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Superconductivity and Spin gap in the zigzag chain t-J model simulating a CuO double chain in $Pr_2Ba_4Cu_7O_{15-\delta}$

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Using the numerical diagonalization method, we examine the one-dimensional t_1-t_2-J_1-J_2 model (zigzag chain t-J model) which represents an effective model for metallic CuO double chain in the superconductor $Pr_2Ba_4Cu_7O_{15-\delta}$. Based on the Tomonaga-Luttinger liquid theory, we calculate the Luttinger-liquid parameter K_ρ as a function of electron density n. It is found that superconductivity is realized in parameter region corresponding to the experimental result. We show phase diagram of spin gap on the $t_2/|t_1|$-n plane by analyzing the expectation value of twist-operator Z_σ in the spin sector. The spin gap appears in the region with large $t_2/|t_1|$, where the phase boundary at half-filling is consistent with that of the known frustrated quantum spin system. The analysis also suggests that the estimated value of the spin gap reaches $\sim 100K$ in the realistic parameter region of $Pr_2Ba_4Cu_7O_{15-\delta}$.

KEYWORDS: zigzag chain t-J model, spin gap, numerical diagonalization, superconductivity, Tomonaga-Luttinger liquid theory

Recently, Matsukawa *et al.* have discovered a new superconductor $Pr_2Ba_4Cu_7O_{15-\delta}$(Pr247) in which CuO double chains are considered to derive the superconductivity at $T_c \sim 20$K.[1,2] Since electronic conduction in CuO_2 plane of Pr247 is suppressed due to the so-called Fehrenbacher-Rice state,[3] the double chains are expected to play a crucial role for metallic state of the material. In fact, anisotropy in the resistivity of a single crystal shows the one-dimensional(1D) conductivity based on the CuO double chains and the NQR experiment also indicates that the superconductivity is realized in the CuO double chains.[4–7] These experiments stimulate our interest in the theoretical aspect for the electronic state and the superconductivity of the double chain system.

Many theoretical works have been performed on the electronic state of double chain systems such as Ladder models and zigzag chain models.[8–23] Generally speaking, the electronic state of these two-band models is characterized by existence of four Fermi points, namely, $\pm k_{F_1}$ and $\pm k_{F_2}$ on the Fermi surface. In the weak coupling regime, bosonaization method reveals that the low-energy excitations of the double chain are given by a single gapless charge mode with a gapped spin mode (labeled as $c1s0$), when the ratio of the two Fermi velocities $|v_{F_1}/v_{F_2}|$ is smaller than a critical value ~ 8.6.[8–10,24] The correlation functions of the superconductivity(SC) and that of the charge density wave (CDW) decay as $\sim r^{-\frac{1}{2K_\rho}}$ and $\sim \cos[2(k_{F_2}-k_{F_1})r]r^{-2K_\rho}$, respectively, while that of the spin density wave (SDW) decays exponentially. Here, K_ρ is the Luttinger liquid

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parameter and determines the critical exponents of various types of correlation functions in the model which is isotropic in spin space.[11–13] In the $c1s0$ region, the SC correlation is dominant for $K_\rho > 1/2$, while, the CDW correlation is dominant for $K_\rho < 1/2$.

In the strong coupling regime, the double chain systems have been studied by using numerical methods.[14–21] At half-filling, the system can be described by a Heisenberg model whose ground state is a spin liquid insulator with a finite spin gap.[15,17,21] Away from half-filling, the system becomes a metallic state which maintains a spin gap.[16,21] 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.

Among them, there are few works which consider the model just corresponding to the Pr247 except our previous work[22] and the very recent work using the fluctuation exchange (FLEX) approximation.[23] In our previous paper, 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 band structure of the local density approximation(LDA). On the basis of the Tomonaga-Luttinger liquid theory, we have obtained K_ρ as a function of the electron density n. The doping dependence of K_ρ is in good agreement with that of T_c in Pr247[2] when we assume that T_c is a monotonically increasing function of K_ρ at $K_\rho > 1/2$. However the Hartree-Fock(HF) approximation has been used in this work and the analysis is limited in the case of the weak coupling region as well as the FLEX approximation.

