Superconductivity in the CuO double chain of $Pr_2Ba_4Cu_7O_{15-\delta}$ on the basis of Tomonaga-Luttinger liquid theory

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Recently, Matsukawa *et al.* have discovered a new superconductor $Pr_2Ba_4Cu_7O_{15-\delta}$ in which metallic CuO double chains are responsible for the superconductivity. To investigate the superconductivity, we employ the *d-p* double chain model where the tight-binding parameters are determined so as to fit the LDA band structure. On the basis of the Tomonaga-Luttinger liquid theory, we obtain the phase diagram including the superconducting phase in the weak coupling limit. We also calculate the Luttinger liquid parameter K_ρ as a function of the electron density n by using the Hartree-Fock approximation. With increasing n from quarter filling, K_ρ increases, and then exceeds 1/2 when the superconducting correlation becomes most dominant. K_ρ has a maximum at an optimal density between quarter- and half-filling. These results are consistent with the experimental observation.

KEYWORDS: $Pr_2Ba_4Cu_7O_{15-\delta}$, CuO double chain, Superconductivity, Tomonaga-Luttinger liquid, *d-p* model

Low-dimensional strongly correlated electron systems have attracted much interest due to the possible relevance to the high-T_c superconductivity. Although the two-dimensional CuO_2 planes play essential roles for the superconductivity, one-dimensional (1D) CuO chains included in some families of high-T_c cuprates have also provided an interesting testing ground for anomalous metallic states due to effects of the electron-correlation.[1–3)]

$PrBa_2Cu_4O_8$ (Pr124) is an excellent system to study the properties of 1D CuO chains, because the electronic conduction in CuO_2 plane is suppressed due to the so-called Fehrenbacher-Rice state formed by the strong hybridization between Pr $4f$ and O $2p$ orbitals.[4)] By studying the anisotropy in the resistivity of a single crystal, it was clarified that the metallic conductivity is caused by conduction in CuO double chains.[5)] Some researchers suggested that the CuO double chain might be in the Tomonaga-Luttinger liquid state.[6)]

$Pr_2Ba_4Cu_7O_{15-\delta}$ (Pr247) has both CuO double chains and CuO single chains and shows metallic conductivity at low temperatures owing to the metallic conduction in the CuO double chains. Furthermore, the carrier density can be varied by controlling the amount of oxygen deficiency in the CuO single chains. In the recent reports, the resistivity in Pr247 was investigated by changing the oxygen content, and superconductivity with $T_c \sim 15$K was found after a reduction treatment.[7,8)] The NQR experiment revealed that the superconductivity is realized at the CuO double chains.[9)] These experiments suggest that the material seems to show the possibility of novel 1D superconductivity.

Many theoretical works have been performed on 1D strongly correlated electron systems confined to a double chain such as the two-chain model and the Ladder model.[10–23)] At half-filling, the system can be described by a Heisenberg model whose ground state is a spin liquid insulator with a finite gap in spin excitation.[24)] Away from half-filling, the system becomes a metallic state which maintains a spin gap.[10–12)] This behavior is explained by the existence of electron pairs produced by the dominant fluctuations of the $4k_F$ charge density wave or the interchain-paring fluctuations. The paring fluctuation is expected to dominate over the other fluctuations in the weak coupling regime of the Hubbard model as well as in the strong coupling regime of the $t-J$ model.

Most of the theoretical works on the double chain systems have been done by using simplified single-band models such as the Hubbard model or the $t-J$ model. As for the single chain systems, two-band models such as the *d-p* model, simulating a CuO linear chain, have also been extensively investigated.[25–30)] They show that the charge fluctuation between d and p orbitals, which is not taken into account in the single-band models, has crucial effect on the superconductivity. In the case of CuO double chain (see Fig. 1), in addition to such effect, the number of the Fermi points and the values of the corresponding Fermi velocity play crucial roles for the superconductivity. They directly depend on parameters included in the *d-p* double chain model. Therefore, we need theoretical studies on the basis of a realistic *d-p* double chain model.

In the present paper, we investigate the *d-p* double

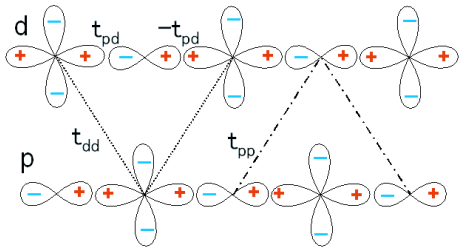

Fig. 1. Schematic diagram of Cu($3d_{x^2-y^2}$) orbitals and O($2p_\sigma$) orbitals in a CuO double chain.

