Phase transition of $S=\frac{1}{2}$ two-leg Heisenberg spin ladder systems with a four-spin interaction

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We study a phase transition and critical properties of the quantum spin ladder system with a four-spin interaction. We determine a phase boundary between a rung singlet and a staggered dimer phases numerically. This phase transition is of a second order in the weak-coupling region. We confirm that this universality class is described by the $k=2$ SU(2) Wess-Zumino-Witten model, analyzing the central charge and scaling dimensions. In the strong-coupling region, phase transition becomes of a first order.

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I. INTRODUCTION

Quantum phase transitions and quantum critical phenomena have attracted much interest in condensed matter and statistical physics.[1] Especially, ground states are not necessarily ordered in low-dimensional quantum systems because of quantum fluctuations. Spin chain systems and spin ladder systems are typical examples of such systems. The quantum spin ladder systems are studied from both theoretical and experimental points of view.[2,3] These systems are related to Haldane's conjecture[4,5] and high-T_c superconductivity.

Effects of many-body spin interactions are much interesting subjects recently. Two-body spin-exchange interactions are derived from second-order perturbations in the strong-coupling limit of the Hubbard model. Thus, it is a natural extension to consider higher-order perturbation terms, for example, four-spin exchange terms are derived from fourth-order perturbations.[6] Many-body interactions are studied in relation to composite spin models.[7,8] By the way, it has been revealed that even the spin ladder model with only two-body terms have a rich phase diagram,[9] therefore we can expect that systems with four-spin interaction terms may have different properties. We know that cyclic spin exchanges play an important role in the solid ^{3}He.[10] Recently, a four-spin cyclic (ring) exchange interaction is found in a two-dimensional square lattice La_2CuO_4 which is a high-T_c superconductor parent compound[11] and in a spin ladder compound $La_6Ca_8Cu_{24}O_{41}$.[12,13]

Ring exchanges have a quite complex form represented by spin operators. Therefore, it is better to investigate a simpler Hamiltonian in order to understand effects of many-body interactions. In this paper, we study a spin ladder model which is described as the following Hamiltonian

$$\mathcal{H} = J_{\text{leg}} \sum_{\alpha=1,2} \sum_{j=1}^{L} \mathbf{S}_{\alpha,j} \cdot \mathbf{S}_{\alpha,j+1} + J_{\text{rung}} \sum_{j=1}^{L} \mathbf{S}_{1,j} \cdot \mathbf{S}_{2,j} + J_4 \sum_{j=1}^{L} (\mathbf{S}_{1,j} \cdot \mathbf{S}_{1,j+1})(\mathbf{S}_{2,j} \cdot \mathbf{S}_{2,j+1}), \quad (1)$$

where $\mathbf{S}_{\alpha,i}$ is $S=\frac{1}{2}$ spin operators at a site (α,i) and we set $J_{\text{leg}}=1$. This model is one of the simplest model with four-spin interactions (see Fig. 1).

In a $J_4=0$ case, this model is known as a usual spin ladder system. The phase diagram of this model has been well studied.[14] In a $J_{\text{rung}}>0$ region, the ground state is the rung-singlet phase which is gapped (see Fig. 2). In a $J_{\text{rung}}<0$ case, the ground state is the Haldane phase which is gapped, too. The $J_{\text{rung}}=0$ point is a phase-transition point. This phase transition is of a second order and the critical properties are described by the two independent Tomonaga-Luttinger liquids with the central charge $c=2$.

In a $J_{\text{rung}}=0$ case, this Hamiltonian is identical with a spin-orbital model. In this case, the model [Eq. (1)] has an $SU(2)\otimes SU(2)$ symmetry, especially at $J_4=4$ point it has an enhanced symmetry, that is, an SU(4) symmetry.[15] In addition, the model [Eq. (1)] on $J_{\text{rung}}=0$, $J_4=4$ point is exactly solvable by the Bethe ansatz.[16] The low-energy theory on this point is described by the $k=1$ SU(4) Wess-Zumino-Witten (WZW) model corresponding to $c=3$ conformal field theory (CFT) which is equivalent to three free bosons.[17,18] The whole phase diagram in the $J_4>0$ has been obtained by Itoi *et al.*[19] In $0<J_4<4$ region, the ground state is the staggered dimer ordered phase (see Fig. 3). This phase is characterized by the twofold-degenerate ground state with the excitation energy gap and the spontaneous symmetry breaking of the one-site translation. In $J_4>4$ region, the ground state is gapless. The low-energy theory of the gapless phase $J_4>4$ is renormalized to the $k=1$ SU(4) WZW model.

