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Unified theory of superconductivity in $La_{2-x}Sr_xCuO_4$ and $Nd_{2-x}Ce_xCuO_4$

Fu-sui Liu†‡¶ and Wan-fang Chen§‖

† Physics Department, Beijing University, Beijing 100871, China
‡ Physics Department, Yunnan University, Kunming 650091, China
§ CCAST (World Laboratory) PO Box 8730, Beijing 100080, China
‖ University of Science and Technology of Staff and Workers of the Academy of Science of China, Beijing 100080, China

E-mail: fsliu@pku.edu.cn (Fu-sui Liu)

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Abstract. Taking the two-local-spin-mediated interaction as a Cooper pair interaction, using the BCS (Bardeen–Cooper–Schrieffer) gap equation and the phase-coherence condition for quantum phase fluctuation, this paper explains basic experimental findings concerning both p-type $La_{2-x}Sr_xCuO_4$ (LSCO) and n-type $Nd_{2-x}Ce_xCuO_4$ (NCCO) at the same time, and predicts that the pseudogap should be clearly observed for underdoped NCCO.

1. Introduction

The pairing mechanism responsible for superconductivity in the high-T_c cuprates is still unknown. We hope that if we study p-type LSCO and n-type NCCO at the same time, then the corresponding pairing mechanism will be more convincing. LSCO and NCCO have the same conductive CuO_2 plane [1]. The crystal structure of NCCO is similar to that of LSCO. The only difference between the two structures is that each copper atom is bonded to four oxygen atoms in NCCO, whereas the copper is surrounded by an octahedron of oxygens in LSCO [1].

LSCO is a p-type superconductor [1], has a d-wave order parameter [2–4], a pseudogap [4], and a very large value of $2\Delta(0\ \mathrm{K})/T_c$ [4]. The doping range of superconductivity for LSCO is $0.5 < x < 0.27$ [4]. Here and in the following, x is the number of carriers in one unit cell in the CuO_2 plane.

NCCO is a n-type superconductor [1]. The doping range of superconductivity for NCCO is $0.12 < x < 0.20$ [5]. Using the phase-sensitive capability of tunnelling spectroscopy, Kashiwaya *et al* did not observe a zero-bias conductance peak (ZBCP), and concluded that the suggestion of d-wave symmetry should be rejected [6]. It was widely believed that NCCO is of s-wave type. The main experimental evidence for this comes from studies of the in-plane penetration depth $\lambda_{ab}(T)$ [7, 8]. Considering the paramagnetism arising from Nd^{3+} ions, Cooper altered the limiting temperature dependence of $\lambda_{ab}(T) - \lambda_{ab}(0)$ from an exponential behaviour to T^1- or T^2-behaviour associated with d-wave pairing [9]. See also reference [10] on this. However, correcting the measured $\lambda_{ab}(T)$ dependence for the temperature-dependent susceptibility due to the Nd^{3+} moments, Alff *et al* still insisted on an

¶ Author to whom any correspondence should be addressed. Address for correspondence: Chang Chun Yuan, Building 56, Room 502, Beijing University, Beijing 100871, People's Republic of China.

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exponential dependence indicating isotropic s-wave pairing [11]. Note that the quasiparticle tunnelling conductance spectra of NCCO closely resemble those of d-wave LSCO and YBCO [6, 11]. Pair tunnelling measurements indicate the product of the critical current and the junction normal-state resistance (I_cR_N) to lie between 0.5 and 6 μV for Pb/NCCO c-axis-oriented films and single crystals [12]—almost three orders of magnitude smaller than the 3 mV Ambegaokar–Baratoff limit expected for an s-wave superconductor. It is noteworthy that the values of ratio $2\Delta(0\ \mathrm{K})/T_c$ obtained by different methods are quite different. The values of $2\Delta(0\ \mathrm{K})/T_c$ from penetration depth experiments are 3.9–4.5 for $T_c = 21$, 21.5, and 22 K [8], and 2.9 for $T_c = 24$ K [11]. The value of $2\Delta(0\ \mathrm{K})/T_c$ measured as the peak-to-peak value in the conductance spectra in the Cu–O bond direction is about 6, and $\Delta(2.2\ \mathrm{K}) = 6.15$ meV for $T_c = 24$ K [11].

Recently, Tsuei and Kirtley presented very powerful and conclusive evidence from a tricrystal phase-sensitive experiment that NCCO has d-wave symmetry [13]. There is no detectable imaginary component of the order parameter for NCCO [13, 14]. Therefore, in our view, the present main problem is that of how to explain the lack of a ZBCP and the 'exponential' behaviour of $\lambda_{ab}(T)$ for NCCO on the premise of the d-wave symmetry, and to put an end to arguments regarding the possibility of s-wave symmetry. A present secondary problem is that of how to judge whether the symmetry in NCCO is a pure d-wave one or a predominantly d-wave one with a small s-wave component. A present third problem is that of discovering why different measurement methods give very different values of $2\Delta(0\ \mathrm{K})/T_c$.

