Universality class of S=$\frac{1}{2}$ quantum spin ladder system with the four spin exchange

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We study $s=\frac{1}{2}$ Heisenberg spin ladder with the four spin exchange. Combining numerical results with the conformal field theory (CFT) [1], we find a phase transition with central charge $c=\frac{3}{2}$. Since this system has an SU(2) symmetry, we can conclude that this critical theory is described by $k=2$ SU(2) Wess-Zumino-Witten model with $\mathbb{Z}_2$ symmetry breaking.

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I. INTRODUCTION

Quantum spin ladder systems [2] have been studied in relation with high-$T_c$ superconductivity and Haldane’s conjecture [3]. These studies have been done mainly with 2-body interaction terms. Recently from experiments on dispersion curve [4], [5], it is suggested that 4-spin exchange interactions play an important role.

In general, spin interactions originate from electron exchange interactions. It is well known that Heisenberg model is derived from the second order perturbation expansion in strong coupling limit of Hubbard model. Similarly higher order terms give many body spin interactions. For example, fourth order terms give the four body spin interactions, e.g. $(\vec{S}_i \cdot \vec{S}_j)(\vec{S}_k \cdot \vec{S}_l)$. In fact, in the one dimensional (1D) two leg ladder, many body spin interactions appear from electron exchanges [6], [7]. Note that 1D nearest neighbor Hubbard model does not give many body interactions, because the cyclic path is impossible on this lattice. Therefore, it is important to understand the spin ladder systems including 4-spin exchange term.

Apart from the spin ladder systems, many-body interactions appear in 2D, 3D systems. It is experimentally known that many-body interaction can not be neglected especially in $^3$He on graphite [8], and Wigner crystal [9]. As another example, in high $T_c$ superconductor described by 2D Hubbard model, many-body spin interactions appear and they may be important physically [10].

This paper is organized as follows. In the next section, we shortly review for $s=1/2$ two-leg spin ladder systems. In Sec. 3, we discuss the phase transition and the universality class from numerical results and the conformal field theory. In Sec. 4, we summarize results. In appendix, we briefly explain theories used in this study, that is, solvable models, WZW model, logarithmic corrections.

II. OVERVIEW OF SPIN LADDER SYSTEMS

We treat the following Hamiltonian

$$H = J_{\text{leg}} \sum_{i=1}^{L} \sum_{\alpha=1,2} \vec{S}_{\alpha,i} \cdot \vec{S}_{\alpha,i+1} + J_{\text{rung}} \sum_{i=1}^{L} \vec{S}_{1,i} \cdot \vec{S}_{2,i} + J_{\text{ring}} \sum_{i=1}^{L} (P_{i,i+1} + P_{i,i+1}^{-1}),$$

(1)

where $J_{\text{leg}}$ is the intrachain coupling, $J_{\text{rung}}$ is the interchain coupling, and $P_{i,j,k,l}$ is the four spin exchange term which is written with spin operators

$$P(i,i+1) + P^{-1}(i,i+1) = \frac{1}{16} + \vec{S}_{1,i} \cdot \vec{S}_{1,i+1} + \vec{S}_{2,i} \cdot \vec{S}_{2,i+1} + \vec{S}_{1,i} \cdot \vec{S}_{2,i+1} + \vec{S}_{2,i} \cdot \vec{S}_{1,i+1} + \vec{S}_{1,i} \cdot \vec{S}_{1,i+1} \vec{S}_{2,i} \cdot \vec{S}_{2,i+1} + 4(\vec{S}_{1,i} \cdot \vec{S}_{2,i})(\vec{S}_{1,i+1} \cdot \vec{S}_{2,i+1}) + (\vec{S}_{1,i} \cdot \vec{S}_{1,i+1})(\vec{S}_{2,i} \cdot \vec{S}_{2,i+1}) - (\vec{S}_{1,i} \cdot \vec{S}_{2,i})(\vec{S}_{2,i} \cdot \vec{S}_{1,i+1}),$$

(2)

and indexes $i$ are for longitudinal direction, $\alpha=1,2$ are indexes of spin chains, (see Fig.1). In this section, we shortly review the model and related studies.
Quantum spin ladder systems have been well studied. Recently several quantum spin ladder materials are found out experimentally, and they attract much attention \[1,11\]. Theoretically, they have been studied with bosonization method and numerical calculations. For only 2-body interaction, there are many studies. See for example, \[2,12,13,4,11\] and references therein.

