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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 is an effective model for metallic CuO double chains in the superconductor $Pr_2Ba_4Cu_7O_{15-\delta}$. Based on the Tomonaga-Luttinger liquid theory, we calculate the Luttinger liquid parameter $K_\rho$ as a function of the electron density $n$. It is found that superconductivity is realized in the parameter region, which is in accordance with experimental results. We show the phase diagram of a spin gap in the $t_2/|t_1|$-$n$ plane by analyzing the expectation value of the twist operator $Z_\sigma$ in the spin sector. The spin gap appears in the region with a 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 $Pr_2Ba_4Cu_7O_{15-\delta}$.

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 the $CuO_2$ plane of Pr247 is suppressed due to the so-called Fehrenbacher-Rice state,[3)] the double chains are expected to play a crucial role in maintaining the metallic state of the material. In fact, 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 superconductivity is realized in the CuO double chains.[4–7)] These experiments stimulate our interest in the theoretical aspects of the electronic state and the superconductivity of the double-chain system.

Many theoretical studies have been performed on the electronic state of double-chain systems, e.g., studies pertaining to ladder models and zigzag-chain models.[8–23)] Generally, the electronic state of these two-band models is characterized by the existence of four Fermi points, namely, $\pm k_{F_1}$ and $\pm k_{F_2}$, on the Fermi surface. In the weak coupling regime, the bosonaization method reveals that the low-energy excitations of the double chain result from 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 $\sim 8.6$.[8–10,24)] The correlation functions of the superconductivity (SC) and those 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 those of the spin density wave (SDW) decay exponentially. Here, $K_\rho$ is the

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Luttinger liquid parameter and determines the critical exponents of various types of correlation functions in models that are 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, 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 that maintains a spin gap.[16,21] This behavior is explained by the existence of electron pairs produced by dominant fluctuations in the $4k_F$ charge density wave or the interchain pairing fluctuations.

Among these theoretical studies, there are few studies that consider a model corresponding to the Pr247, apart from our previous study[22] and a very recent study using the fluctuation exchange (FLEX) approximation.[23] In our previous paper, we investigated superconductivity in the *d-p* double -chain model simulating a CuO double chain of Pr247 in which the tight-binding parameters were determined so as to fit the band structure of the local density approximation (LDA). On the basis of the Tomonaga-Luttinger liquid theory, we obtained $K_\rho$ as a function of the electron density $n$. The doping dependence of $K_\rho$ was in good agreement with that of $T_c$ in Pr247[2] when we assumed that $T_c$ is a monotonically increasing function of $K_\rho$ at $K_\rho > 1/2$. However, the Hartree-Fock (HF) approximation was used in the study and the analysis was 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 determining the electronic state and superconductivity of Pr247, a nonperturbative and reliable approach is required. In this study, 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 $K_\rho$ and address the behavior of the spin gap in the strong coupling regime beyond previous studies.

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 $\sigma$ 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 $J_2$ represent the exchange coupling between the nearest-neighbor sites and between the next nearest-neighbor sites,

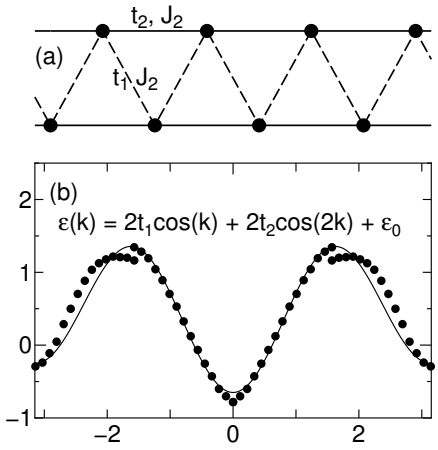


Fig. 1. (a) Schematic diagram of the $t_1$-$t_2$-$J_1$-$J_2$ model for the zigzag chain. (b) Energy dispersion relation for the noninteracting $t_1$-$t_2$ model for the zigzag chain. Solid lines are the tight-binding result with $t_1 = -0.1$ eV and $t_2 = -0.45$ eV. Closed circles are the LDA result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

respectively. We consider 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 CuO double chains with a lattice structure identical to that of CuO double chains 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 from the exchange interaction between electrons at the nearest-neighbor $d$-sites. The value of $J_1$ is given by the second-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 0.01 eV. On the other hand, $J_2$ is considered to cause the superexchange interaction between the next nearest-neighbor Cu sites connecting through O sites. Our previous study on $d$-$p$ single-chain and ladder models[27] indicates that the exchange interaction $J/t_{pd}$ is $\sim 0.14$ for the $d$-$p$ single chain, and about 0.09 for the $d$-$p$ ladder at $\Delta/t_{pd} \sim 2.6$ and $U_d/t_{pd} = 8$. Here, we note that the fourth-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] Then, we regard the adequate value of $J_2$ as $\sim 0.15$ eV. These values are close to those of the corresponding parameters obtained in a $CuO_2$ 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 of sites. The critical exponent $K_\rho$ is related to the charge susceptibility $\chi_c$ and the Drude weight