This paper gives a unified explanation for all of the above experimental facts by taking the two-local-spin-mediated interaction (TLSMI) as a pairing interaction, and predicts that the pseudogap should be observed clearly for underdoped NCCO. In section 2 we derive a generic formula for T_c independent of any special mechanism by using the long-range phase-coherence condition. In section 3 we briefly introduce the concept of TLSMI proposed in references [16, 17]. The basic theoretical method given in references [16, 17] is the extended Abrikosov pseudo-fermion method [18, 16]. In section 4 we discuss the values of related parameters. In section 5 we give the results from our numerical calculations in order to explain the experimental facts, and to make some predictions. In section 6 we make some interesting conjectures.

2. Determination of T_c

In this section, we derive a generic formula for T_c independent of any special mechanism by using the long-range phase-coherence condition. There are many papers in which T_c is determined from the long-range phase-coherence condition [19–22]. We decided to use the quantum XY-model described in reference [21]. There are three reasons for this.

- First, Emery and Kivelson [19, 20] showed that the value of T_c determined using the quantum XY-model in reference [21] is less than that determined using the classical XY-model in references [19, 20, 22].
- Second, in our view, the classical XY-model is not appropriate to the high-T_c cuprates. According to the classical XY-model, $T_c \propto x$. Therefore, the value of T_c can never become zero at $x = 0.05$ and 0.12 in the cases of LSCO and NCCO, respectively. However, the experimental values of T_c at $x = 0.05$ and 0.12 are zero for both LSCO and NCCO. Although Uemura *et al* claimed that their experiments show $T_c \propto x/m^*$ [23, 24], we should note that they never measured T_c at small values of x for the high-T_c cuprates.
- Third, the deviations of the theoretical values of T_c from the experimental values are too large [19, 20].

In our picture, the disappearance of superconductivity above T_c does not involve Cooper pair breaking as it would for phonon-mediated superconductors where the BCS coherence length is generally longer than the mean free path for the carriers; instead, it is associated with the loss of long-range superconducting phase coherence as the Coulomb energy required to suppress charge fluctuations prevails over the tendency towards long-range superconducting phase order maintained by the Ginzburg–Landau phase-stiffness parameter, $J_{\text{stiffness}}$. Doniach and Inui gave the critical value of $J_{\text{stiffness}}$, J_c, at T_c as [21]

$$J_c \geqslant \frac{2e^2}{\epsilon_\infty a_0(T_c)} \tag{1}$$

where ϵ_∞ is the high-frequency dielectric constant, typically in the range from 1 to 4 [25], e the free-electron charge, and $a_0(T_c)$ the mean pair spacing at T_c. For $J_{\text{stiffness}} \geqslant J_c$, the system remains a superconductor. The phase-stiffness parameter may be computed from an expansion of the appropriate Cooper pair correlation function in powers of the wavenumber q [21]. The formula used in reference [21] to determine the value of T_c from the condition for appearance of long-range phase coherence is approximately

$$|\Psi(T_c)|^2 \lim_{q\to 0} \frac{1}{a_0^2(T_c)} \frac{\partial}{\partial q^2}[L(q)]^{-1} = \frac{2e^2}{\epsilon_\infty a_0(T_c)} \tag{2}$$

where $\Psi(T_c)$ is the order parameter at T_c, and q the wavenumber. For the CuO_2 plane of the high-T_c cuprates,

$$a_0^2(T_c) = \frac{2a_{\text{Cu}}^2}{x|\Psi(T_c)|^2}. \tag{3}$$

Note that equation (2) does not involve the form of the pair interaction. Also,

$$L(q) = \sum_{\boldsymbol{k}} \left[\frac{1}{2E_{\boldsymbol{k}}} - \frac{E_{\boldsymbol{k}}E_{\boldsymbol{k}+\boldsymbol{q}} + \xi_{\boldsymbol{k}}\xi_{\boldsymbol{k}+\boldsymbol{q}}}{E_{\boldsymbol{k}}E_{\boldsymbol{k}+\boldsymbol{q}}(E_{\boldsymbol{k}} + E_{\boldsymbol{k}+\boldsymbol{q}})} \right] \tag{4}$$

$$E_{\boldsymbol{k}} = \xi_{\boldsymbol{k}} + \Delta(\boldsymbol{k}, 0) \tag{5}$$

$$\xi_{\boldsymbol{k}} = \epsilon(\boldsymbol{k}) - E_F \tag{6}$$

where $\Delta(\boldsymbol{k}, 0)$ is the gap at 0 K:

$$\Delta(\boldsymbol{k}, T) = \Delta(T)G(\boldsymbol{k}). \tag{7}$$

Assume that the maximum value of $G(\boldsymbol{k})$ is one. Note that $\Delta(\boldsymbol{k}, T)$ in equation (7) can be caused by any pairing mechanism. Then equation (2) can be simplified by making the following two approximations: the effective-mass approximation for $\epsilon(\boldsymbol{k})$; and using $\Delta(0)/2$ as the average value of $\Delta(\boldsymbol{k}, 0)$. Hence for the CuO_2 plane,