Returning to the general coupling case of model [Eq. (1)], effects of four-body interactions are studied about ground-state properties by Bethe ansatz (only on the special line $J_4=4$, $J_{\text{rung}}\neq 0$),[20] numerical calculations,[21] effective-field theory,[22] and thermodynamics properties by transfer-matrix renormalization group.[23] The model [Eq. (1)] with $J_{\text{rung}}<0$, $J_4<0$ is investigated by Nersesyan and Tsvelik.[24] This

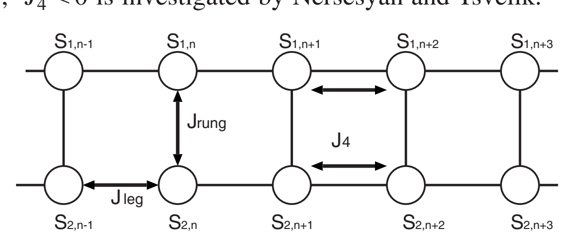

FIG. 1. Schematic structure of a $S=\frac{1}{2}$ two-leg spin ladder of Eq. (1).

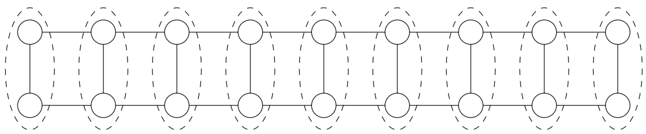

FIG. 2. A schematic picture of rung-singlet state. Two spins $\mathbf{S}_{1,i}, \mathbf{S}_{2,i}$ enclosed by a dotted line is a singlet $\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$.

case is directly linked to an $S=1$ bilinear-biquadratic (BLBQ) chain.

In this study we treat the $J_4, J_{\mathrm{rung}} > 0$ case in a weak-coupling region where J_4, J_{rung} are not enough large. We will investigate the ground-state phase diagram and critical properties of the phase transition in an antiferromagnetic region near the $J_{\mathrm{rung}} = J_4 = 0$ point where the model is described by the $c=2$ CFT.

This paper is organized as follows. In Sec. II, we discuss the relation between symmetry and boundary condition in some phases. In Sec. III, we show our numerical results. In Sec. IV, we summarize our results.

II. SYMMETRY AND BOUNDARY CONDITIONS

In this section, we discuss symmetries and boundary conditions. At first, we describe several quantum numbers. As usual, we define $S_T^z \equiv \Sigma_{\alpha,j} S_j^z$ as a total magnetization and q as a wave number. We introduce a rung parity P_{r} which is related to the inversion along the rung direction. And we introduce a leg parity P_{l} which is related to the inversion along the leg direction.

The ground state of the rung-singlet phase is unique, whereas the ground state of the staggered dimer phase is twofold degenerate in the thermodynamic limit. On the other hand, the spontaneously symmetry breaking does not occur in finite systems. We consider the finite system. We call the ground state of the rung-singlet phase as RS, and one of the linear combination of ground states of the staggered dimer phase with $P_{\mathrm{r}}=1$ as SD1, another state with $P_{\mathrm{r}}=-1$ as SD2. In Table I, we summarize the quantum numbers of these three states. Note that under the periodic boundary condition (PBC), the quantum numbers of RS and SD1 are the same, thus we cannot distinguish these two states. Although, in principle, one can determine the phase boundary between the rung-singlet phase and the staggered dimer phase, examining the energy-gap size dependence, this method needs large size data. Therefore, we will consider another approach, that is, using the twisted boundary condition (TBC).

Next we introduce the TBC.

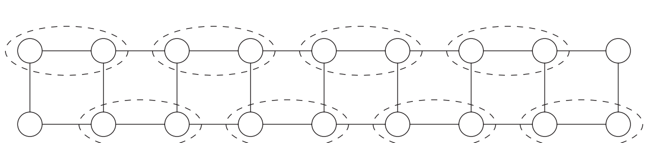

FIG. 3. A schematic picture of a staggered dimer order state under the open boundary condition. Two spins $\mathbf{S}_{\alpha,i}, \mathbf{S}_{\alpha,i+1}$ enclosed by a dotted line is a singlet. This phase is characterized by the order parameter $\langle \mathbf{S}_{\alpha,i-1} \cdot \mathbf{S}_{\alpha,i} \rangle$-$\langle \mathbf{S}_{\alpha,i} \cdot \mathbf{S}_{\alpha,i+1} \rangle$.