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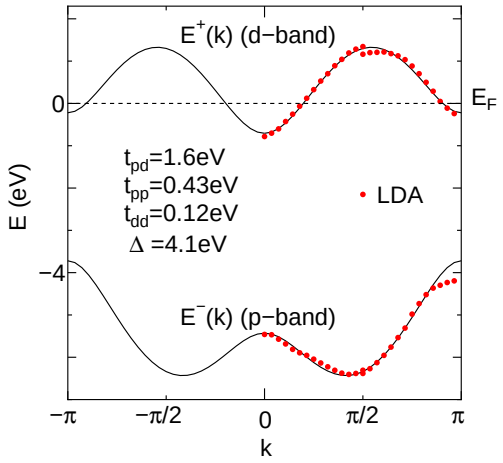

Fig. 2. A typical energy dispersion relation for the CuO double chain. Solid lines are the tight-binding result $E^{\pm}(k)$ with $t_{pd} = 1.6$eV, $t_{pp} = 0.43$eV, $t_{dd} = 0.12$eV and $\Delta = 4.1$eV. Closed circles are the LDA result for Y124.[36] Dotted line indicates the Fermi level with $n = 0.57$.

chain model, simulating a CuO double chain composed of Cu($3d_{x^2-y^2}$) orbitals and O($2p_\sigma$) orbitals as shown in Fig. 1. The tight-binding parameters, *i.e.* the hopping integrals and the charge transfer energy are estimated to fit the LDA band structure. By using the weak coupling theory,[31–33] we obtain the phase diagram including the superconducting phase.

We also calculate the Luttinger liquid parameter K_ρ[34,35] as a function of the electron density for a finite Coulomb interaction between d electrons U_d by within the Hartree-Fock (HF) approximation.

The Hamiltonian of the d-p double chain model is given by

$$\begin{aligned} H &= t_{pd}\sum_{i,\sigma}(p^\dagger_{i\sigma}d_{i+1\sigma} + h.c.) + U_d\sum_i \hat{n}_{di\uparrow}\hat{n}_{di\downarrow} \\ &+ t_{pp}\sum_{i,\sigma}(p^\dagger_{i\sigma}p_{i+1\sigma} + h.c.) + \epsilon_p\sum_{i,\sigma} p^\dagger_{i\sigma}p_{i\sigma} \\ &+ t_{dd}\sum_{i,\sigma}(d^\dagger_{i\sigma}d_{i+1\sigma} + h.c.) + \epsilon_d\sum_{i,\sigma} d^\dagger_{i\sigma}d_{i\sigma}, \quad (1) \end{aligned}$$

where $d^\dagger_{i\sigma}$ and $p^\dagger_{i\sigma}$ stand for creation operators for a electron with spin σ in a Cu($3d_{x^2-y^2}$) orbital at site i and for a hole with spin σ in a O($2p_\sigma$) orbital at site i, respectively, and $\hat{n}_{di\sigma} = d^\dagger_{i\sigma}d_{i\sigma}$. Here, t_{pd} is the hopping energy between the nearest-neighbor d and p sites and t_{pp} (t_{dd}) is the hopping energy between the nearest-neighbor p (d) sites. The atomic energy levels for p and d orbitals are given by ϵ_p and ϵ_d, respectively. The charge-transfer energy Δ is defined as $\Delta = \epsilon_d - \epsilon_p$. U_d is the on-site Coulomb interaction between d electrons.

In the noninteracting case with $U_d = 0$, the Hamiltonian eq. (1) is easily diagonalized. It yields a dispersion relation: $E^{\pm}(k) = \frac{1}{2}\{\epsilon_d + \epsilon_p + 2(t_{dd} + t_{pp})\cos k \pm \sqrt{(\Delta + 2(t_{dd} - t_{pp})\cos k)^2 + 16(t_{pd}\cos(k/2))^2}\}$, where k is a wave vector and $E^+(k)$ ($E^-(k)$) represents the upper (lower) band energy. A typical energy dispersion relation $E^{\pm}(k)$ is depicted in Fig. 2. As the charge transfer energy is positive, $\Delta = \epsilon_d - \epsilon_p > 0$, the upper band $E^+(k)$ corresponds to the d band, while the lower band $E^-(k)$ corresponds to the p band.