Since the strong correlation effect may play an important role in the electronic state and the superconductivity of Pr247, a nonperturbative and reliable approach is required. In this work, we employ the numerical diagonalization method for the double chain t-J model whose parameters are selected to cover the realistic band structure of the CuO double chains. We calculate the Luttinger liquid parameters K_ρ and address the behavior of the spin gap in the strong coupling regime beyond the previous works.

We consider the following Hamiltonian for the one-dimensional t_1-t_2-J_1-J_2 model(zigzag chain t-J model);

$$\begin{aligned} H &= t_1 \sum_{i,\sigma} (c^\dagger_{i,\sigma} c_{i+1,\sigma} + h.c.) + t_2 \sum_{i,\sigma} (c^\dagger_{i,\sigma} c_{i+2,\sigma} + h.c.) \\ &+ J_1 \sum_{i,\sigma} (\mathbf{S}_i \cdot \mathbf{S}_{i+1} - \frac{1}{4} n_i n_{i+1}) \\ &+ J_2 \sum_{i,\sigma} (\mathbf{S}_i \cdot \mathbf{S}_{i+2} - \frac{1}{4} n_i n_{i+2}), \end{aligned}$$

where $c^\dagger_{i,\sigma}$ stands for the creation operator of an electron with spin σ at site i and $n_{i,\sigma} = c^\dagger_{i,\sigma} c_{i,\sigma}$. Here, t_1 is the hopping energy between the nearest-neighbor sites and t_2 is that between the next nearest-neighbor sites as shown in Fig.1(a). The interaction parameters J_1 and J_2 stand for the

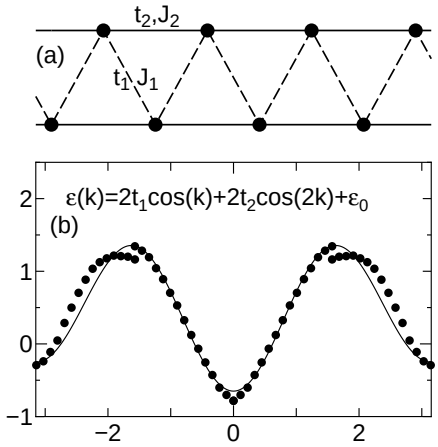

Fig. 1. (a) Schematic diagram of $t_1 - t_2 - J_1 - J_2$ model on the zigzag chain. (b) Energy dispersion relation for the noninteracting $t_1 - t_2$ model on the zigzag chain. Solid lines are the tight-binding result with $t_1 = -0.1$eV and $t_2 = -0.45$eV. Closed circles are the LDA result for the d-band of the CuO double chain.

exchange coupling between the nearest-neighbor sites and between the next nearest-neighbor sites, respectively. We take account of the infinite on-site repulsion by removing states with doubly occupied sites from the Hilbert space.

To determine the hopping energies t_1 and t_2, we compare the noninteracting t_1-t_2 band with the d-band of the CuO double chain obtained by the LDA band structure in $YaBa_2Cu_4O_8$(YBCO).[25] Here YBCO includes the CuO double chains with the same lattice structure as those in Pr247. As shown in Fig.1(b), both bands are in good agreement with each other, when we select $t_1 = -0.1$eV and $t_2 = -0.45$eV.[26]

As for the exchange coupling energies, J_1 is considered to originate in the exchange interaction between electrons in the nearest neighbor d-sites. The value of J_1 is given by the 2nd order perturbation with respect to the hopping t_{dd}, *i.e.* $J_1 = 4t_{dd}^2/U_d$, where U_d is the on-site Coulomb interaction between d electrons. When we assume $t_{dd} = 0.12$eV[26] and $U_d = 6$eV, J_1 is estimated as 0.01eV. On the other hand, J_2 is considered to the superexchange interaction acting between the next nearest neighbor Cu-sites connecting through O-site. Our previous study for d-p single chain and Ladder models[27] indicates that the exchange interaction J/t_{pd} is ~ 0.14 for d-p single chain, and about 0.09 for d-p Ladder at $\Delta/t_{pd} \sim 2.6$ and $U_d/t_{pd} = 8$. Here, we note that the 4th order perturbation[28] with respect to t_{pd} overestimates the value of J/t_{pd} in the case of $\Delta/t_{pd} \lesssim 4$.[27] By reference from the above, we regard the adequate value of J_2 as ~ 0.15eV. These values are close to that of corresponding parameters obtained in CuO_2 plain system.[29]

