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ScienceDirect
Journal of Magnetism and Magnetic Materials 310 (2007) 1108–1109
Journal of magnetism and magnetic materials
www.elsevier.com/locate/jmmm

Chemical potential-electron density curve of the zigzag Hubbard ladder for Pr247

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Available online 7 November 2006

Abstract

We investigate the filling dependence of the zigzag Hubbard ladder, which is a relevant model to the recently synthesized quasi-one-dimensional super conductor $Pr_2Ba_4Cu_7O_{15-\delta}$(Pr247). Using the density matrix renormalization group method, we calculate chemical potential–electron density (μ–ρ) curve of the model and then discuss the relation between the oxygen-deficiency and transition temperature in Pr247.

Keywords: μ–ρ curve; DMRG; Spin gap

Recently, a novel Cu-based compound $Pr_2Ba_4Cu_7O_{15-\delta}$ (Pr247) was found to exhibit superconductivity below $T_c \simeq 12$ K [1–3]. This compound has a layered structure of CuO single chains, CuO double chains, and two-dimensional CuO_2 planes. An important point is that the usual CuO_2 plane is insulating due to the hybridization between Pr-4f and O-2p orbits [4], and thus the metallic conductivity is originating from the zigzag double chain structure. This suggests that the superconductivity in Pr247 may be driven by the one-dimensional mechanism. Moreover, the CuO single chain site is easily defected by deoxidization and then electrons are effectively doped into the zigzag double chain sites. This implies that this compound can be regarded as a "filling controlled system" of the zigzag chain structure, depending on deficiency of the CuO chain site. In fact, the superconductivity transition temperature of Pr247 strongly depends on the oxygen deficiency δ. Thus, it is important to investigate the filling dependence of Pr247.

For this purpose, we consider an effective Hubbard model on the zigzag lattice [3]. The Hamiltonian of the model is written as

$$H = \sum_{i\sigma} [t_1 c^\dagger_{i\sigma} c_{i+1\sigma} + t_2 c^\dagger_{i\sigma} c_{i+2\sigma} + h.c.] + U \sum_i n_{i\uparrow} n_{i\downarrow}, \quad (1)$$

where $c_{i\sigma}$ is the electron annihilation operator at i site with spin σ, $n_{i\sigma} \equiv c^\dagger_{i\sigma} c_{i\sigma}$, $t_1(t_2)$ is the nearest(next-nearest) hopping term of the electron, and U is the on-site coulomb interaction. We consider $t_2 < 0$ and $t_1 \leqslant |t_2|$ region, which is relevant to Pr247. This model has been investigated extensively by analytical and numerical methods. In particular, Fabrizio sketched a qualitative phase diagram by invoking the weak coupling theory for the unfrustrated Hubbard ladder [5]. Daul and Noack have presented an approximated phase diagram in the context of ferromagnetisizm [6]. However, the precise filling dependence of (1) has not been clarified, which is essential in analyzing the superconductivity of Pr247. In this paper, we focus on the filling dependence of (1). In particular, we perform density matrix renormalization group (DMRG) calculation and illustrate the chemical potential–electron density (μ–ρ) curve. We then discuss the characteristic properties of the low-energy excitation of Eq. (1).

We define $E_L(N, S^z)$ as the lowest energy of a L-site system with electron number N and total magnetization S^z. We then calculate chemical potential μ with $\mu = -[E_L(N+1, \frac{1}{2}) - E_L(N, 0)]$ for N = even and $\mu = -[E_L(N+1, 0) - E_L(N, \frac{1}{2})]$ for N = odd. In Fig. 1, we show the μ–ρ curves of $L = 60$ for $U = 8$. In order to analyze the μ–ρ curves, it is primely important to resolve the one particle dispersion curve, which is easily obtained as $\varepsilon(k) = 2t_1 \cos k + 2t_2 \cos 2k$. The μ–ρ

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0304-8853/$ - see front matter © 2006 Published by Elsevier B.V.
doi:10.1016/j.jmmm.2006.10.300