TABLE I. States and their symmetries. 1 denotes "even" and −1 denotes "odd." $(\cdots)$ are eigenvalues under the TBC. We use a symbol P^* for parity P under the TBC.

	S_T^z	P_{r}	P_{l}	q
RS	0	1	1	0
SD1	0	1	1(−1)	0
SD2	0	−1	1(−1)	π

$$S^+_{\alpha,L+j} = S^+_{\alpha,j} \exp[i\Phi],$$

$$S^-_{\alpha,L+j} = S^-_{\alpha,j} \exp[-i\Phi],$$

$$S^z_{\alpha,L+j} = S^z_{\alpha,j}, \qquad (2)$$

where Φ is called a twist angle. The case with $\Phi=0$ is equivalent to the PBC. Usually $\Phi=\pi$ is called the twisted boundary condition.

Twist angle Φ does not affect S_z^T and P_{r}. The leg parity is well defined in the case with only $\Phi=0,\pi$. Under the TBC, the system is not translationally invariant. But we can introduce an extended wave number using some unitary transformation. This is discussed by Kolb[25] and Fáth-Sólyom.[26]

Although the leg parity P_{l} of RS is the same under the TBC as the PBC case, the meaning of the leg parity P_{l} of SD1 drastically changes under the TBC, as can be seen in Table I. Therefore, using P_{l} under the TBC, we can clearly distinguish the RS state and SD1 state. In other words, in order to determine the phase boundary between the rung-singlet phase and the staggered dimer phase, we can use the level crossing of energy eigenvalues of the RS state and the SD1 state under the TBC.

From the other point of view, we can use the field theoretical approach. As is well known, Takhtajan-Babujian point in $S=1$ BLBQ model is the second-order phase-transition point with $\mathbf{Z}_2$ symmetry breaking in SU(2) symmetric models. This phase transition has the central charge $c=3/2$.[17,27] By the way, Fáth and Sólyom[26] have found that a degeneracy occurs at Takhtajan-Babujian point under the TBC but they did not give the theoretical explanation of this degeneracy. After that, Kitazawa and Nomura[28] have proved that one can determine the Takhtajan-Babujian-type critical point using the level crossing of the energy eigenvalues under the TBC. More precisely, they have done a renormalization-group analysis for the $k=2$ SU(2) WZW model with the SU(2) relevant term under the TBC.

From the analogy between the $S=1$ BLBQ model and the present model [Eq. (1)], we expect that the level crossing of $S=1$ BLBQ model under the TBC corresponds to one between a rung-singlet phase and a staggered dimer ordered phase under the TBC in the model [Eq. (1)].

We predict that the level crossing of $S=1$ BLBQ model under TBC corresponds to one between the rung-singlet phase and staggered dimer ordered phase under the TBC. Later we will confirm the universality class numerically in order to check the validity of this prediction.

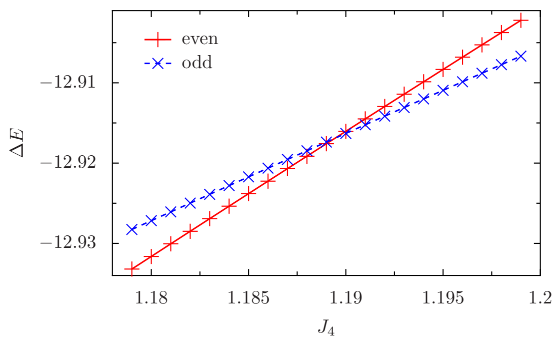

FIG. 4. (Color online) Level crossing in the system with the twisted boundary conditions. + is the lowest energy with $P_1^*=1$, $P_r^*=1$, $S_T^z=0$, × is the lowest energy with $P_1^*=-1$ $P_r^*=1$, $S_T^z=0$ for $L=14(N=28)$ at $J_{\text{rung}}=1.0$.

III. NUMERICAL RESULTS

Here we assume that a direct phase transition occurs between the staggered dimer phase and the rung-singlet phase. This is plausible in a small (J_{rung},J_4) region. We first determine the phase boundary between the staggered dimer phase and the rung-singlet phase. In order to determine the transition points, we use the TBC method. In this case, the boundary condition is the following:

$$S^{\pm}_{\alpha,j+L}=-S^{\pm}_{\alpha,j},\quad S^{z}_{\alpha,j+L}=S^{z}_{\alpha,j}, \tag{3}$$