We numerically diagonalize the Hamiltonian up to 24 sites using the standard Lanczos algorithm and calculate the ground state energy E_0. We use the periodic boundary condition for $N_e = 4m + 2$ and the antiperiodic boundary condition for $N_e = 4m$, where N_e is the total number of electrons and m is an integer. The filling n is defined by $n = N_e/N$, where N is the total number

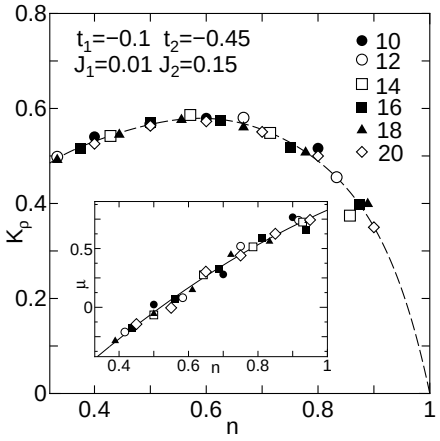

Fig. 2. K_ρ as a function of n for $t_1 = -0.1$eV, $t_2 = -0.45$eV, $J_1 = 0.01$eV and $J_2 = 0.15$eV. The dashed line is a guide for eyes. Inset shows the chemical potential μ as a function of n. The solid line represents a fitting line using a second order polynomial by the least square method.

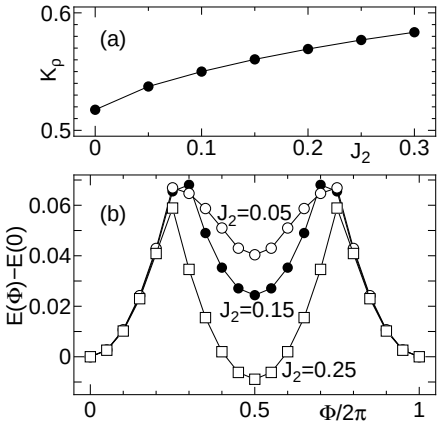

Fig. 3. (a) K_ρ as a function of J_2 for $n = 2/3$(12electrons/18sites). (b) The energy difference $E_0(\phi) - E_0(0)$ as a function of an external flux ϕ for $n = 2/3$(12electrons/18sites) at J_2=0, 0.15 and 0.30eV with $t_1 = -0.1$eV, $t_2 = -0.45$eV and $J_1 = 0.01$eV.

of sites. The critical exponent K_ρ is related to the charge susceptibility χ_c and the Drude weight D by $K_\rho = \frac{1}{2}(\pi\chi_c D)^{1/2}$, with $D = \frac{\pi}{N}\frac{\partial^2 E_0(\phi)}{\partial\phi^2}$, where $E_0(\phi)$ is the total energy of the ground state as a function of magnetic flux $N\phi$.[13] Here, the flux is imposed by introducing the following gauge transformation: $c_{m\sigma}\dagger \to e^{im\phi}c^\dagger_{m\sigma}$ for an arbitrary site m. When the charge gap vanishes in the thermodynamic limit, the uniform charge susceptibility χ_c is obtained from $\chi_c = \frac{\partial n}{\partial\mu}$, where the chemical potential $\mu(N_e, N)$ is defined by $\mu(N_e, N) = \frac{E_0(N_e+1,N)-E_0(N_e-1,N)}{2}$. Using the above χ_c and D, we calculate the K_ρ from the ground state energy E_0 of the finite size system.