When there is the four spin exchange, it is expected that strange phase transitions may appear. In this region, there are few studies. Brehmer et al. numerically calculated the dispersion curve in the $s=\frac{3}{2}$ spin ladder with the four spin exchange \[10\]. They discussed it from the viewpoint of the symmetry breaking. Sakai et al. \[13\] studied with numerical calculation for the system with the magnetization plateau. In that paper, they found out that this system is Tomonaga-Luttinger (TL) liquid with central charge $c = 1$, when magnetization $m=\frac{1}{2}$, and that BKT transition occurs between TL phase and plateau phase region. Honda et al. \[27\] investigated the energy gap and the spin-spin correlation function with the density matrix renormalization group method. Recently experimentists found the real material with 4-spin cyclic exchange, i.e., La$_6$Ca$_8$Cu$_{24}$O$_{41}$. In that experiment, the dispersion relation was observed by neutron scattering, which suggests four-body terms \[3,11\].

When $J_{\text{rung}} < 0$, $s=\frac{1}{2}$ quantum spin two-leg ladder systems can be mapped to $s=1$ systems. Thus they can be considered as a generalization of Haldane’s conjecture \[3\] for ladder systems. Haldane phase is characterized by the string order parameter, which is related to a hidden $Z_2 \times Z_2$ symmetry breaking. In $s=\frac{1}{2}$ ladder systems with four spin exchanges, the string order parameter was discussed by Fath et al. \[15\]. In that paper, there are two type gapped phases. One is a rung singlet type, another is the AKLT type \[19\]. Using density matrix renormalization group, Legeza et al. \[15\] pictured phase diagram in these systems. But they have not decided phase boundary properly. Nersesyan et al. \[20\] referred to the relation between $s=\frac{1}{2}$ ladder system with four spin exchange and $s=1$ quantum spin chain with bilinear-biquadratic term (see Appendix A). In that paper, they examined behaviors of a correlation function of relative staggered magnetization and a correlation function of relative dimerization field, and suggested the phase transition with central charge $c = \frac{3}{2}$.

When $J_{\text{rung}} < 0$, we can relate $s=\frac{1}{2}$ quantum spin ladder system with four spin exchange to $s=1$ quantum spin chain with bilinear-biquadratic term. When $J_{\text{rung}} > 0$, is it obvious? The discussion of Legeza et al. \[15\] is different from that of Nersesyan et al. \[20\]. Legeza et al. \[15\] wrote that this phase transition is between a nondegenerate singlet state and a fourfold-degenerate ground state. The fourfold-degenerate ground state realizes because the singlet-triplet gap disappear. Nersesyan et al. \[20\] wrote that, there is the region where the triplet Majorana excitation is lower than the singlet one, in which it is enough to consider only the triplet Majorana excitation, thus the phase transition belongs to the second order type with $c = \frac{3}{2}$. Although both of them predicted Takhtajan-Babujian type transition point ($c = \frac{3}{2}$) in the $s = 1/2$ spin ladder (with four-body terms), there is a difference on other critical phenomena between them. Nersesyan et al. \[20\] referred to $c = 1/2$ (the singlet Majorana field becomes massless in another region), Legeza et al. \[15\] referred to $c = 2$ Uimin-Lai-Sutherland model \[30\]. There remains controversial in this region.

III. RESULTS AND DISCUSSION

We study $J_{\text{leg}}=J_{\text{rung}}=1$ case with varying $J_{\text{ring}}$ coupling in the system (1) with no magnetizations, combining numerical calculation and conformal field theory (CFT).

A. numerical results and universality discussion

At first, we study the size dependence of the ground state energy, in order to see the type of periodicity ($Z_2$ or $Z_3$) under periodic boundary condition (PBC). In Fig.2, we can see that the ground state energy per site $E_g(L)/L$ oscillates according to $L$ even or odd (even cases are lower). This suggests that translational invariance by one site may be spontaneously broken. For another evidence of $Z_2$ symmetry breaking, we study the dispersion curve, which shows that the lowest excitation has soft modes at $q = \pi$ (see Fig.3). Thus we will study the system size $L=N/2=6,8,10,12$.