$$L(q) = \frac{a^2 m^*}{4\pi} \left[1 + \frac{k_F^2 q^2}{9(m^*)^2(\Delta(0)/2)^2} \right] \tag{8}$$

where m^* is the effective mass of the carrier. The relation between the order parameter and the gap is

$$|\Psi(T_c)| = \frac{\Delta(T_c)}{\Delta(0)}. \tag{9}$$

Substituting equations (3), (8), and (9) into equation (2) yields

$$|\Psi(T_c)|^3 = \frac{\Delta(0)^2}{\sqrt{x}k_F^2} \frac{9\sqrt{2}a_{\text{Cu}}^3 e^2 (m^*)^3}{8\pi\epsilon_\infty}. \tag{10}$$

Equation (10) is a general theoretical formula for T_c versus x, which is still independent of any particular model for the pair interaction in the CuO_2 plane. The key point as regards using equation (10) is that one needs to know the relation between the gap and temperature T—which is needed to solve the BCS gap equation—and, therefore, to know the relation describing the concrete pair interaction.

The value of T_c determined above corresponds to establishing the long-range phase coherence of the order parameter. Therefore, T_c should be called the pairing temperature with phase coherence. Correspondingly, the temperature T^* for the opening of a gap at the Fermi surface should be called the pairing temperature without phase coherence. A gap appearing in the range $T_c < T < T^*$ is called a pseudogap.

3. The pairing interaction

The effective Hamiltonian of the Hubbard–Emery d–pσ model used to describe the CuO_2 plane of p-type cuprates is given clearly by reference [26]; it is

$$H = -\sum_{i\alpha\beta s} T_{\alpha\beta} p^+_{\alpha s} p_{\beta s} + J_K \sum_{i\alpha\beta ss'} \widehat{\boldsymbol{S}}_i \cdot \vec{\boldsymbol{\sigma}}_{ss'} p^+_{\alpha s} p_{\beta s'} + J \sum_{i\neq j} \widehat{\boldsymbol{S}}_i \cdot \widehat{\boldsymbol{S}}_j \tag{11}$$

where the summation over α and β is for the oxygen sites around the ith Cu^{2+} site, $p_{\alpha s}$ annihilates an $O_{p\sigma}$ hole with spin s at site α, $\widehat{\boldsymbol{S}}_i$ is the local spin operator of Cu^{2+} at site i, $\vec{\boldsymbol{\sigma}}$ is the Pauli matrix vector, and i and j are the nearest neighbours. Expand $p_{\alpha s}$ in $\boldsymbol{k}$-space. Here $\boldsymbol{k}$ is the wave vector in the Brillouin zone of the oxygen lattice in the CuO_2 plane. The second term in equation (11) is the Kondo Hamiltonian, H_K, which implies that the $O_{p\sigma}$ holes with wave vectors $\boldsymbol{k}\uparrow$ and $-\boldsymbol{k}\downarrow$ can have interactions with the local spins of Cu^{2+} at sites i and j, respectively. The third term in equation (11), on the other hand, is the Heisenberg interaction, H_H, between the two local spins at sites i and j. The effective interaction between the two $O_{p\sigma}$ holes with wave vectors $\boldsymbol{k}\uparrow$ and $-\boldsymbol{k}\downarrow$, mediated by H_K, H_H, and H_K, is called the TLSMI.

Using the extended Abrikosov pseudo-fermion method described in references [16, 18], the expression for the TLSMI $U_{\boldsymbol{k}\boldsymbol{k}'} = -A(T)F_{\boldsymbol{k}\boldsymbol{k}'}$ is [16, 17]

$$U_{\boldsymbol{k}\boldsymbol{k}'} = -A(T)F_{\boldsymbol{k}\boldsymbol{k}'} \tag{12}$$

$$A(T) = \frac{JJ_K^2(1+C)N''/N'w(J/T)}{T^2 + 16JJ_K^2\sum_{\boldsymbol{k}\boldsymbol{p}} g(\boldsymbol{k},\boldsymbol{p})/\{1+32\pi^2 J_K^2[N(E_F)]^2\overline{h(\boldsymbol{q})}\}} \tag{13}$$

$$g(\boldsymbol{k},\boldsymbol{p}) = \left(\frac{1}{2N_{Cu}}\right)^2 \frac{f[\epsilon(\boldsymbol{k}) - E_F]F_1(\boldsymbol{k})F_1(\boldsymbol{p})F_5(\boldsymbol{k})F_5(\boldsymbol{p})}{\epsilon(\boldsymbol{k}) - \epsilon(\boldsymbol{p})} \tag{14}$$