where L is the system size. As discussed in the previous section, from the analogy with the $S=1$ BLBQ model, we will determine the phase boundary using the level crossing between the lowest energy eigenvalue with quantum numbers $S_T^z=0$, $P_r^*=1$, $P_1^*=-1$ under the TBC and the lowest energy eigenvalue with $S_T^z=0$, $P_r^*=1$, $P_1^*=1$ under the TBC (see Table I).[26,28] Note that this level crossing is different from the $c=1$ Gaussian line case.[29,30] After determining the phase boundary, we will confirm the universality class of this transition, and we will justify this type of level-crossing method under the TBC to determine the phase boundary. Note that this method is exact to determine the $k=2$ SU(2) WZW-type critical point, except the finite-size corrections from the irrelevant fields with the scaling dimension $x=4$ such as $L_{-2}\bar{L}_{-2}\mathbf{1}$ and $L_{-4}\mathbf{1}$, $\bar{L}_{-4}\mathbf{1}$,[31–33] which are related to the lattice effect not included in the continuum theory.

Here we show numerical results of $L=6,8,10,12,14$ (the number of sites $N=12,16,20,24,28$) using the exact diagonalization. In Fig. 4, we show the level crossing in the subspace $\Sigma_{\alpha,i}S^z_{\alpha,i}=0$ with the TBC for $L=14$ and $J_{\text{rung}}=1.0$.

In Fig. 5, we show the size dependence of the crossing point for $J_{\text{rung}}=1.0$. Since there remain finite-size corrections from irrelevant term $x=4$, we extrapolate crossing points as follows:

$$J_4^{\text{cross}}(L)=J_4^{\text{cross}}+a\frac{1}{L^2}+b\frac{1}{L^4}+(\text{higher-order terms}), \tag{4}$$

where we neglect higher-order terms. We show the partial phase diagram (level-crossing points) in Fig. 6.

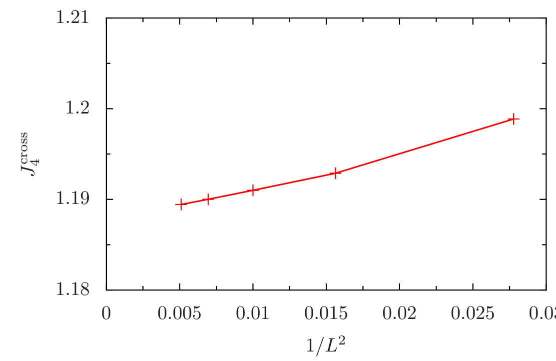

FIG. 5. (Color online) Size dependence of the crossing point for $J_{\text{rung}}=1.0$ as a function of $1/L^2$.

Next, we investigate the properties of this phase transition. Since $(J_{\text{rung}},J_4)=(0,0)$ is a gapless point, we can expect that the phase transition is of the second order, at least in a weak-coupling region. It is believed that the ground states of one-dimensional quantum system on the second-order phase-transition point are expected to be conformal invariant. So we can determine the universality class based on the CFT.[34] The finite-size scaling of the ground-state energy on a critical point with the PBC has a following form:

$$E_g(L)\simeq \varepsilon L-\frac{\pi v c}{6L}, \tag{5}$$

where $E_g(L)$ is the ground-state energy of the system with the size L, ε is the energy per site in the infinite system limit, v is the spin-wave velocity, and c is the central charge.[27,35] By the way, this central charge can be obtained from the entropy profile of finite systems.[36–38] But numerically very long systems have to be investigated to obtain accurate results obtained from the entropy.[39]

The formula (5) is correct only in critical cases. Here we define an effective central charge as follows:

$$E_g(L)\simeq \varepsilon L-\frac{\pi v\tilde{c}}{6L}, \tag{6}$$

where $\tilde{c}$ is the effective central charge. This effective central charge is equivalent to the central charge on the critical point

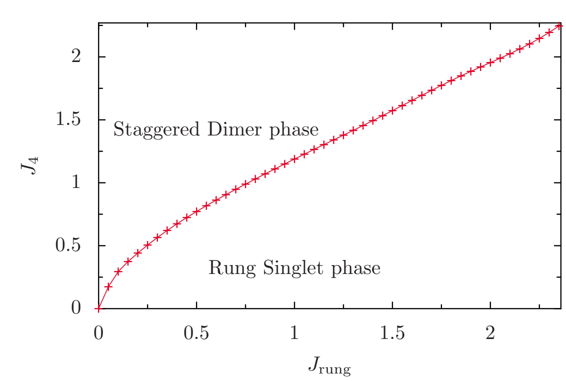

FIG. 6. (Color online) Phase diagram of the spin ladder system (1), which is obtained from $L=6,8,10,12,14$, in the weak-coupling region. Staggered order phase appears on an upper side of the crossing line, rung-singlet phase appears on its lower side.