In order to discuss what type of phase transitions may occur, we use the effective central charge $c$, obtained from the finite size scaling of the ground state energy. From the conformal field theory at the critical point, the finite size scaling of ground state energy under the periodic boundary condition (PBC) is the following \[21,22\].

$$E_g(L) = \epsilon L - \frac{\pi v c}{6L},$$

where $E_g(L)$ is the ground state energy for size $L$, $\epsilon$ is the energy per site in the infinite limit, $v$ is the spin wave velocity.
In addition to the ground state energy, we should obtain $v$ numerically to decide $c$ in equation (3). The spin wave velocity $v$ is obtained from

$$v(L) = \frac{L}{2\pi} \left[ E \left( q = \frac{2\pi}{L} \right) - E(q = 0) \right],$$

where $q$ is a wave number. Then we extrapolate $v(L)$ as

$$v(L) = v + a \frac{1}{L^2} + b \left( \frac{1}{L^2} \right)^2 + \text{higher order}. \quad (5)$$

In Fig.4, we show the obtained effective central charge. The effective central charge shows a maximum value $c=1.49$ at $J_{ring}=0.192$. According to Zamolodchikov’s c-theorem [23], the effective central charge shows maximum at the infrared fixed point. Thus we can conclude that there is a phase transition with the central charge $c=\frac{3}{2}$.

Only from the central charge, there remain several possibilities for universality class. But considering the symmetry of the system, we can discuss in detail. Combining the overall SU(2) symmetry of Hamiltonian, we can relate central charge $c=\frac{3}{2}$ in conformal field theory to the topological coupling constant (Kac-Moody central charge) $k$ in SU(2) Wess-Zumino-Witten model. The relation between $k$ and $c$ is given by

$$c = \frac{3k}{k + 2}. \quad (6)$$

Thus the critical theory $c=\frac{3}{2}$ with SU(2) symmetry is described as the $k = 2$ SU(2) Wess-Zumino-Witten model. This universality class is characterized with scaling dimensions $x = \frac{3}{2}$ (parity odd,$q = \pi$), $x = 1$ (parity even,$q = 0$) for the primary field (in Kac-Moody algebra), $x = 2$ (parity even,marginal,$q = 0$) for the (Kac-Moody) descendant field (see appendix B). They mean that a second order transition occurs with $Z_2$ symmetry breaking. And the mass (energy) gap is generated near the critical point as $\Delta E \propto |J_{ring} - J_{cring}|$ from $x = 1$ term. Here the mass gap $\Delta E$ is related with the correlation length $\xi$ as $\Delta E \propto \xi^{-1}$.

Next we study lowest excitations with wave number $q = \pi$, which consist of $s = 0$ (singlet) and $s = 1$ (triplet). We can expect that these excitation are related with the scaling dimension ($x = \frac{3}{2}$,$q = \pi$) in the $k = 2$ SU(2) WZW model. In general, from CFT, scaling dimension can be calculated from the excitation energy for finite size under PBC as [24]

$$\Delta E_i = E_i - E_0 = \frac{2\pi v}{L} x_i. \quad (7)$$

Unfortunately, in the $k = 2$ SU(2) WZW model, there are marginal corrections, $1/\ln L$, which are difficult to treat. Thus we should remove them with the method in appendix C. After removing logarithmic corrections, scaling dimension is almost independent on the system size at critical point $J_{ring} = 0.192$ (See Fig.5). Therefore, we can conclude that this universality class belongs to the $k = 2$ SU(2) WZW type.

Finally, we comment on the effect of the marginal operator to the ground state energy and the velocity. For ground state energy, it is proved that,

$$E_g(L) = \epsilon L - \frac{\pi v}{6L} \left( c + \frac{b}{(\ln L)^3} \right),$$

where $o\left(\frac{1}{L}\right)$, $o\left(\frac{1}{(\ln L)^2}\right)$ terms do not exist [25]. We have neglected the $o\left(\frac{1}{(\ln L)^3}\right)$ contribution (which is small enough) to obtain the effective central charge. For the velocity, it is proved that there is not $o\left(\frac{1}{\ln L}\right)$ term in current-current correlation [26]. Therefore, we have neglected logarithmic correction in equation (5).

**B. symmetry breaking and boundary condition**

After studying the universality class, we proceed to discuss the symmetry breaking and the order parameter. Although finite size effect prevents us from drawing a definite conclusion, we can consider several clues relating to the ordered state.
At first, for $J_{\text{ring}} < J'_{\text{ring}}$, the triplet excitation is lower than the singlet excitation at $q = \pi$, whereas for $J_{\text{ring}} > J'_{\text{ring}}$, the singlet excitation is inclined to be under the triplet excitation. But this is not clear in terms of the finite size effect. Secondary, besides the translational symmetry breaking, it is observed a rung-parity symmetry breaking, reversing each spin chain ($S_{1,i} \leftrightarrow S_{2,i}$), which Brehmer et al. discussed on the dispersion curve. We confirmed their dispersion curves at $J_{\text{ring}} = 0.15$ (see Fig. 4). In summary, in the $L \to \infty$ limit under PBC, it is expected that, for $J_{\text{ring}} > J'_{\text{ring}}$, the ground state ($q = 0, S_z^{\text{tot}} = 0, P_{\text{ring}} = \text{even}$) will be degenerate with the lowest state ($q = \pi, S_z^{\text{tot}} = 0, P_{\text{ring}} = \text{odd}$), while for $J_{\text{ring}} < J'_{\text{ring}}$, there is no symmetry breaking.