Fig. 2 shows the Luttinger parameter K_ρ as a function of the electron density n for $t_1 = -0.1$eV, $t_2 = -0.45$eV, $J_1 = 0.01$eV and $J_2 = 0.15$eV. Inset shows the chemical potential μ as a function of n, where data of μ is fitted to a second-order polynomial as a function of n by the least square method and the value of χ_c is estimated from differential coefficient of the polynomial. K_ρ increases

with increasing n and then have a maximum at an optimal electron density at $n \sim 0.6$. In the region of $0.4 \lesssim n \lesssim 0.8$, the value of K_ρ exceeds 0.5 when the SC correlation becomes most dominant as compared with the other correlations (SC phase). The overall behavior of K_ρ is consistent with our previous work obtained by the HF approximation[22] except near the half-filling.

Figure 3(a) shows the value of K_ρ as a function of J_2 for the 12electrons/18sites system. As J increases, K_ρ increases and it becomes larger than 0.5 even if $J_2 = 0$. To confirm the superconductivity, we calculate the ground state energy $E_0(\phi)$, as a function of an external flux ϕ. As shown in Fig. 2(b), anomalous flux quantization clearly occurs at $J \gtrsim 0.05$. It suggests that the SC phase appears at $K_\rho > 0.5$.

Next, we consider the phase diagram of the spin gap Δ_σ. Generally speaking, it is not easy for numerical methods to estimate Δ_σ preciously in the case of the energy scale being small. Especially, it is very difficult to determine the phase boundary of the spin gap which is defined by $\Delta_\sigma = 0$. To overcome this difficulty, we introduce *twist-operator* Z_σ, given as

$$Z_\sigma = \exp[\frac{2\pi i}{N} \sum_{j=1}^{N} j(n_{j\uparrow} - n_{j\downarrow})]. \tag{1}$$

When the expectation value $\langle Z_\sigma \rangle > 0 (< 0)$, the system becomes spin gapfull(gapless) as has already been well examined by Nakamura *et al.* in the study of 1D extended Hubbard model.[30] We expect that this method is applicable to our zigzag chain model as well.

In Fig.4, we show the size dependence of the critical point $t_{2c}/|t_1|$ determined by $\langle Z_\sigma \rangle = 0$, where we set the relation between the electron hopping and the exchange interaction as $(t_2/|t_1|)^2 = J_2/J_1$. For $n = 1$, our system reduces to the J_1-J_2 Heisenberg model and the critical point $t_{2c}/|t_1|$ is well scaled by $1/N^2$. The extrapolated value $|t_{2c}/t_1| = 0.491$ is very close to the known result of the Heisenberg model, $J_{2c}/J_1 = (t_{2c}/t_1)^2 = 0.241$.[31] For $n < 1$, we obtain the extrapolated value by assuming the same size dependence, where we set $J_1/|t_1| = 0.4$, and $J_2/J_1 = (t_2/t_1)^2$ to correspond to the zigzag chain Hubbard model(t_1-t_2-U model).

Fig.5 shows the phase diagram on the $t_2/|t_1|$-n plane together with the result of the weak coupling theory. It shows that the phase boundary of the spin gap is close to that from the weak coupling theory for the region with $n \gtrsim 0.5$ and $t_2/|t_1| \lesssim -1$. It also suggests that the boundary is almost independent of U in the t_1-t_2-U model, as has already reported for $n = 1$.[32,33] We note that the phase diagram suggests that the parameter region corresponding to Pr247 belongs to the spin gapped phase with $Z_\sigma > 0$.

