Superconductivity due to spin fluctuations originating from multiple Fermi surfaces in a double chain superconductor Pr$_2$Ba$_4$Cu$_7$O$_{15−δ}$

Tsunghito Nakano,$^1$ Kazuhiko Kuroki,$^1$ and Seiichiro Onari$^2$

$^1$Department of Applied Physics and Chemistry, The University of Electro-Communications, Chofu, Tokyo 182-8585, Japan
$^2$Department of Applied Physics, The University of Nagoya, Nagoya 464-8603, Japan

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The mechanism of superconductivity in Pr$_2$Ba$_4$Cu$_7$O$_{15−δ}$ is studied using a quasi-one dimensional double chain model with appropriate hopping integrals, on-site $U$, and off-site repulsion $V_t$. Applying the fluctuation exchange method to this model and solving the Eliashberg equation, we obtain the doping dependence of superconductivity that is consistent with the experiments. The superconducting gap has an extended $s$-wave-like form, which gives a temperature dependence of the spin lattice relaxation rate that does not contradict with the experimental results.

It goes without saying that unconventional superconductivity (SC) appears on the CuO$_2$ planes or ladder structures in some cuprates.$^{1,2}$ Recently, SC in the cuprates has been found in another structure, namely, the CuO double chain. Pr$_2$Ba$_4$Cu$_7$O$_{15−δ}$ (Pr247/δ), which consists of metallic CuO double-chain and semiconducting single-chain besides the Mott insulating CuO$_2$ plane, shows SC with $T_c^{max} \sim 15$ K in a moderate oxygen defect concentration range of $δ = 0.2 \div 0$, which controls the band filling of the double chain block. Recent NQR study has revealed that the SC occurs in the double-chain, and further observed a "charge freezing" just like the one observed in Pr$_{1−δ}$Ba$_2$Cu$_4$O$_{6+δ}$ at, and only at, $δ = 0$, which implies that the double chain is near 1/4-filling in Pr247($δ = 0$) (although there remains some ambiguity in the band filling estimation)$^9,10,11$.

Theoretically, Sano et al. proposed a superconducting mechanism using a one dimensional (1D) double chain model$^{12}$ which is essentially based on a superconducting mechanism proposed generally by Fabrizio$^{13}$ and also studied by one of the present authors$^{14}$ about a decade ago. In a purely 1D double chain system, the band dispersion can have a double well structure, resulting in four Fermi points for appropriate band fillings, which in turn results in an opening of the spin gap and dominating superconducting correlation. Sano et al. determined the tight binding (TB) parameters for a purely 1D system using the LDA band dispersion between the X and S point for the double chain of YBa$_2$O$_4$O$_y$ (Y124) (See Fig. 2.$^{15}$)

From this band structure, they have suggested that the appearance of SC upon oxygen reduction is due to the increase of the number of Fermi points from two to four as the band filling is increased from $\sim 1/4$-filling.

Although we believe that this theory is correct in that the existence of four Fermi surfaces (FS) is essential in the occurrence of SC, there remain several problems, which have motivated the present study. First, if we look into the band structure in the entire two dimensional Brillouin zone (BZ) shown in Fig. 2, the number of the FS along the Γ-Y line remains to be four down to very low band fillings (i.e., the inner FS is 2D).$^{16,19}$ so the variance of the FS around 1/4-filling is not simply a change of their number between two and four as in the pure 1D theory.

Therefore, the reason for the absence of $T_c$ before oxygen reduction is not clear. Secondly, a previous estimation of the spin gap using density matrix renormalization group (DMRG) has shown that the spin gap in a double chain Hubbard model is, if any, very small at 1/4-filling$^{15}$ although the values of the hopping integrals taken there do not directly correspond to Pr247. Moreover, a recent DMRG analysis shows that the spin gap, if any, is too small to be estimated numerically when the ratio between the interchain and the intrachain hopping is smaller than $\sim 0.3$ while this ratio is estimated to be around 0.2 in Pr247 from first principles calculations.$^{19}$ Thirdly, it is of interest whether the relatively high $T_c$ of 15K can be explained within a Hubbard-type model with the above mentioned ratio as small as $\sim 0.2$, because it is obvious that SC does not occur when this ratio is too small, namely, when the system is essentially a single chain repulsive Hubbard model.$^{20}$ To resolve these problems, we propose in this paper a spin fluctuation mediated pairing mechanism, where the origin of the spin fluctuation is indeed the presence of multiple FS. We adopt the fluctuation exchange (FLEX) method to a quasi-one dimensional (Q1D) extended Hubbard model for the CuO double chain.$^{22}$ A set of TB parameters are determined from the results of LDA calculation for Y124.$^{16,19}$ By solving the linearized Eliashberg equation, we obtain a finite $T_c$ for an extended $s$-wave SC, whose band filling dependence is qualitatively similar to the experimental results.