$$h(\boldsymbol{q}) = [\cos(q_x a/2)\cos(q_y a/2)]^4 \tag{15}$$

$$F_{\boldsymbol{k}\boldsymbol{k}'} = \sum_{i=1}^{4} F_i(\boldsymbol{k})F_i(\boldsymbol{k}')F_5(\boldsymbol{k})F_5(\boldsymbol{k}') \tag{16}$$

$$F_1(\boldsymbol{k}) = \cos(k_x a)\cos(k_y a) \tag{17}$$

$$F_2(\boldsymbol{k}) = \sin(k_x a)\sin(k_y a) \tag{18}$$

$$F_3(\boldsymbol{k}) = \sin(k_x a)\cos(k_y a) \tag{19}$$

$$F_4(\boldsymbol{k}) = \cos(k_x a)\sin(k_y a) \tag{20}$$

$$F_5(\boldsymbol{k}) = \cos^2(k_x a/2)\cos^2(k_y a/2) \tag{21}$$

where $f(x)$ is the Fermi distribution, $\epsilon(\boldsymbol{k})$ is the energy of the $O_{p\sigma}$ holes, E_F is the Fermi energy, $N(E_F)$ is the density of states, C is the weak tunnelling coupling between two CuO_2 planes if the cuprates have two CuO_2 planes in a unit cell, N' is the number of Cu^{2+} in a cluster with antiferromagnetic short-range order in the CuO_2 plane, and N'' is the number of Cu^{2+} in the nearest-neighbour position in the same cluster. The bar represents the average over a Fermi surface. $w(J/T)$ is the transformation factor in the extended Abrikosov pseudo-fermion method [16].

If $J > 0$, then the TLSMI between two $O_{p\sigma}$ holes with wave vectors $\boldsymbol{k}\uparrow$ and $-\boldsymbol{k}\downarrow$, $U_{\boldsymbol{k}\boldsymbol{k}'}$, is negative, which means that the TLSMI can become the Cooper pair interaction of the two $O_{p\sigma}$ holes in regions with, at least, antiferromagnetic short-range order. There are also the phonon-mediated interaction, V_{ep}, and the effective Coulomb interaction, V_c^*, between the two $O_{p\sigma}$ holes with wave vectors $\boldsymbol{k}\uparrow$ and $-\boldsymbol{k}\downarrow$ besides the TLSMI. Considering all the interactions, the BCS gap equation is [16]

$$\Delta'(T,\boldsymbol{k}) = -\sum_{\boldsymbol{k}'} \frac{V_{\boldsymbol{k}\boldsymbol{k}'}\Delta'(T,\boldsymbol{k}')}{2m(T,\boldsymbol{k}')} \tanh\frac{m(T,\boldsymbol{k}')}{2T} \tag{22}$$

$$m(T,\boldsymbol{k}) = \sqrt{[\epsilon(\boldsymbol{k}) - E_F]^2 + |\Delta'(T,\boldsymbol{k})|^2} \tag{23}$$

$$V_{\boldsymbol{k}\boldsymbol{k}'} = \begin{cases} V_{ep} + V_c^* & 0 \leqslant |\epsilon(\boldsymbol{k}) - E_F|, |\epsilon(\boldsymbol{k}') - E_F| \leqslant E_D \\ U_{\boldsymbol{k}\boldsymbol{k}'} & 0 \leqslant |\epsilon(\boldsymbol{k}) - E_F|, |\epsilon(\boldsymbol{k}') - E_F| \leqslant E_F \\ 0 & \text{otherwise} \end{cases} \tag{24}$$

where $\Delta'(T,\boldsymbol{k})$ is a gap function in the CuO_2 plane, and E_D the Debye energy. Considering that $\epsilon(\boldsymbol{k})$ generally has even parity, V_{ep} and V_c^* are constants, $F_1(\boldsymbol{k})$, $F_2(\boldsymbol{k})$, and $F_5(\boldsymbol{k})$ have even parity, and $F_3(\boldsymbol{k})$ and $F_4(\boldsymbol{k})$ have odd parity, the BCS gap equation can be separated into four decoupled equations, and has the following four solutions:

$$\Delta'_{\rm s}(T,\boldsymbol{k}) = \Delta_1(T) + \Delta_2(T)F_1(\boldsymbol{k})F_5(\boldsymbol{k}) \tag{25}$$

$$\Delta'_{\rm d}(T,\boldsymbol{k}) = \Delta_3(T)F_2(\boldsymbol{k})F_5(\boldsymbol{k}) \tag{26}$$

$$\Delta'_{\rm p1}(T,\boldsymbol{k}) = \Delta_4(T)F_3(\boldsymbol{k})F_5(\boldsymbol{k}) \tag{27}$$

$$\Delta'_{\rm p2}(T,\boldsymbol{k}) = \Delta_5(T)F_4(\boldsymbol{k})F_5(\boldsymbol{k}). \tag{28}$$

Note that in a coordinate system $\boldsymbol{k}'$ obtained by rotating the system $\boldsymbol{k}$ by 45°,

$$F_2(\boldsymbol{k}') = [\cos(k'_x a_{\rm Cu}) - \cos(k'_y a_{\rm Cu})]/2.$$

That is, $F_2(\boldsymbol{k}')$ is the frequently encountered d wave. Because $\Delta'_{\rm d}(T,\boldsymbol{k})$ contains $F_5(\boldsymbol{k})$ besides $F_2(\boldsymbol{k})$, we call $\Delta'_{\rm d}(T,\boldsymbol{k})$ the composite d wave.