In the region $0.5 \lesssim t_2/|t_1| \lesssim 1.9$, we find that the ground state of finite systems is a spin polarized ferromagnetic state in part as shown in Fig.5,[14,16,34] where we use the systems for $n = 4/14, 8/14, 12/14, 4/16, 8/16, 12/16, 4/18, 8/18, 12/18$ and $16/18$. This ferromagnetic state is disconnected in respect to $t_2/|t_1|$, but it might be caused by finite size effect. Although the phase boundary of $\langle Z_\sigma \rangle = 0$ is masked by the ferromagnetic state in the region, we have confirmed that

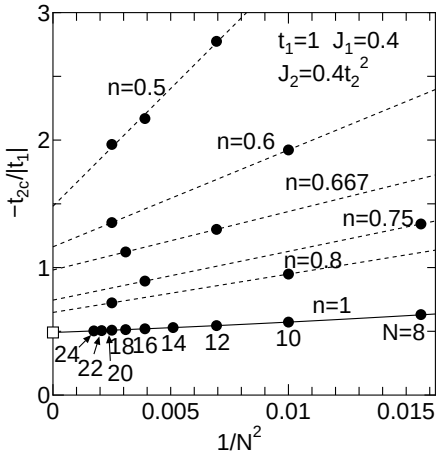

Fig. 4. Size dependence of the critical point t_{2c} for $n = 1/2, 3/5, 3/4, 4/5$, and 1 determined by the condition $\langle Z_\sigma \rangle = 0$. The open square stands the well known result of the J_1-J_2 Heisenberg model in the limit $N \to \infty$.

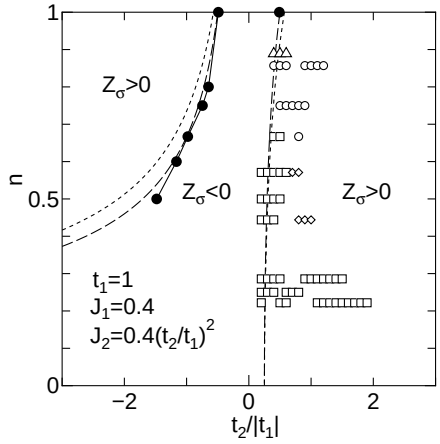

Fig. 5. Phase diagram on the $t_2/|t_1|$-n plane. The solid circles stand the extrapolated value of the critical point $t_{2c}/|t_1|$. The open symbols, △, ♢, ◯ and □ indicate spin polarized ground state of finite size systems with $S_{total}/S_{max} = 1/4$, $S_{total}/S_{max} = 1/3$, $S_{total}/S_{max} = 1/2$ and $S_{total}/S_{max} = 1$, respectively, where S_{total} is the total spin of the ferromagnetic state and S_{max} is the maximum possible value of S_{total}. The broken lines are the phase boundary between c2s2 and c1s0 obtained by the weak coupling theory.[8] The dashed lines present the boundary between the region of four Fermi points and that of two Fermi points in the noninteracting model.

the sign of $\langle Z_\sigma \rangle$ is positive for $t_2/|t_1| \gtrsim 1$ and negative for $t_2/|t_1| \lesssim 0$ except the ferromagnetic phase.

Finally, we consider the relationship between $\langle Z_\sigma \rangle$ and the value of the spin gap Δ_σ. It is known that $\langle Z_\sigma \rangle$ corresponds to the expectation value of the nonlinear term $\cos(\sqrt{8}\phi_\sigma)$ in the sine-Gordon model which is the effective Hamiltonian of 1D electron system.[30] Because this term becomes a source producing the gap, there is a close relation between Δ_σ and $\langle Z_\sigma \rangle$.[37] We find that Δ_σ of the infinite system is almost proportional to the product of v_σ and $\langle Z_\sigma \rangle$ of the 18-sites system in wide range of the parameter $t_2/|t_1|$ at $n = 1$, where v_σ is the spin velocity corresponding to the energy scale of the spin part of the effective Hamiltonian.[35] In Fig.6, we plot $\langle Z_\sigma \rangle$ in the 18-sites system