We estimate the tight-binding parameters in the d-p model eq. (1) so as to fit the energy dispersion $E^{\pm}(k)$ to the LDA band structure. Since the LDA results for Pr247 have not been available so far, we employ the LDA result for $YaBa_2Cu_4O_8$ (Y124)[36] in which CuO double chains are included with the same lattice structure as those in Pr247.[7] Therefore, the energy dispersions corresponding to the CuO double chain for the both compounds are expected to be almost equivalent. Using the least squares method, we obtain the parameters as $t_{pd} \simeq 1.6$eV, $t_{pp} \simeq 0.43$eV, $t_{dd} \simeq 0.12$eV and $\Delta \simeq 4.1$eV, respectively. Here, the fitting weight of the d band is taken to be one hundred times as large as that of the p band. This choice gives better fitting near E_F than the fitting with equal weight for both bands.

These estimated values are of the same orders of the well known values for the corresponding energies in the CuO_2 plane.[37] The hopping energies satisfy the relations: $t_{pd} > t_{pp} > t_{dd} > 0$, which are consistent with the values of the overlap integrals between atomic orbitals (see Fig. 1). Then, we expect that the obtained tight-binding parameters are realistic to describe the electronic state of the CuO double chain in Pr247.

Since the d band dispersion relation $E^+(k)$ has a double minimum (maximum) structure as shown in Fig. 2, the number of the Fermi points depends on the electron density n in the d band of the CuO double chain. There are two Fermi points for small n, while, four Fermi points for large n. This difference plays crucial role for the superconductivity as will be discussed later.

The LDA calculation for Y124[36] has predicted that there are four Fermi points in the d band of the CuO double chain with the electron density $n \simeq 0.57$. As for the case with Pr247, it is considered to be nearly quarter filling $n \approx 0.5$ due to the Fehrenbacher-Rice effect mentioned before.[4] Then, the CuO double chain of Pr247 is in the boundary between the two Fermi point system and the marginal four Fermi point system as seen in Fig. 2 where the Fermi level for $n = 0.57$ is plotted.

On the basis of the Tomonaga-Luttinger liquid theory,[31–35] various types of correlation functions show power-low dependence with critical exponents. These exponents are determined by a single parameter K_ρ in the model which is isotropic in spin space. For the single-band model with two Fermi points, $\pm k_F$, the SC correlation function decays as $\sim r^{-(1+\frac{1}{K_\rho})}$, while the CDW and SDW correlation functions decay as $\sim \cos(2k_F r)r^{-(1+K_\rho)}$. When the system is in the Tomonaga-Luttinger regime, both of the charge and spin excitations are gapless (we label this regime as $c1s1$). In this case, the SC correlation is dominant for $K_\rho > 1$, while the CDW or SDW correlation is dominant for $K_\rho < 1$.

In contrast to the single-band model, the situation is rather complicated in the two-band model with four Fermi points, $\pm k_{F_1}$ and $\pm k_{F_2}$. When the ratio of the two Fermi velocities $|v_{F_1}/v_{F_2}|$ is smaller than a critical value

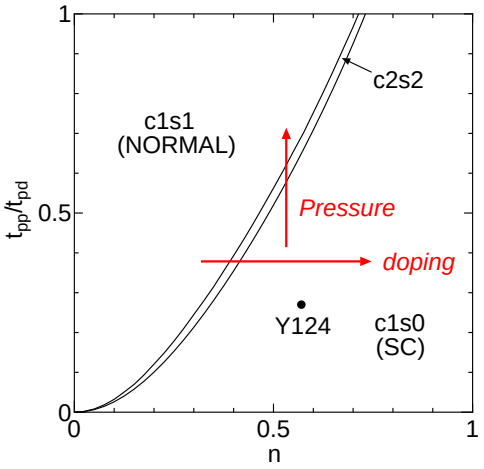

Fig. 3. Phase diagram on the n-t_{pp} plane in the weak coupling limit for $t_{pd} = 1.6$eV, $\Delta = 4.1$eV and $t_{dd}/t_{pp} = 0.28$. Closed circle stands for the parameter point corresponding to the LDA calculation for Y124.