It is easy to understand that the effective Hamiltonian (11) can also describe the CuO_2 plane of the n-type cuprates in principle, because the structures of the d–pσ model Hamiltonian in equation (2.1) of reference [26] should be similar for LSCO and NCCO. The main difference between the two types is in the form of the Fermi surface. The Fermi surfaces are near the lower Hubbard band top and the upper Hubbard band bottom for LSCO and NCCO, respectively. The Fermi surfaces of LSCO and NCCO with $x = 0.15$ are shown in figure 1.

4. Values of related parameters

The values of the parameters appearing in the expressions for the TLSMI in equations (12) and (13) and in the BCS gap equation, equations (22), (23), and (24), have been determined from experiments and first-principles calculations for the p-type cuprates, and they are given

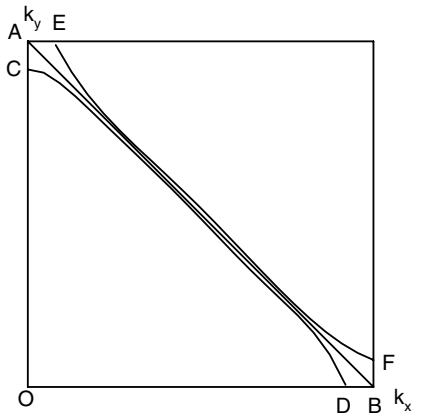

Figure 1. Fermi surfaces of LSCO and NCCO in one quadrant. The line AB is the lower Hubbard band top and upper Hubbard band bottom for LSCO and NCCO, respectively. The lines CD and EF are the Fermi surfaces for LSCO and NCCO, respectively. The line CD has negative energy. The mathematical expression for line CD is given in reference [16]. The line EF has positive energy. The lines CD and EF are symmetric, in contrast to line AB.

in reference [16]. Because the CuO_2 plane of NCCO is nearly the same as that of LSCO, the values of related parameters should also be nearly the same for the two. For example, $J = 0.126$ eV and 0.107 eV for LSCO and NCCO at $x = 0$, respectively [27, 28]. For NCCO the AF long-range coherence length persists until $x = 0.12$ [28, 29]. Therefore, $N''/N' = 2$ from the definition of N'' and N' in section 3. To obtain the values of N''/N' from x for LSCO, reference [16] uses figure 3 of reference [17], which gives the relation between N''/N' and the AF short-range coherence length ξ, and the experimental data, which give the values of ξ derived from x. In the case of NCCO, we lack experimental data relating ξ and x. Qualitatively, the smaller the value of x, the larger the value of ξ. We know from figure 3 of reference [17] that the larger the value of ξ, the larger the value of N''/N'. We take it that the values of N''/N'

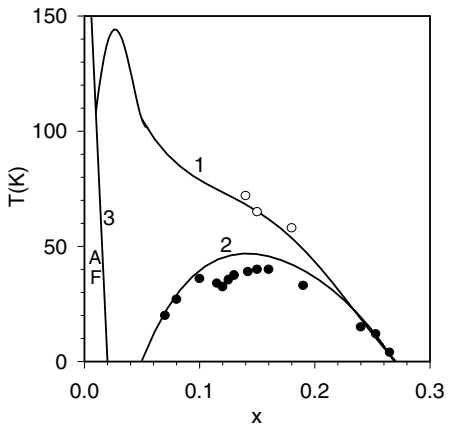

Figure 2. The phase diagram of LSCO. Lines 1 and 2 are our theoretical curves for T^* and T_c versus x, respectively. The solid circles and the open circles are the data for T_c and T^* versus x, respectively [4]. The AF insulator is at $x < 0.02$ [28, 29]. The Cooper pairs without phase coherence are in the region enclosed by lines 1, 2, and 3.

decrease approximately linearly from 2 at $x = 0.12$ to 1.1 at $x = 0.2$. The electron–phonon coupling constant $\lambda = N(E_F)V_{ep} \cong 0.1$ for LSCO [30]. $\mu^* = N(E_F)V_c^* = 0.15$ [31].