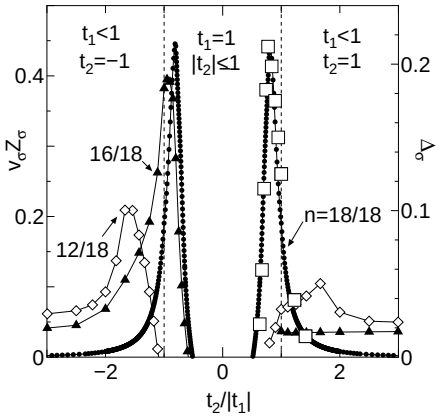

Fig. 6. The value of $v_\sigma\langle Z_\sigma\rangle$ as a function of $t_2/|t_1|$ at $n = 12/18, 16/18, 18/18$ (18-sites systems with 12,16,18-electrons), where we set $t_2 = -1$ for $t_2/|t_1| < -1$, $t_1 = 1$ for $|t_2/t_1| \leq 1$, and $t_2 = 1$ for $t_2/|t_1| > 1$, respectively. For all values of $t_2/|t_1|$, we set $J_1 = 0.5t_1^2$, and $J_2 = 0.5t_2^2$ to correspond to the t_1-t_2-U model with $U = 8$. The open squares stand the spin gap of Δ_σ obtained from the DMRG method for $n = 1$.[38]

together with Δ_σ obtained by DMRG method for $n = 1$.[38]

Remarkably, a phenomenological relation, $\Delta_\sigma = 0.48 v_\sigma\langle Z_\sigma\rangle$, is observed at $n = 1$ for all values of $t_2/|t_1|$. Assuming the same relation is satisfied even for $n < 1$, we estimate the spin gap Δ_σ from the value of $v_\sigma\langle Z_\sigma\rangle$ of the 18-sites system. To confirm this assumption, we compare our result with Δ_σ of the t_1-t_2-U model obtained by the recent DMRG method.[21] As shown in Fig.6, we obtain $\langle Z_\sigma\rangle \sim 0.25$ and $v_s \sim 1.5$ resulting in $\Delta_\sigma \sim 0.18$ for $n = 16/18$ (18-sites system with 16-electrons) with the parameters: $|t_1| = 1.0$, $t_2 = -1.0$, $J_1 = 0.5$, and $J_2 = 0.5$. The result is in good agreement with the DMRG result, i.e., $\Delta_\sigma \sim 0.16$ of the corresponding t_1-t_2-U model with $|t_1| = 1.0$, $t_2 = -1.0$ and $U = 8$.[21] Then, we expect that our analysis is useful to estimate the spin gap, even for $n < 1$. When we apply the above method to the realistic parameter region of Pr247, we obtain $\Delta \simeq 0.0072$eV for $n = 16/18$ with $t_1 = -0.1$eV, $t_2 = -0.45$eV, $J_1 = 0.01$eV and $J_2 = 0.15$eV. In the case of $n = 12/18$, we find $\Delta_\sigma \simeq 0.011$eV. These results suggest that the order of the spin gap amounts to $\Delta_\sigma \sim 100$K in the realistic parameter region of Pr247 and is larger than $T_c \simeq 20$K.

In summary, we investigate the one-dimensional t_1-t_2-J_1-J_2 model as an effective model for metallic CuO double chain of Pr247 using the numerical diagonalization method. The hopping parameters of electron are chosen so as to fit the d-band from the CuO double chain obtained from LDA calculation and the exchange coupling energies J_1 and J_2 are estimated by the known results of 1D d-p models. In a realistic parameter region, we show that the Luttinger liquid parameter K_ρ is greater than 0.5 and the anomalous flux quantization is found. It suggests that the CuO double chain is responsible for the superconductivity of Pr 247 on the basis of the Tomonaga-Luttinger liquid theory. We also calculate the expectation value of the twist-operator Z_σ and obtain the phase boundary of the spin gap including the region with large value of $t_2/|t_1|$. By comparing with

the known result of the J_1-J_2 Heisenberg model, we estimate the value of the spin gap Δ_σ through $\langle Z_\sigma \rangle$ and spin velocity v_σ, and find the spin gap becomes $\sim 100K$ in the realistic parameter region of Pr247. This result is consistent with the recent NQR experiment, where $(T_1T)^{-1}$ is suppressed in the superconducting sample as compared with the non-superconducting sample even above T_c.

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