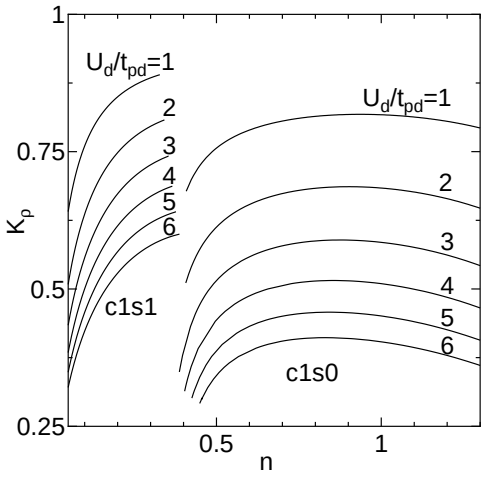

Fig. 4. The Luttinger parameter K_ρ as a function of the electron density n for several U_d for $t_{pd} = 1.6$eV, $t_{pp} = 0.43$eV, $t_{dd} = 0.12$eV and $\tilde{\Delta} = 4.1$eV.

~ 8.6, the low-energy excitations are given by a single gapless charge mode with a gapped spin mode (labeled as $c1s0$).[31–33] In this case, the SC and the CDW correlations decay as $\sim r^{-\frac{1}{2K_\rho}}$ and $\sim \cos[2(k_{F_2} - k_{F_1})r]r^{-2K_\rho}$, respectively, while the SDW correlation decays exponentially. Hence, the SC correlation is dominant for $K_\rho > 0.5$, while, the CDW correlation is dominant for $K_\rho < 0.5$. When the ratio $|v_{F_1}/v_{F_2}|$ is larger than the critical value ~ 8.6, the low energy excitations are given by two gapless charge modes and two gapless spin modes (labeled as $c2s2$).

In the non-interacting case with $U_d = 0$, the Luttinger liquid parameter K_ρ is always unity. In the weak coupling limit $U_d \to 0$, *i.e.*, in the limit $K_\rho \to 1$, the SC correlation is most dominant in the $c1s0$ region (SC phase), while, the CDW or SDW correlation is most dominant in the $c1s1$ and $c2s2$ regions (normal phases).[31–33] In Fig. 3, we plot the phase diagram in the weak coupling limit on the n-t_{pp} plane. The values of $t_{pd} = 1.6$eV and $\Delta = 4.1$eV together with the ratio $t_{dd}/t_{pp} = 0.28$ are fixed to the corresponding values in Fig. 2.

As mentioned before, the CuO double chain of Pr247 is expected to be in the boundary region between the $c1s1$ and the $c1s0$ phases. When the system is initially in the $c1s1$ phase, the electron doping effect brings about the phase transition from the $c1s1$ to the $c1s0$ (see Fig. 3). This is consistent with the experimental observation in Pr247, where the superconductivity is caused by the oxygen reduction corresponding to the electron doping effect in the CuO double chain.[7,8]

When the distance between the two chains of a CuO double chain decreases, the hopping terms t_{pp} and t_{dd} are expected to increase. Therefore, the pressure effect might lead to the phase transition from the $c1s0$ to the $c1s1$ as shown in Fig. 3. This is again consistent with the recent experiment in Pr247 under high pressure,[38] where the superconductivity is suppressed and finally disappears due to the pressure effect.

Now, we calculate the Luttinger liquid parameter K_ρ for finite Coulomb interaction U_d. Based on the Tomonaga-Luttinger liquid theory, K_ρ is related to the charge susceptibility χ_c and the Drude weight D by the following equation:[35] $K_\rho = \frac{1}{2}(\pi\chi_c D)^{1/2}$ with

$$\chi_c^{-1} = \frac{\partial^2 E_g}{\partial n^2}, \qquad D = \pi\frac{\partial^2 E_g}{\partial \phi^2}, \tag{2}$$

where E_g is the ground state energy per unit cell as a function of the electron density n and the magnetic flux ϕ. To calculate K_ρ in the d-p model eq.(1), we estimate E_g within the HF approximation and substitute it into eq.(2). The obtained value of K_ρ is valid up to the first order of U_d and a good approximation in the weak coupling regime. The reliability of this approximation has been checked for the Hubbard model[13,14] and the d-p model.[29,30] These results show that K_ρ of the HF approximation agrees well with that of the second order perturbation together with the available exact results up to the intermediate coupling regime except for $n \sim 1$ (half-filling) where the umklapp process, which is neglected in the HF approximation, becomes dominant.[39]