Honda et al. studied the same system as ours \[27\]. Using the density matrix renormalization group method, they calculated the spin gap and spin-spin correlation function. They claimed that there occurs a phase transition from a massive phase to a massless phase at $J_{\text{ring}} > J'_{\text{ring}}$, the ground state ($q = 0, S_z^{\text{tot}} = 0, P_{\text{ring}} = \text{even}$) will be degenerate under the open boundary condition \[28\]. The four lowest energy states are almost degenerate, whose energy gap decays exp ($-H/L$), and there is a Haldane gap between them and the continuum energy spectrum. On the finite size effect, the edge state is well defined when it is sufficiently localized, that is, the system size is large enough compared with the correlation length. However, since the correlation length becomes very long near the critical point, so the finite size effect becomes large. Therefore, considering edge states, it is possible to explain why Honda et al. estimated the critical point $J'_{\text{ring}}$ larger than ours. Numerically, edge states can be confirmed by investigating the ground state energies under open boundary condition with higher magnetizations. Note that edge states can be detected experimentally.

### IV. SUMMARY

In the present paper, we studied $s = \frac{1}{2}$ quantum spin ladder with four spin exchange, in order to see the phase transition type in this system.

We saw the behavior of the central charge and the scaling dimension, which have logarithmic corrections. At first, we calculated the central charge, since its correction is small. The central charge has the maximum value $c = 1.49$ at $J_{\text{ring}} = 0.192$. Removing the logarithmic correction for the scaling dimension, we obtained $x \approx \frac{3}{2}$ near $J_{\text{ring}} = 0.192$. In this region, the scaling dimension do not have a significant size dependence. So we can conclude that this phase transition belongs to a $k = 2$ SU(2) WZW type.

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APPENDIX A: $S=1$ QUANTUM SPIN CHAIN WITH BILINEAR-BIQUADRATIC TERM

We shortly review the following Hamiltonian.

$$H = \sum_n \left( \cos \theta \left( \vec{S}_n \cdot \vec{S}_{n+1} \right) + \sin \theta \left( \vec{S}_n \cdot \vec{S}_{n+1} \right)^2 \right). \tag{A1}$$

This model is well researched. The phase diagram of this model is known in numerically \[28\], \[30\]. And this model is exactly solved by Bethe Ansatz, at the special point $\theta = -\frac{\pi}{4}, 0$. The critical point $\theta = -\frac{\pi}{4}$ is Takhtajan-Babujian point \[31\], \[32\]. This is the critical point between dimer phase and Haldane phase. It is known that this critical theory is described as $c = \frac{3}{2}$ CFT or $k = 2$ SU(2) WZW model \[33\], which is equivalent to three Majorana fermions.

For general spin $s$, Takhtajan-Babujian type solvable models are described as Wess-Zumino-Witten non-linear $\sigma$ model(WZW model) with topological coupling constant $k = 2s$ \[32\], \[33\], in terms of the analysis for quantum spin systems using non-Abelian bosonization \[33\].

Another Bethe Ansatz solvable point at $\theta = \frac{\pi}{4}$ is equivalent to $k = 1$ SU(3) WZW model with $c = 2$. This is known as Uimin-Lai-Sutherland model \[36\]. Above $\theta > \frac{\pi}{4}$, although there is not SU(3) symmetry, the massless region extends with the $Z_3$ symmetry quasi breaking, and soft modes appear at $q = \pm \frac{2\pi}{3}$. Recently from non-Abelian
bosonization and renormalization group analysis, it is shown that this is a variant of the BKT transition (but the different universality class [37]).

