Superconductivity and Spin gap in the zigzag chain $t$-$J$ model simulating a CuO double chain in Pr$_2$Ba$_4$Cu$_7$O$_{15-\delta}$

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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$_2$Ba$_4$Cu$_7$O$_{15-\delta}$. Based on the Tomonaga-Luttinger liquid theory, we calculate the Luttinger-liquid parameter $K_\rho$ 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 $t_2/|t_1|\cdot n$ plane by analyzing the expectation value of twist-operator $Z_\sigma$ 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 $\sim 100$K in the realistic parameter region of Pr$_2$Ba$_4$Cu$_7$O$_{15-\delta}$.

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$_2$Ba$_4$Cu$_7$O$_{15-\delta}$ (Pr247) which CuO double chains are considered to derive the superconductivity at $T_c \sim 20$K. Since electronic conduction in CuO$_2$ plane of Pr247 is suppressed due to the so-called Fehrenbacher-Rice state, 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 that the superconductivity is realized in the CuO double chains.

Among them, there are few works which consider the model just corresponding to the Pr247 except our previous work and the very recent work using the fluctuation exchange (FLEX) approximation. 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 $K_\rho$ as a function of the electron density $n$. The doping dependence of $K_\rho$ is in good agreement with that of $T_c$ in Pr247 when we assume that $T_c$ is a monotonically increasing function of $K_\rho$ 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.

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. Away from half-filling, the system becomes a metallic state which maintains a spin gap. 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.
dimensional $t_1$-$t_2$-$J_1$-$J_2$ model (zigzag chain $t$-$J$ model);

$$H = t_1 \sum_{i,\sigma} (c_i^\dagger c_{i+1,\sigma} + h.c.) + t_2 \sum_{i,\sigma} (c_i^\dagger c_{i+2,\sigma} + h.c.)$$

$$+ J_1 \sum_{i,\sigma} (S_i \cdot S_{i+1} - \frac{1}{4}n_in_{i+1})$$

$$+ J_2 \sum_{i,\sigma} (S_i \cdot S_{i+2} - \frac{1}{4}n_in_{i+2}),$$

where $c_i^\dagger$ stands for the creation operator of an electron with spin $\sigma$ at site $i$ and $n_i=\sum_\sigma c_i^\dagger c_i$. 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 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 YBa$_2$Cu$_4$O$_8$ (YBCO). Here YBCO includes the CuO double chains with the same lattice structure as those in Pr$_2$47. As shown in Fig.1(b), both bands are in good agreement with each other, when we select $t_1 = -0.1eV$ and $t_2 = -0.45eV$.

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 $t_{dd} = 0.12eV$ and $U_d = 6eV$, $J_1$ 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 indicates that the exchange interaction $J_2/t_{pd}$ is $\sim 0.14$ 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 with respect to $t_{pd}$ overestimates the value of $J_2/t_{pd}$ in the case of $\Delta/t_{pd} \lesssim 4$. By reference from the above, we regard the adequate value of $J_2$ as $\sim 0.15eV$. These values are close to that of corresponding parameters obtained in CuO$_2$ plain system.

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 $N_c = 4m + 2$ and the antiperiodic boundary condition for $N_c = 4m$, where $N_c$ is the total number of electrons and $m$ is an integer. The filling $n$ is defined by $n = N_c/N$, where $N$ is the total number of sites. The critical exponent $K_\rho$ is related to the charge susceptibility $\chi_c$ and the Drude weight $D$ by $K_\rho = \frac{1}{2}(\pi\chi_c D)^{1/2}$, with $D = \frac{\pi}{N} \frac{\partial^2 E_\phi(\phi)}{\partial \phi^2}$, where $E_\phi(\phi)$ is the total energy of the ground state as a function of magnetic flux $N\phi$. Here, the flux is imposed by introducing the following gauge transformation: $c_{m\sigma}^\dagger \rightarrow e^{im\phi}c_{m\sigma}^\dagger$ for an arbitrary site $m$. When the charge gap vanishes in the thermodynamic limit, the uniform charge susceptibility $\chi_c$ is obtained from $\chi_c = \frac{\partial n}{\partial \mu}$, where the chemical potential $\mu(N_c, N)$ is defined by $\mu(N_c, N) = E_0(N_c+1,N) - E_0(N_c-1,N).$ Using the above $\chi_c$ and $D$, we calculate the $K_\rho$ from the ground state energy $E_0$ of the finite size system.