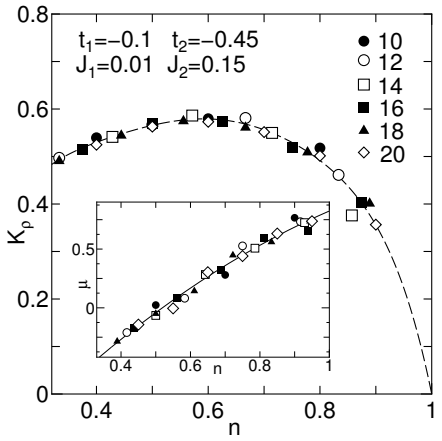


Fig. 2. $K_\rho$ as a function of $n$ for $t_1 = -0.1$ eV, $t_2 = -0.45$ eV, $J_1 = 0.01$ eV and $J_2 = 0.15$ eV. The dashed line is a guide for the eyes. The inset shows $\mu$ as a function of $n$. The solid line represents the fitting line obatained using a second-order polynomial by employing the least square method.

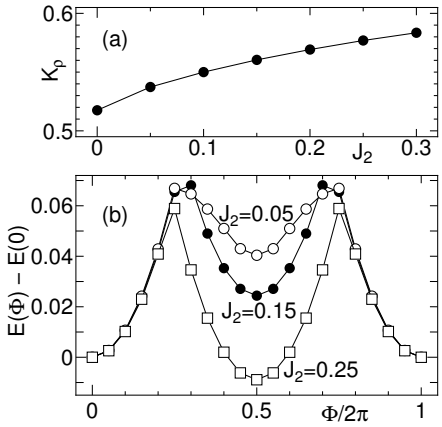


Fig. 3. (a) $K_\rho$ as a function of $J_2$ for $n = 2/3$ (12 electrons/18 sites). (b) The energy difference $E_0(\phi) - E_0(0)$ as a function of an external flux $\phi$ for $n = 2/3$ (12 electrons/18 sites) at $J_2 = 0$, 0.15, and 0.30 eV with $t_1 = -0.1$ eV, $t_2 = -0.45$ eV and $J_1 = 0.01$ eV.

$D$ 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 the magnetic flux $N\phi$.[13] Here, the flux is imposed by introducing the following gauge transformation: $c^\dagger_{m\sigma} \to e^{im\phi}c^\dagger_{m\sigma}$ for an arbitrary site $m$. When the charge gap vanishes in the thermodynamic limit, $\chi_c$ 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 $\chi_c$ and $D$, we calculate $K_\rho$ from the value of $E_0$ for the finite-size system.

Figure 2 shows $K_\rho$ 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 inset shows $\mu$ as a function of $n$, where the data for $\mu$ is fitted to a second-order polynomial as a function of $n$ by the least square method; the value of $\chi_c$ is estimated from the differential coefficient of this polynomial. $K_\rho$ increases with $n$ and then has a maximum at the optimal value of $n \sim 0.6$. In the region with $0.4 \lesssim n \lesssim 0.8$, the value of $K_\rho$ exceeds 0.5 when the

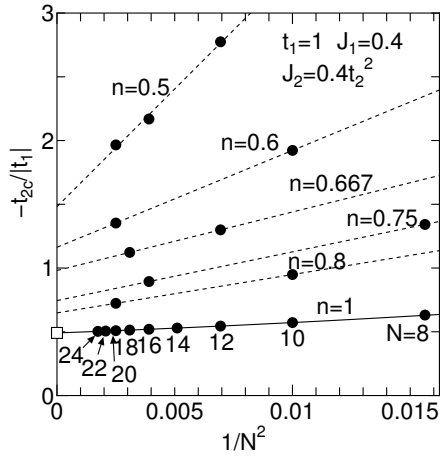


Fig. 4. Size dependence of the critical point $t_{2c}$ for $n = 1/2, 3/5, 3/4, 4/5$, and 1 determined by the condition $\langle Z_\sigma \rangle = 0$. The open square represents the well-known result of the $J_1$-$J_2$ Heisenberg model in the limit $N \to \infty$.

SC correlation becomes the most dominant as compared with the other correlations (SC phase). The overall behavior of $K_\rho$ is consistent with the behavior obtained in our previous study through the HF approximation,[22] except near the half filling.

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

Next, we consider the phase diagram of the spin gap $\Delta_\sigma$. Generally, it is not easy for numerical methods to estimate $\Delta_\sigma$ accurately when the energy scale is small. In paricular, it is very difficult to determine the phase boundary of the spin gap defined by $\Delta_\sigma = 0$. To overcome this difficulty, we introduce the *twist operator* $Z_\sigma$, which is 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 has a spin gap (is 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 using $\langle Z_\sigma \rangle = 0$, where we set the relation between 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).