Note that the original model on the zigzag lattice

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**FIG. 1:** (a) The effective single band 1D double chain model. (b) Q1D double chain model.
(which has two sites in a unit cell and thus results in a two band system) can be mapped to a single band model having distant hopping integrals as shown Fig. 2. Such a mapping is often adopted in the study of zigzag chains. Note that after this single band mapping, the BZ will be unfolded in the \( k_b \) direction. Hereafter, our FLEX results will be shown in the unfolded BZ. The Hamiltonian of the extended Hubbard model for the double chain is given by

\[
H = \sum_{i,j,\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} + \frac{1}{2} \sum_{i,j} V_{ij} n_i n_j, \tag{1}
\]

where \( c_{i\sigma}^\dagger \) creates an electron of spin \( \sigma \) at site \( i \), \( t_{ij} \) is a hopping parameter between site \( i \) and \( j \), and \( U \) and \( V_{ij} \) is an electron-electron interaction between such sites. The values of \( t_{ij} \) are determined by fitting the TB dispersion to the results of the LDA calculations for the double chains of Y124. The fitting result is shown in Fig. 2. With the obtained values of the hopping parameters, we have found that for the noninteracting case the inner FS around the \( \Gamma \) point remains unless \( n \leq 0.1 \) (\( n = \) band filling=number of electrons/number of sites), although a topological change does occur near the X point at \( n \sim 0.3 \) (Fig. 2b), which corresponds to the change of the number of Fermi points discussed in ref. 12. In the FLEX, the dressed Green’s function is obtained by solving the Dyson’s equation for the noninteracting case the inner FS around the \( \Gamma \) point remains unless \( n \leq 0.1 \) (\( n = \) band filling=number of electrons/number of sites), although a topological change does occur near the X point at \( n \sim 0.3 \) (Fig. 2b), which corresponds to the change of the number of Fermi points discussed in ref. 12. In the FLEX, the dressed Green’s function is obtained by solving the Dyson’s equation

\[
\bar{G}(k) = \left[ G_0^{-1}(k) - \Sigma(k) \right]^{-1}
\]

self-consistently, where \( G_0(k) \) is the undressed Green’s function and \( \Sigma(k) \) is the self energy written by the spin and charge susceptibilities \( \chi_s(q) = \chi(q)[I + \tilde{V}_m.d(q)\chi(q)]^{-1} \) with \( k \equiv (k,\varepsilon_n = (2n+1)\pi T) \) and \( q \equiv (q,\omega_l = 2l\pi T) \). \( \tilde{\chi}(q) \) is the irreducible susceptibility which is composed of a product of \( G(k) \), and \( \tilde{V}_m.d(q) \) is the magnetic and density coupling vertices described with \( U \) and \( V_{ij} \). \( \chi_{s,c}(q) \) and \( V_{d,m}(q) \) are the matrices indexed by the initial (final) relative displacement of particle-hole pair \( \Delta r \) (\( \Delta r' \)). The sizes of these matrices increase as the number of off-site interactions increases; namely if \( U \) and the nearest neighbor (n.n.) repulsion \( V_1 \) exist, the matrix size becomes \( 3 \times 3 \). The pairing interactions are given by

\[
\Gamma_s(k,k') \propto \sum_{\Delta r,\Delta r'} \left[ \frac{1}{2} \bar{V}_m \bar{\chi}_s \bar{V}_m - \frac{1}{2} \bar{V}_d \bar{\chi}_s \bar{V}_d \right](k-k')
\]

for singlet pairing and

\[
\Gamma_t(k,k') \propto \sum_{\Delta r,\Delta r'} [-\frac{1}{2} \bar{V}_m \bar{\chi}_s \bar{V}_m - \frac{1}{2} \bar{V}_d \bar{\chi}_s \bar{V}_d](k-k')
\]

for triplet pairing. With the obtained \( G(k) \) and \( \Gamma(k,k') \), the linearized Eliashberg equation

\[
\lambda \Delta(k) = \frac{1}{2} \sum_{k',k} \Gamma(k-k')G(k')G(-k')\Delta(k')
\]

is solved. \( T_c \) is defined as \( T_c = T(\lambda = 1) \). In order to assure the convergence of the calculation, the system size and the number of Matsubara frequencies are taken as \( N = 512 \times 16 \) sites and 16384, respectively, when only \( U \) exists, and \( 256 \times 16 \) sites and 16384 are taken when both \( U \) and \( V_1 \) are present. As for the band filling range, we have investigated in the range of \( n = 0.3 \) to near half filling. In the following, we show the irreducible susceptibility \( \chi(q) \), spin and charge susceptibilities \( \chi_{s,c}(q) \) defined as the largest eigenvalues of \( \tilde{\chi}(q), \chi_{s,c}(q) \), respectively. Along with the gap function are plotted at the lowest Matsubara frequency.