5. Results from numerical calculations

Our numerical calculations show that the order parameter of LSCO is the d-wave one given in equation (26). For LSCO, $\lambda < \mu^*$. Therefore the electron–phonon interaction makes no contribution to the superconductivity of LSCO. From figure 2 we see that the theoretical curve for T_c versus x fits the data in reference [4] well. T^* in figure 2 is determined only by the zero-gap condition for the BCS gap equation. Therefore, there is a pseudogap at $T_c < T < T^*$, which comes from the formation of a Cooper pair without long-range phase coherence. Figure 3 shows clearly that the values of the ratio $2\Delta(0\text{ K})/T_c$ can be very large for LSCO. For completeness, we give the theoretical curve and the experimental data for $\Delta(0\text{ K})$ versus x in figure 4.

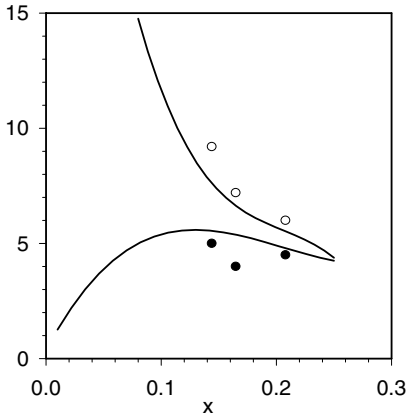

Figure 3. The lower and the upper solid lines are our theoretical curves for $2\Delta(0\text{ K})/T^*$ and $2\Delta(0\text{ K})/T_c$ versus x for LSCO, respectively. The solid circles and open circles are the corresponding data [4]. Here and in all the following diagrams, $\Delta(0\text{ K})$ is the d-wave gap in equation (26), at $T = 0$ K and along the Cu–O bond direction.

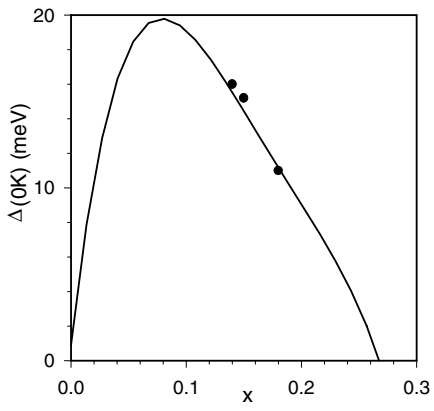

Figure 4. The theoretical curve for $\Delta(0\text{ K})$ versus x for LSCO. The data come from reference [4].

Figure 5 is our theoretical phase diagram for NCCO. Its basic structure is the same as that of LSCO. Both our theory and the experiment in reference [5] show that the doping range of superconductivity for NCCO is much narrower than that of LSCO. The pseudogap exists in the range enclosed by the lines 1, 2, and 3, which has not yet been found by experiment. Figure 6 shows that the theoretical value of $2\Delta(0)/T_c$ can be much larger than the BCS value, 3.53. Figure 7 indicates that the smaller the value of x, the larger the value of $\Delta(0\ \mathrm{K})$ for $x > 0.12$. Figure 8 shows the gap anisotropy of NCCO. It is very important to note that there is no state between the two directions of the lines OF and OB in figure 1.

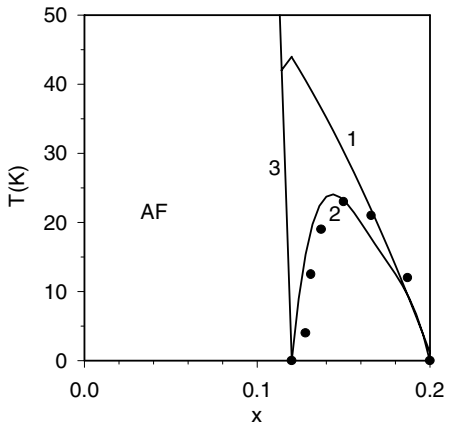

Figure 5. The phase diagram of NCCO. The lines 1 and 2 are our theoretical curves for T^* and T_c versus x, respectively. The solid circles are the data for T_c versus x from reference [5].

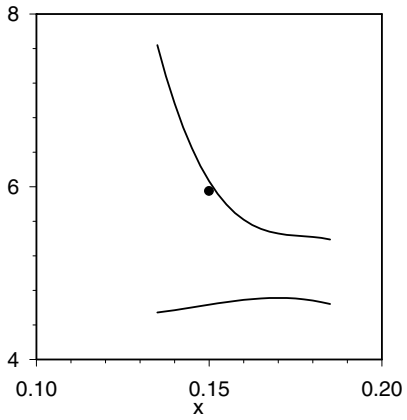

Figure 6. The lower and the upper solid lines are our theoretical curves for $2\Delta(0\ \mathrm{K})/T^*$ and $2\Delta(0\ \mathrm{K})/T_c$ versus x for NCCO, respectively. The solid circle represents data from reference [6].