Fig. 4 shows K_ρ as a function of n for several values of U_d/t_{pd} with $t_{pd} = 1.6$eV, $t_{pp} = 0.43$eV, $t_{dd} = 0.12$eV and $\tilde{\Delta}|_{n=0.57} = 4.1$eV, where $\tilde{\Delta}$ is the renormalized charge-transfer energy within the HF approximation and is explicitly given by $\tilde{\Delta} = \Delta + \frac{U_d n_d}{2}$. As $\tilde{\Delta}$ depends on n and U_d, we determine the bare charge transfer energy Δ so as to fix $\tilde{\Delta}$ to the corresponding value in Fig. 2: $\tilde{\Delta} = 4.1$eV at $n = 0.57$ for each U_d.

As shown in Fig. 4, the $c1s1$ phase appears for $n \lesssim 0.4$, while the $c1s0$ phase appears for $n \gtrsim 0.4$. In $c1s0$ phase, K_ρ increases with increasing n and then have a maximum at an optimal electron density between quarter- and half-filling. In the $c1s0$ phase with $U_d/t_{pd} \lesssim 4$, the value of K_ρ exceeds $1/2$ when the SC correlation becomes most dominant as compared with the other correlations (SC phase). On the other hand, in the $c1s1$ phase, K_ρ is always smaller than unity and the CDW or SDW correlation is most dominant (normal phase).

Experimentally, the superconductivity of Pr247 is ob-

served only for a range of the oxygen reduction rate $\delta \gtrsim 0.3$ and T_c shows a maximum at an optimal reduction rate $\delta \sim 0.45$.[8] When we assume the electron density of the CuO double chain in Pr247 with $\delta = 0$ to be $n \simeq 0.4$, we can guess $n \simeq 0.4+\delta$ for finite δ. Then, for $U_d/t_{pd} = 4$ corresponding to $U_d = 6.4$eV, the SC region ($n \gtrsim 0.7$) with $K_\rho > 1/2$ as well as the optimal electron density ($n \simeq 0.85$) with a maximum in K_ρ seems to be consistent with the experimental observation mentioned above. Although the effect of the umklapp process may result in the reduction of K_ρ obtained from the HF approximation,[39] the essential feature of the doping dependence away from half-filling is expected to be unchanged as previously observed in the Hubbard ladder model.[13,14]

To summarize, we have investigated the superconductivity in the *d-p* double chain model, simulating a CuO double chain of Pr247, where the tight-binding parameters are determined so as to fit the LDA band structure. On the basis of the Tomonaga-Luttinger liquid theory, we have obtained the phase diagram in the weak coupling limit, which provides us a clear understanding of the doping and the pressure dependence of the superconductivity in Pr247.[8,38]

The Luttinger liquid parameter K_ρ has also been obtained as a function of the electron density n using the Luttinger-liquid relation combined with the HF approximation. The doping dependence of K_ρ is in good agreement with that of T_c in Pr247,[8] when we assume that T_c is finite for $K_\rho > 1/2$ in the $c1s0$ phase and is monotonically increasing function of K_ρ. Although the finite value of T_c is not obtained in purely one-dimensional systems, an approximate value of T_c could be estimated as a function of K_ρ by taking into account of a three-dimensionality due to the effect of couplings between the double chains. We will report it in a subsequent paper.

Even in the normal state above T_c, a kind of transition between the $c1s1$ phase and the $c1s0$ phase is expected. In fact, such a transition has been observed in the doping and/or the pressure dependence of transport properties such as the resistivity and the Hall coefficient.[8,38] In addition to the transport properties, a spin gap is expected to exist in the $c1s0$ phase. A spin gap like behavior has been observed in the recent NQR experiment,[9,40] where $(T_1T)^{-1}$ is suppressed in the superconducting sample as compared with the non-superconducting sample even above T_c.

Taking account of the LDA calculation and our result, we can expect that the CuO double chain of Y124 is also in the $c1s0$ phase and shows the superconductivity as well as Pr247. We note that a rapid decrease in the resistivity below 15K has been observed in $YBa_2(Cu_{1-x}Zn_x)_4O_8$ with high Zn doping $0.05 < x < 0.1$.[41] In this case, the superconductivity in the CuO_2 plane is considered to disappear, but the CuO double chain might preserve the superconductivity. To be more conclusive, we need further investigation in this regard.

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