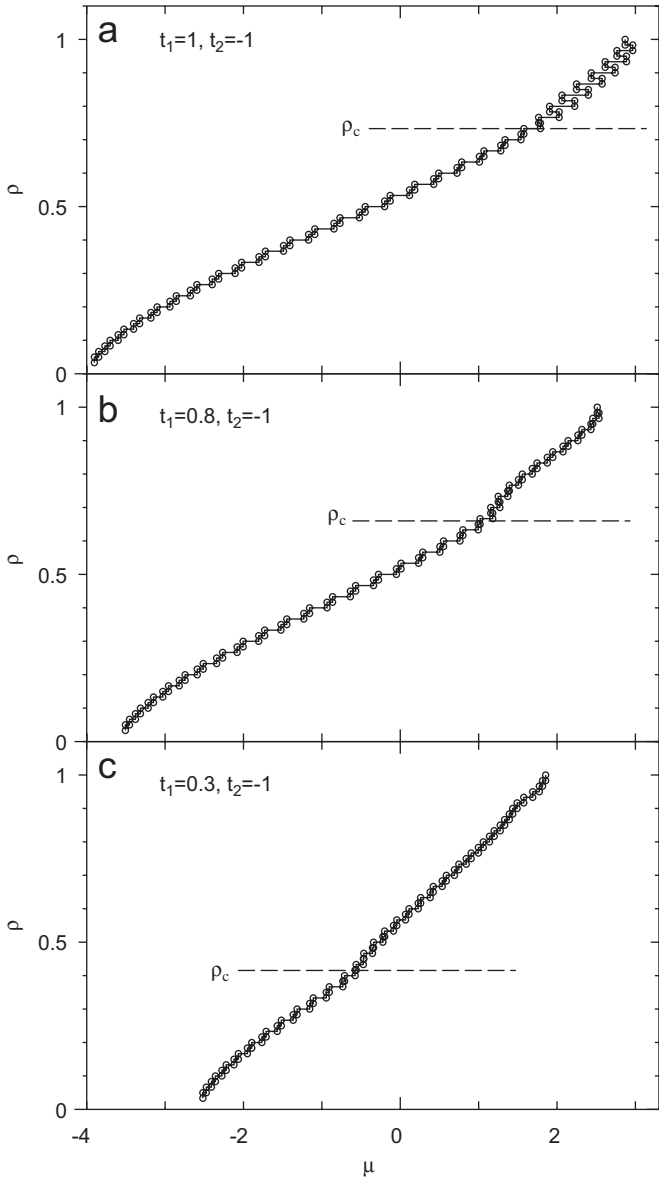

Fig. 1. μ–ρ curves of the zigzag Hubbard model for $U = 8$: (a) $t_1 = 1$, $t_2 = -1$, (b) $t_1 = 0.5$, $t_2 = -1$, and (c) $t_1 = 0.3$, $t_2 = -1$. Broken lines are guides for ρ_c.

curve for the noninteracting case ($U = 0$) can be illustrated by the shape of this dispersion curve. Depending on the ratio $\alpha \equiv |t_1/t_2|$, the dispersion curve continuously changes between single-band-like and two-band-like shapes, reflecting single chain and double chain natures of the zigzag lattice. For $\alpha < 2$, the van Hove singularity is located below half-filing. Accordingly, the cusp-like singularity appears in the μ–ρ curve. Hereafter, we denote the corresponding electron density as ρ_c, which is shown as broken lines in Fig. 1. As α decreases, ρ_c shifts down to the lower electron-density region. Then the system is essentially described by the single band below ρ_c, while it has the two band like nature above ρ_c. For the case of finite U, Fig. 1 shows that these features are basically maintained. However, we can see that the μ–ρ curve in the two band region clearly exhibits oscillating behavior, which can be attributed to the bound state pair of the electrons; If two electrons conform a bound state, $N =$ even sector becomes energetically more stable than $N =$ odd sector. Thus, the μ–ρ curve in the present definition of μ is expected to show oscillating behavior depending on $N =$ even or odd in the spin gap region. Indeed, it is well known that, for $\alpha < 1.8$, there is the dimer spin gap at half filling [7–9]. For $0.7 < \alpha < 1.8$, the oscillating behavior of the μ–ρ curve appears down to ρ_c, suggesting the spin gap phase extends down to ρ_c. For $\alpha < 0.7$, however, such an oscillating behavior disappears below the half filling and the anomalous oscillation may appear near ρ_c again. This suggests that a spin gap may emerge in a restricted range of ρ above ρ_c. Since the model parameter for Pr247 is in $|t_2| \gg t_1$, this result is important to analyze the superconductivity of Pr247. As α decreases, the energy scale of the amplitude of the even–odd oscillation itself becomes small, and thus it is difficult to analyze the spin gap for small α region ($\alpha < 0.3$). Here, we note that the oscillation below ρ_c, where the system is essentially single band, certainly disappears with the $L \to \infty$ extrapolation.

As was seen in the μ–ρ curves, we can expect that the spin gap is enhanced above ρ_c. Detailed calculations of the spin gap indicate that it actually appears in a narrow range of ρ above ρ_c, which suggests that the superconductivity in Pr247 may appear in the corresponding region in vicinity of ρ_c. The experimentally measured transition temperature is rapidly raised above the critical value of δ [1,2], and, moreover, it is very sensitive to the high pressure effects. The μ–ρ curves basically support these experimental results. However, it is still an interesting problem to precisely determine the phase boundary of the spin gap phase. We hope that our results stimulate further investigations of the zigzag Hubbard model for full-understanding of Pr247 superconductivity.

This work has been partly supported by Grants-in-Aid for Scientific Research (18740230,17340100,17038011) from the Ministry of Education, Culture, Sports, Science and Technology of Japan. It is also supported by Grant-in-Aid for Scientific Research(18040044) on priority Areas "High Field Spin Science in 100T". A part of numerical computations was performed with SX8 at Yukawa Institute in Kyoto University.

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