Our theory can provide answers to the three problems regarding the contradictory experimental results on NCCO posed in section 1. We do not know the value of λ for NCCO. If we assume $\lambda = 0.2$, which is already much larger than the experimental value for LSCO, $\mu^* = 0.15$, and $E_D = 1000\ \mathrm{K}$, then $T_{c,\mathrm{phonon}} = 10^{-4}\ \mathrm{K}$, which means that the electron–phonon interaction does not make a contribution to the superconductivity of NCCO. Our numerical calculations also indicate that the s wave of the TLSMI in equation (12) makes no contribution

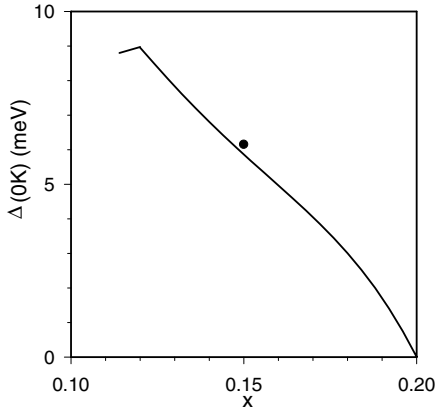

Figure 7. The theoretical curve for $\Delta(0\ \mathrm{K})$ versus x for NCCO. The solid circle comes from reference [11].

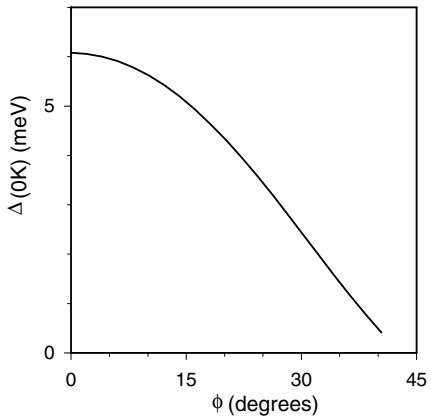

Figure 8. The gap anisotropy at $T = 0$ K for NCCO with $x = 0.15$. 0° corresponds to the direction of the Cu–O bond. The gap at 40.42° corresponds to the gap at point F in figure 1.

to the superconductivity of NCCO. Briefly, our theory shows that the superconductivity of NCCO should be the pure d-wave one described by equation (26).

Now we answer the main problem posed in section 1. Alff *et al* obtained values for the gap at $T = 0$ K for identical samples using two different methods in reference [11]. The first method is that in which Alff *et al* measured the tunnelling conductance spectra of NCCO with $T_c = 24$ K and $x = 0.15$, and obtained $\Delta(2.2\ \mathrm{K}) = 6.15$ meV in the Cu–O bond direction. The second method is that on the basis of which Alff *et al* reached the conclusion that NCCO is of isotropic s-wave type, by fitting the $\lambda_{ab}(T)$ data with $\Delta(0\ \mathrm{K}) = 3$ meV. It is obvious that the two values are too different. Our theory can explain this difference. Figure 8 indicates that $\Delta(0\ \mathrm{K}) = 6.02$ meV along the Cu–O bond direction, and the average value of the gap at 0 K in all directions is about 3.2 meV. Therefore, combining the two values in reference [11] and our theory, we can say that the isotropic s-wave conclusion is unreliable. Figure 8 shows that although there is no gap node in NCCO, the gap at 40.42° is only 0.4 meV, i.e., really very small. This is why Luke *et al* cannot reliably distinguish between possible forms, i.e., T^1, T^2, and exponential, of $\lambda_{ab}(T)$ at low temperature [10].

Why is it that Kashiwaya *et al* cannot observe a ZBCP if the symmetry of the superconductivity in NCCO is a d-wave one? As is well known, many experiments support the suggestion that the origin of the ZBCP is an Andreev bound state at the surface of a d-wave superconductor [15]. Figure 1 shows that there is no state for the angles between the lines OF and OB. Therefore, there is definitely no Andreev bound state for a small angle of the quasiparticle trajectory to the surface normal for a (110)-oriented surface. It must also be noted that—besides our theory—the ZBCP can be suppressed by disorder [15].

Combining reference [11] and our theory, we know that the value of the gap along the Cu–O bond direction measured from conductance spectra is maximal, and the value of the gap obtained by fitting measured penetration depths is only an average value for an anisotropic gap. Therefore, it is easy to understand why the values of $\Delta(0\ \mathrm{K})$ and $2\Delta(0\ K)/T_c$ derived in the former manner are larger than the values derived in the latter manner.

6. A possible s-wave superconductor

If we can make a compound $M_{2-x}N_xCuO_4$, then we can definitely make the lower Hubbard band not full through changing the valences of M and N, and the magnitude of x. If this material exhibits superconductivity caused by the TLSMI, then the symmetry of the order parameter should be the s-wave one, given by equation (25). The reason for this is as follows. The TLSMI in equation (12) and the gap in equation (25) contain a term $\cos(k_xa)\cos(k_ya)$. This term will make a larger contribution to the gap equation due to the small values of k_xa and k_ya near the bottom of lower Hubbard band. In contrast, the d wave makes only a small contribution to the gap equation, due to the factor $\sin(k_xa)\sin(k_ya)$ and the small values of k_xa and k_ya in this case. The s-wave expression of equation (25) contains two terms. One comes from the TLSMI. The other comes from electron–phonon interaction. The superconductivity caused by both the TLSMI and the electron–phonon interaction might have a higher value of T_c than that caused by just one interaction.