First, we present the result for \( U = 2.0 \) eV without the off-site interaction. The obtained \( T_c \) is shown in Fig. 3 as functions of \( n \), and the largest eigenvalue \( \lambda \) as \( T \) for various band fillings is also shown in the inset. Finite values of \( T_c \) are obtained in a wide range of band filling, and its value gradually increases with increasing \( n \). The FS (defined as \( \varepsilon_k - \mu + \text{Re} \langle \Sigma(k) \rangle = 0 \) along with the nodes of the gap function, and the spin susceptibility, \( \chi_s(q) \), are plot-
and the values of $\chi_\nu$ differ so much from the results for $V_1$, particularly for $N = 0.5$, turns out to be smaller. As seen in Fig. 6 (a) and (b), where the obtained FS and the values of $U\chi(Q_1)$ for $V_1 = 0$ and $0.7$ eV are plotted, this reduction of $\chi_s$ is caused by the degradation of the nesting condition due to the renormalization of the band for $V_1 \neq 0$, which results in a stronger warping of the FS especially around $1/4$ filling. The reduction of $\chi_s$ is reflected in the reduction of SC especially near $n \approx 0.5$. As for the direct contribution of the charge fluctuation to the pairing interaction through the $\frac{1}{4}V_d\bar{\chi}_dV_d$ term, although $\chi_d(Q_1)$ near $1/4$ filling is relatively large compared to those for other band fillings, the peak value itself is much smaller than that of the spin susceptibility, so that this contribution should hardly affect SC. Thus the main contribution of the charge fluctuation is through the self-energy renormalization.

Although we cannot obtain $T_c$ within the investigated temperature range, judging the obtained temperature dependence of $\lambda$, it does not seem unnatural to linearly extrapolate $\log(\lambda)$ up to $\lambda = 1$ against log(T) in order to estimate the value of $T_c$. In the inset of Fig. 5 the estimated values of $T_c$ are shown. If we assume that the band filling of Pr247/δ = 0 is $n \simeq 0.5$, this result shows qualitative agreement with the experimental result in that the SC appears with moderate electron doping.

Finally, we discuss the validity of the obtained form of the gap function in the light of the experimental results. The NQR measurement has observed $1/T_1 \propto T^2$ ($T_1$ is the spin-lattice relaxation rate) without exhibiting a coherence peak below $T_\lambda$. This result seems to suggest that the nodes of the gap intersect the FS. However, if we assume that a small amount of oxygen defects controlling the band filling work as scatterers, we find that the observed $1/T_1$ can be accounted for as follows. Taking into account the effect of the impurities and the defects in the unitarity limit, we have calculated $1/T_1$ for the gap functions and the FS obtained by FLEX. As for the temperature dependence of the gap...
function, $\Delta(k, T) = \Delta_0 \phi(k) \tanh(2\sqrt{(T_c/T) - 1})$ with $\Delta_0/(k_BT_c) = 4$ is assumed, where $\phi(k)$ is proportional to the gap function obtained within the FLEX+Eliashberg eq. approach. In Fig. 8, the obtained $1/T_1$ is shown for $U = 2.0$ eV, $V_1 = 0.7$ eV. The values of $\alpha/\Delta_0$ are chosen as 0.0, 0.2 and 0.4, where $\alpha = c/\pi N_0(0)$ is the pair breaking parameter, $c$ is the impurity concentration and $N_0(0)$ is the density of states at the Fermi level in the normal state. When $\alpha/\Delta_0 = 0$, $1/T_1$ decays exponentially since a full gap opens on the FS. For finite $\alpha/\Delta_0$, $1/T_1$ shows a power-law-like decay without exhibiting a coherence peak, which resembles the experimental result. Therefore, from these results, we can safely say that the observed $1/T_1$ does not necessary rule out the possibility of the fully gapped extended s-wave pairing.

To summarize, we have investigated the superconductivity of Pr$_2$Ba$_2$Cu$_4$O$_{15-\delta}$ using an extended Hubbard model on a Q1D double chain with the TB parameters determined from the LDA calculation. By applying the FLEX to the model and solving the Eliashberg equation, in the absence of $V_1$, we have obtained singlet superconductivity with moderately varying $T_c$ in a wide band filling range. By introducing the n.n interaction $V_1$, the superconductivity is suppressed at a band filling near 1/4-filling, which at least qualitatively explains the $\delta$ dependence of superconductivity. NQR relaxation rate $1/T_1$ is also calculated taking into account the effect of the impurities and the defects. Power-law-like decaying $1/T_1$ resembling the experimental result is obtained with a moderate impurity concentration.

We should comment on the higher $\delta$ regime ($\delta > 0.5$), where $T_c$ is found to decrease with increasing $\delta$ and vanishes at $\delta \sim 0.6$ Considering that the nesting vector $Q_1$, $Q_2$ and $Q_3$ all become close to $(\pi/2, q_n)$ near half filling (see Fig. 4 and Fig. 6), umklapp processes can be allowed to result in a Mott insulating state which cannot be dealt with in the present method. More study on this issue will be carried out elsewhere. In a zigzag system as in the present case, next n.n. interactions may also play some role as suggested in experimental and theoretical studies. Unfortunately, the calculation including such interactions within the present approach has to be restricted to small system sizes. Therefore the study on this effect also remains as future study.

Present results somewhat resemble that of the recent study on Na$_x$CoO$_2$·yH$_2$O in that the extended s-wave superconductivity occurs due to the inner-outer FS nesting in a disconnected FS system. Further studies on such systems may open interesting new physics.

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