**APPENDIX B: WESS-ZUMINO-WITTEN MODEL (KAC-MOODY ALGEBRA)** [1],[34]

The minimal conformal field theory with the smallest spectrum containing currents obeying the Kac-Moody algebra with central charge \( c \) is the Wess-Zumino-Witten non-linear \( \sigma \) model, with topological coupling constant \( k \). Thus the relation between \( c \) and \( k \) is

\[
c = \frac{k \dim G}{k + \frac{2\pi}{C_A^2}}, \tag{B1}
\]

where \( \dim G \) is dimension for an arbitrary representation and \( \frac{2\pi}{C_A^2} \) is called as the dual Coxeter number. In the present case, since the system has SU(2) symmetry, we have \( \dim G = 3 \), and \( \frac{2\pi}{C_A^2} = 2 \).

Now we think of the case with the SU(2) symmetry. In this case, primary fields can be classified according to their left and right moving spin. There are operators with \( s_L = s_R = 0 \) (singlet) case, \( s_L = 1 \), \( s_R = 0 \) (triplet) case, \( s_L = 1 \), \( s_R = 1 \) which forms 1 (singlet) and a singlet \( s=0 \). The states with momentum \( \pi/L \) have the conformal weight \( (h, \bar{h}) = (1, 0) \) which has the scaling dimension \( x = h + \bar{h} = 2 \) and the conformal spin 0, i.e. wave number \( q = 0 \).

Current operators \( J_L, J_R \) themselves have conformal spin \( \pm 1 \), corresponding to the wave number \( q = \pm 2\pi/L \), thus they are related with the spin wave velocity.

**APPENDIX C: LOGARITHMIC CORRECTION TO SCALING DIMENSION (OR ENERGY GAP)** [34]

According to the non-Abelian bosonization, in SU(2) symmetric gapless system, the excitation energies (for \( q = \pi \) states), including logarithmic corrections, are

\[
\Delta E = E_\pi - E_0 \approx \frac{2\pi v}{L} \left( x_i - \frac{\langle \vec{S}_L \cdot \vec{S}_R \rangle}{\ln L} \right). \tag{C1}
\]

where \( L \) is a system size, and \( v \) is a spin wave velocity. Here \( \vec{S} = \vec{S}_L + \vec{S}_R \) is total spin which is a conserved quantity. Note that

\[
\vec{S}_L \cdot \vec{S}_R = \frac{1}{2} \left( \vec{S}_L + \vec{S}_R \right)^2 - \frac{1}{2} S_L^2 - \frac{1}{2} S_R^2
= \frac{1}{2} s(s+1) - \frac{1}{2} s_L(s_L+1) - \frac{1}{2} s_R(s_R+1). \tag{C2}
\]

In the case of \( s_L = s_R = \frac{1}{2} \), since \( s_L \otimes s_R = \frac{1}{2} \oplus \frac{3}{2} = 0 \oplus 1 \), it forms a triplet \( s=1 \) and a singlet \( s=0 \). The states \( s_L = s_R = \frac{1}{2} \) correspond to a wave vector \( q = \pi \). For \( s=1 \) (triplet) case, we obtain

\[
\langle \text{triplet} \mid \vec{S}_L \cdot \vec{S}_R \mid \text{triplet} \rangle = \frac{1}{4}. \tag{C4}
\]

On the other hand, for \( s=0 \) (singlet) case,

\[
\langle \text{singlet} \mid \vec{S}_L \cdot \vec{S}_R \mid \text{singlet} \rangle = \frac{3}{4}. \tag{C5}
\]
Therefore we obtain

$$\Delta E(s = 1) = E_i - E_0 \approx \frac{2\pi v}{L} \left( x_i - \frac{1}{4 \ln L} \right),$$  \hspace{1cm} (C6)

and

$$\Delta E(s = 0) = E_i - E_0 \approx \frac{2\pi v}{L} \left( x_i + \frac{3}{4 \ln L} \right),$$  \hspace{1cm} (C7)

thus we can remove logarithmic corrections of energy gap.

$$x_i = \frac{L}{8\pi v} \left[ 3\Delta E(s = 1) + \Delta E(s = 0) \right].$$  \hspace{1cm} (C8)

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FIG. 1: Two-leg spin ladder of eq. (1)

FIG. 2: Size dependence of the ground state energy at $J_{\text{ring}} = 0.3$, 0.3.

FIG. 3: Dispersion curve at $J_{\text{ring}}=0.1$ and $J_{\text{ring}}=0.3$ for the system size $L=12$ (N=24).
FIG. 4: Effective central charge

FIG. 5: Scaling dimension $x$ at $q = \pi$.

FIG. 6: $L=12$ ($N=24$) dispersion curve with rung parity at $J_{\text{ring}} = 0.15$. 