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References

[1] Khurana A 1989 *Phys. Today* **42** 17
[2] Paget K M, Cuha S, Cieplak M Z, Trofimov I F, Turneaure S J and Lemberger R 1999 *Phys. Rev.* B **59** 641
[3] Fisher R A, Phillips N E, Schilling A, Buffeteau B, Calemczuk R, Hargreaves T E, Marcenat C, Dennis K W, McCallum R W and Marcenat C 2000 *Phys. Rev.* B **61** 1473
[4] Nakano T, Momono N, Oda M and Ido M 1998 *J. Phys. Soc. Japan* **67** 2622
[5] Naito M, Sato H and Yamamoto H 1997 *Physica* C **293** 36
[6] Kashiwaya S, Ito T, Oka K, Ueno S, Takashima H, Koyanagi M, Tanaka Y and Kajimura K 1998 *Phys. Rev.* B **57** 8680
[7] Andreone A, Cassinese A, Chiara A D, Vaglio R, Gupta A and Sarnelli E 1994 *Phys. Rev.* B **49** 6392
[8] Wu D H, Mao J, Mao S N, Peng J L, Xi X X, Venkatesan T, Greene R L and Anlage S M 1993 *Phys. Rev. Lett.* **70** 85
[9] Cooper J R 1996 *Phys. Rev.* B **54** R3753
[10] Luke G M, Fudamoto Y, Kojima K, Larkin M, Merrin J, Nachumi B, Uemura Y J, Sonier J E, Ito T, Oka K, de Andrade M, Maple M B and Uchida S 1997 *Physica* C **282–287** 1465
[11] Alff L, Meyer S, Kleefish S, Schoop U, Marx A, Sato H, Naito M and Gross R 1999 *Phys. Rev. Lett.* **83** 2644
[12] Woods S I 1999 *IEEE Trans. Appl. Supercond.* **9** 3917

[13] Tsuei C C and Kirtley J R 2000 *Phys. Rev. Lett.* **85** 182
[14] Tsuei C C 2000 private communication, June
[15] Aprili M, Corington M, Paraoanu E, Neidermeier B and Greene L H 1998 *Phys. Rev.* B **57** R8139
[16] Liu Fu-sui and Chen Wan-fang 1998 *Phys. Rev.* B **58** 8812
[17] Liu Fu-sui 1997 *Phys. Lett.* A **224** 185
[18] Liu Fu-sui, Wang Zhongcheng, Chen Wan-fang and Yuan Xiao-jian 1995 *Phys. Rev.* B **51** 12 491
[19] Emery V J and Kivelson S A 1995 *Nature* **374** 434
[20] Emery V J and Kivelson S A 1995 *Phys. Rev. Lett.* **74** 3253
[21] Doniach S and Inui M 1990 *Phys. Rev.* B **41** 6668
[22] Chakraverty B K and Ramakrishnan T V 1997 *Physica* C **282–287** 290
[23] Uemura Y J, Luke G M, Sternlieb B J, Brewer J H, Carolan J F, Hardy W N, Kadono R, Kempton J R, Kiefl R F, Kreitzman S R, Mulhern P, Riseman T M, Williams D L, Yang B X, Uchida S, Tagagi H, Gopalakrishnan J, Slaight A W, Subramanian M A, Chien C L, Cieplak M Z, Xiao Gang, Lee V Y, Statt B W, Stronach C E, Kossler W J and Yu X H 1989 *Phys. Rev. Lett.* **62** 2317
[24] Uemura Y J, Le L P, Luke G M, Sternlieb B J, Wu W D, Brewer J H, Riseman T M, Seaman C L, Maple M B, Ishikawa M, Hinks D G, Jorgensen J D, Saito G and Yamochi H 1991 *Phys. Rev. Lett.* **66** 2665
[25] Timusk T and Tanner D B 1988 *Physical Properties of High Temperature Superconductors* vol 1, ed D M Ginsberg (Singapore: World Scientific) p 346
[26] Matsukawa H and Fukuyama H 1989 *J. Phys. Soc. Japan* **58** 2845
[27] Lyons K B, Fleury P A, Singh R R and Sulewski P E 1991 *Proc. NATO Advanced Research Workshop on Dynamics of Magnetic Fluctuations in High-Temperature Superconductors* ed G Reiter, P Horsch and G Psaltakis (New York: Plenum) p 159
[28] Brenig W 1995 *Phys. Rep.* **251** 153
[29] Dagoto E 1994 *Rev. Mod. Phys.* **66** 763
[30] Tanner D B and Timusk T 1992 *Physical Properties of High Temperature Superconductors* vol 3, ed D M Ginsberg (Singapore: World Scientific) p 363
[31] Schruter M A 1993 *Mater. Sci. Eng.* B **19** 129