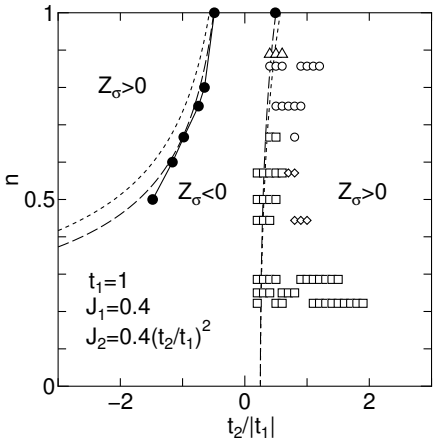


Fig. 5. Phase diagram on the $t_2/|t_1|$-$n$ plane. The solid circles represent the extrapolated values of the critical point $t_{2c}/|t_1|$. The open symbols, △, ◯, ◇, and □ indicate the spin-polarized ground state of finite-size systems with $S_{total}/S_{max} = 1/4$, $S_{total}/S_{max} = 1/3$, $S_{total}/S_{max}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

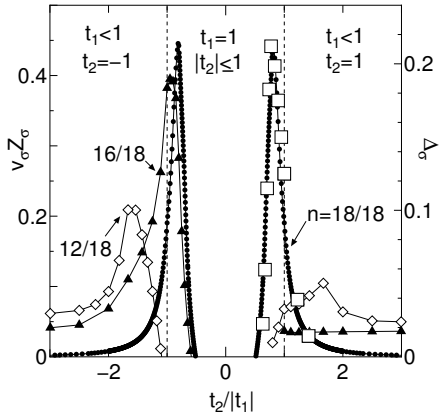


Fig. 6. The value of $v_\sigma\langle Z_\sigma\rangle$ as a function of $t_2/|t_1|$ at $n = 12/18, 16/18$, and $18/18$ (18-site systems with 12,16, and 18 electrons), where we set $t_2 = -1$ for $t_2/|t_1| < -1$, $t_1 = 1$ for $|t_2/t_1| \le 1$, and $t_2 = 1$ for $t_2/|t_1| > 1$, respectively. For all 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 represent $\Delta_\sigma$ obtained from the DMRG method for $n = 1$.[38]

Fig.5 shows the phase diagram in 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 of the spin gap in 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 been 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 the finite system is partly a spin-polarized ferromagnetic state, as shown in Fig.5;[14,16,34] in this figure, 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 ferromag-

netic state is disconnected with regard 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 for the ferromagnetic phase.

Finally, we consider the relationship between $\langle Z_\sigma \rangle$ and the value of $\Delta_\sigma$. 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 a 1D electron system.[30,35] Because this term becomes the source producing the gap, there is a close relation between $\Delta_\sigma$ and $\langle Z_\sigma \rangle$.[36] We find that $\Delta_\sigma$ for the infinite system is almost proportional to the product of $v_\sigma$ and $\langle Z_\sigma \rangle$ for the 18-site system for a 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.[37] In Fig.6, we plot $\langle Z_\sigma \rangle$ in the 18-site system together with $\Delta_\sigma$ obtained the by the 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 that the same relation is satisfied even for $n < 1$, we estimate $\Delta_\sigma$ from the value of $v_\sigma \langle Z_\sigma \rangle$ for the 18-site system. To confirm this assumption, we compare our result with the $\Delta_\sigma$ in the $t_1$-$t_2$-$U$ model that is obtained by the recent DMRG method.[21] As shown in Fig.6, we obtain $\langle Z_\sigma \rangle \sim 0.25$ and $v_s \sim 1.5$, which gives $\Delta_\sigma \sim 0.18$ for $n = 16/18$ (18-site system with 16 electrons) with the parameters $|t_1| = 1.0$, $t_2 = -1.0$, $J_1 = 0.5$, and $J_2 = 0.5$. This result is in good agreement with the DMRG result, i.e., $\Delta_\sigma \sim 0.16$ for the corresponding $t_1$-$t_2$-$U$ model with $|t_1| = 1.0$, $t_2 = -1.0$, and $U = 8$.[21] Therefore, we expect our analysis to be useful for estimating 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 chains of Pr247 by using the numerical diagonalization method. The hopping parameters of electrons are chosen so as to fit the $d$-band from the CuO double chain obtained from the 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 $K_\rho$ is greater than 0.5 and anomalous flux quantization is found. These facts suggest that the CuO double chain is responsible for the superconductivity of Pr247. We also calculate the expectation value of the twist operator $Z_\sigma$ and obtain the phase boundary of the spin gap in the $t_2/|t_1|$-$n$ plane. By comparing those results with the known result of the $J_1$-$J_2$ Heisenberg model, we estimate the value of $\Delta_\sigma$ using $\langle Z_\sigma \rangle$ and $v_\sigma$ and find that the spin gap becomes $\sim 100$ K in the realistic parameter region of Pr247. This result is consistent with the recent NQR experiment in which $(T_1 T)^{-1}$ is suppressed

in the superconducting sample as compared with the nonsuperconducting sample, even above $T_c$.

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