconductivity\[30, 31, 40\] dominates, $\Delta_{\text{Max}}$ is approximately proportional to $\Delta_{\text{CT}}$ with almost the same slope. This can be explained simply. As $\Delta_{\text{CT}}$ increases from 0, doublon number begins to decrease significantly and consequently the number of singly occupied sites or spinon increases (see Fig. 6a). Once the CTG values reach a critical magnitude, the strong correlation Mott physics begins to take hold, then the increase of $\Delta_{\text{CT}}$ will result in a decrease of pairing order which should be inversely proportional to the CTG in the form of $t^2/\Delta_{\text{CT}}$. This is consistent with the result in Ref. [18] that $T_{c,\text{Max}}$ is roughly proportional to $1/\Delta_{\text{CT}}$ for one- and two-layer cuprates. Their data also shows when the CTG is reduced by 25% from one layer CCOC to Bi2201, the $T_{c,\text{Max}}$ increases 45%. By choosing $t = 0.3eV$ and consider $\bar{t} = 0.4t$, we get the enhancement of maximum pairing amplitude about 23% when $\Delta_{\text{CT}}/t$ is reduced from 6.5 to 5. This result is quite satisfactory considering that the parameters of these two different cuprates are roughly estimated.
Since the introduction of the CTG provides an additional superexchange interaction for pairing, this sure will enhance $\Delta_{\text{Max}}^{\text{SC}}$ and $T_{\text{c}}^{\text{Max}}$. However, we were surprised to find that pairing order parameter is not uniformly enhanced for all the doped hole density when CTG is reduced as shown in Fig. 4. The enhancement is larger in the UD regime and with no enhancement or pairing is even suppressed in the OD phase. As noted by Anderson[6] a long time ago, the $d$-wave pairing caused by the superexchange interaction favors the singly occupied sites or spinons. In Fig 6a, we examine the effect of spinon density on pairing. The parameters used are $\bar{t} = t_d = t$, $J = 0.33$ and $t' = t'_d = t' = 0$ so this is same as $t - J - U$ model. For all the concentrations, the spinon density first increases quickly with CTG and then approaches a plateau with a very small increase around $\Delta_{CT} = 8 - 10$ which enters the strong correlation regime. The increase of spinon density is much rapid and larger in the UD regime than in OD regime. Thus we can expect pairing will be quickly enhanced in the UD regime but much milder in the OD regime. Accordingly, one would also expect $\Delta_{\text{SC}}^{\text{Max}}$ to be larger in the UD regime. This is exactly what we found in Fig. 6b, where the pairing order parameter is plotted as a function of CTG for various hole densities. For hole density less than 0.18, the pairing order rapidly increases with CTG. Once the maximum value is reached at some critical CTG, the system enters the strongly correlated regime and the increase of $\Delta_{CT}$ only reduces the additional superexchange interaction thus pairing order decreases as $1/\Delta_{CT}$. At very large values of $\Delta_{CT}$, the system is essentially the same as the $t - J$ model and the pairing order is quite small as it is proportional to the hole density in the UD regime. In the OD regime, although the spinon density still gradually increases as CTG is increased, it is weaker than the effect of decreases of additional superexchange interaction as $1/\Delta_{CT}$. 

Figure 5: Maximum $d$-wave pairing order parameter vs. CTG with $t_d = 1$ and $t' = 0$. 
3.3. Examine the effect of pressure

When pressure is applied, the in-plane distance between Cu and Oxygen will decrease, hence $t_{pd}$ will increase. As shown from previous sections, not only $\Delta_{CT}$ but also $t_d$ and $\bar{t}$ can affect the superconducting dome shape. According to standard perturbation derivation: $t \sim t_{pd}^2$, $t_d \sim t_{pd}$, $J \sim t_{pd}^4$. Hence as $t_{pd}$ increases, $t_d/t$ hardly changes, $t/t$ is inversely proportional to $t_{pd}$, thus it will decreases, $\Delta_{CT}/t$ will decreases as $1/t_{pd}^2$, and $J/t$ is proportional to $t_{pd}^2$. So assuming that we set the parameter at ambient pressure ($J/t$, $\Delta_{CT}/t$, $t_d/t$, $t/t$) to be $(0.33, 8, 1, 1)$. If we increase $t_{pd}$ by a ratio $\alpha$ then the parameters will turn into $(0.33\alpha^2, 8/\alpha^2, 1, 1/\alpha)$. As pressure is increased, $\alpha$ increases from 1 to 1.04 and 1.08 as shown in Table 2 with all other parameters. In Fig.7, the two sets of parameters show the similar result that as
pressure or $t_{pd}$ increases, pairing order parameter increases in UD regime but decreases in OD. This is very consistent with high pressure experiment [23].