Fig. 2 shows the Luttinger parameter $K_\rho$ as a function of the electron density $n$ for $t_1 = -0.1eV$, $t_2 = -0.45eV$, $J_1 = 0.01eV$ and $J_2 = 0.15eV$. Inset shows the chemical potential $\mu$ as a function of $n$. The solid line represents a fitting line using a second order polynomial by the least square method.

$$\chi_c \sim n^{\nu_c},$$

$$D \sim n^{-\nu_D},$$

$$K_\rho \sim n^{-\nu_K}.$$
In Fig. 3(a), we obtain the extrapolated value by assuming $J_\rho$ as a function of $J_2$ for $n = 2/3(12$electrons/18sites). The energy difference $E_0(\phi) - E_0(0)$ as a function of an external flux $\phi$ for $n = 2/3(12$electrons/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.

The extrapolated Hubbard model is applicable to our zigzag chain model as well. It is extended Hubbard model. It is consistent with our previous work obtained by the weak coupling theory. It is well scaled by $1/N^2$.

When the expectation value $\langle Z_\sigma \rangle > 0 (< 0)$, the system becomes spin gap full (gapless) as has already been well examined by Nakamura et al. in the study of 1D extended Hubbard model.\cite{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, $J_{2c}/J_1 = (t_{2c}/|t_1|)^2 = 0.241.$\cite{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 $n \geq 0.5$ and $t_2/|t_1| < -1$. It also suggests that the boundary is almost independent of $U$ in the $t_1$-$t_2$-$U$ model, as has already reported for $n = 1.\cite{32,33}$ We note that the phase diagram suggests that the parameter region corresponding to Pr$_{247}$ belongs to the spin gapped phase with $Z_\sigma > 0$.

In the region $0.5 \leq t_2/|t_1| \leq 1.9$, we find that the ground state of the finite system is a spin polarized ferromagnetic state in part as shown in Fig. 5,\cite{14,16,34} where we use the systems for $n = 4/14, 8/14, 12/14, 4/16, 8/16, 12/16, 4/18, 8/18, 12/18 and 16/18$. The region of the ferromagnetic state is discon-
Fig. 6. The value of $v_\sigma(Z_\sigma)$ 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 $J_2 = 0.5t_1^2$ to correspond to the $t_1$-$t_2$-$U$ model with $U = 8$. The open squares stand the spin gap of $\Delta_\sigma$ obtained from the DMRG method for $n = 1$.$^{38}$

connected in respect to $t_2/|t_1|$, which is considered to be caused by a 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 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 $\Delta_\sigma$. 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 $\Delta_\sigma$ and $\langle Z_\sigma \rangle$.$^{37}$ We find that $\Delta_\sigma$ of the infinite system is almost proportional to the product of $v_\sigma$ and $\langle Z_\sigma \rangle$ of the 18-sites system in wide range of the parameter $t_2/|t_1|$ at $n = 1$, where $v_\sigma$ 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 together with $\Delta_\sigma$ obtained by DMRG method for $n = 1$.$^{38}$

Remarkably, a phenomenological relation, $\Delta_\sigma = 0.48v_\sigma\langle Z_\sigma \rangle$, 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 $\Delta_\sigma$ from the value of $v_\sigma\langle Z_\sigma \rangle$ of the 18-sites system. To confirm this assumption, we compare our result with $\Delta_\sigma$ 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 $v_\sigma \sim 1.5$ 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 $\Delta \sim 0.0072\text{eV}$ for $n = 16/18$ with $t_1 = -0.1\text{eV}$, $t_2 = -0.45\text{eV}$, $J_1 = 0.01\text{eV}$ and $J_2 = 0.15\text{eV}$. In the case of $n = 12/18$, we find $\Delta \sim 0.011\text{eV}$. These results suggest that the order of the spin gap amounts to $\Delta_\sigma \sim 100\text{K}$ in the realistic parameter region of Pr247 and is larger than $T_c \sim 20\text{K}$.

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 $\Delta_\sigma$ 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 $Z_\sigma$ 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 $\Delta_\sigma$ through $\langle Z_\sigma \rangle$ and spin velocity $v_\sigma$, and find the spin gap becomes $\sim 100\text{K}$ in the realistic parameter region of Pr247. This result is consistent with the recent NQR experiment, where $(T/T_c)^{-1}$ is suppressed in the superconducting sample as compared with the non-superconducting sample even above $T_c$.

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Superconductivity and Spin gap in the zigzag chain $t$-$J$ model

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