### Table 2

| data label | A1 | A2 | A3 | B1 | B2 | B3 |
|------------|----|----|----|----|----|----|
| $\alpha$   | 1  | 1.04 | 1.08 | 1  | 1.04 | 1.08 |
| $J/t$      | 0.33 | 0.357 | 0.385 | 0.33 | 0.357 | 0.385 |
| $\Delta_{CT}/t$ | 8 | 7.4 | 6.86 | 8 | 7.4 | 6.86 |
| $t_{d}/t$  | 1 | 1 | 1 | 0.5 | 0.5 | 0.5 |
| $\bar{t}/t$ | 1 | 0.961 | 0.926 | 0.4 | 0.384 | 0.37 |

![Figure 7](image)

(a) $\Delta_{SC}$ vs $\delta$

(b) $\Delta_{SC}$ vs $\delta$

**Figure 7:** Simulation of pressure effect, parameter at ambient pressure ($J/t$, $\Delta_{CT}/t$, $t_{d}/t$, $\bar{t}/t$) are selected to be (0.33, 8, 1, 1) for (a) and (0.33, 8, 0.5, 0.4) for (b). The detail parameters are listed in Table 2.

On the other hand, the hydrostatic pressure will also decrease the apical oxygen distance. When the apical Oxygen is brought closer to the Cu atom, it will increase the repulsion to electrons on the copper, hence the increase of charge transfer gap [63, 64]. Distance. To simulate this effect, we increase $\Delta_{CT}$ a little bit, say 2.5% or 5%. Assuming at ambient pressure the parameter ($J/t$, $\Delta_{CT}/t$, $t_{d}/t$, $\bar{t}/t$) is (0.33, 8, 0.5, 0.4) as data of B1 in Table 2. With increasing pressure, the $t_{pd}$ becomes $\alpha t_{pd}$ and $\Delta_{CT}$ becomes $\beta \Delta_{CT}$. Hence, as pressure is applied, the parameters becomes (0.33$\alpha^2$, 8$\beta/\alpha^2$, 0.5, 0.4/$\alpha$). The detailed parameters are listed in Table 3. Fig. 8 shows similar result as Fig. 7 although we have included the effect that CTG is increased by reducing the apical oxygen distance from Cu. The UD side has its pairing enhanced while the OD side is reduced under pressure as the pairing dome is shifted or tilted toward the UD side.

### Table 3

| data label | B1 | B2' | B3' | B2'' | B3'' |
|------------|----|-----|-----|------|------|
| $\alpha$   | 1  | 1.04 | 1.08 | 1.04 | 1.08 |
| $\beta$    | 1  | 1.025 | 1.025 | 1.05 | 1.05 |
| $J/t$      | 0.33 | 0.357 | 0.385 | 0.357 | 0.385 |
| $\Delta_{CT}/t$ | 8 | 7.58 | 7.03 | 7.77 | 7.2 |
| $t_{d}/t$  | 0.5 | 0.5 | 0.5 | 0.5 | 0.5 |
| $\bar{t}/t$ | 0.4 | 0.384 | 0.37 | 0.384 | 0.37 |
Figure 8: Simulation of pressure effect that include the apical oxygen effect, parameter at ambient pressure $(J/t, \Delta_{CT}/t, t_d/t, \bar{t}/t)$ are selected to be $(0.33, 8, 0.5, 0.4)$. As pressure is applied, the parameters becomes $(0.33\alpha, 8\beta/\alpha^2, 0.5, 0.4/\alpha)$. The detail parameter for the data is listed in Table 3.

4. Conclusion

In summary, motivated by the recent experiments [65], we have studied the CF effect of the Copper-Oxygen three-band model with an effective one-band model similar to the t-J-U model. But now $U$ or $\Delta_{CT}$ is the charge transfer gap. The formation of this doublon and its hopping as well as the size of the charge transfer gap all played an important role in the CF effect. The inclusion of these effects provides a simple understanding of the enhancement of maximum pairing when the $\Delta_{CT}$ is reduced as observed by the experiment [18]. Additionally, we also found that there is a minimum $\Delta_{CT}$ for enhancement. On the other hand, this enhancement only occurs in the UD regime but not in OD. This dichotomy between UD and OD is further examined by considering the effect of applying pressure. Our model provides a very simple explanation for the observations in several pressure experiments that $T_c$ is always enhanced in the UD regime but reduced in the OD.

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