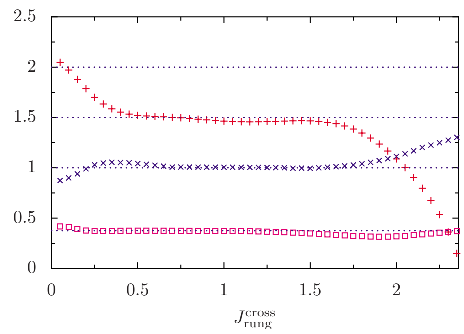

FIG. 7. (Color online) The effective central charge (+) and scaling dimensions (×), (□) on the phase boundary (obtained by the crossing points). Scaling dimensions are extrapolated after logarithmic corrections removed. (×) denotes the scaling dimension $x=1$ for a $q=0$ mode. (□) denotes the scaling dimension $x=3/8$ for a $q=\pi$ mode. Dotted lines are 3/8, 1, 3/2, and 2.

or in the critical (massless) region. The effective central charge decreases to zero in the noncritical (massive) region since the finite-size correction of the ground-state energy is exponentially decaying ($\sim\exp[-L/\xi]$: ξ is a correlation length), with increasing the system size. This means that the effective central charge rapidly decreases from a massless region to a massive region.[40,41] Actually, with a marginal irrelevant field (operator), there are logarithmic corrections for the ground-state energy of the finite system in the critical systems,

$$E_g(L) \simeq \varepsilon L - \frac{\pi v}{6L}\left(c + \frac{b}{(\ln L)^3}\right) + \text{higher order}, \qquad (7)$$

where b is constant. Note that it is proved that there are no $o(\frac{1}{\ln L})$, $o[\frac{1}{(\ln L)^2}]$ terms.[42–44] Hereafter we will neglect the term $1/(\ln L)^3$, which is small enough. So we calculate the effective central charge from Eq. (6).

In order to obtain the effective central charge $\tilde{c}$, we need the spin-wave velocity. The spin-wave velocity v is obtained from the lowest-excitation energy with the momentum $q=2\pi/L$ and the total spin 1 which corresponds to the SU(2) current

$$v(L) = \frac{L}{2\pi}\left[E\left(q=\frac{2\pi}{L}\right) - E_g\right]. \qquad (8)$$

Since there is no logarithmic correction in a current-current correlation,[45] we extrapolate $v(L)$,

$$v(L) = v + a\frac{1}{L^2} + b\frac{1}{L^4} + \text{higher order terms}, \qquad (9)$$

where a and b are fitting parameters. Neglecting higher-order terms, we finally obtain the effective central charge $\tilde{c}$ numerically. In Fig. 7, we show the effective central charge on the crossing line. It can be observed that $\tilde{c}\simeq 2$ at $J_{\rm rung}=0$ and $\tilde{c}\simeq 3/2$ in a weak-coupling region, whereas $\tilde{c}$ rapidly decreases in $J_{\rm rung}>1.5$. This behavior is interpreted as the phase transition between the rung-singlet phase and the staggered dimer phase is of the second order with the central charge $c=3/2$ in the weak-coupling region, and it becomes of the first order in $J_{\rm rung}>1.5$.

Universality class of this phase transition cannot be completely determined only by the central charge. Therefore we need to check consistency. From nonAbelian bosonization,[46] a relation between the central charge and the level k of SU(2) WZW model is the following:[44]

$$c = \frac{3k}{k+2}. \qquad (10)$$

From a symmetry of the systems and this relation, the critical properties with the central charge $c=3/2$ are expected to be described by the $k=2$ SU(2) WZW model.

Next, the scaling dimensions x of primary fields in Kac-Moody algebra[47,48] can be classified according to their left and right spin $s_{\rm R}=s_{\rm L}=0,1/2,\ldots,k/2$,

$$x = \frac{2s_{\rm L}(s_{\rm L}+1)}{k+2}, \qquad (11)$$

where k is a level of the WZW model. For the $k=2$ SU(2) WZW case, the lowest-excitation state has $s_{\rm R}=s_{\rm L}=1/2$, thus $x=3/8$, and the total spin $S=0,1$. Since the operators with half-odd integer $s_{\rm L}$ are odd under one-site translation, these states have momentum $q=\pi$. The next lowest-excitation state has $s_{\rm R}=s_{\rm L}=1$, thus $x=1$, and total spin $S=0,1,2$. Since the operators with integer $s_{\rm L}$ are even under one-site translation, these states have momentum $q=0$.[44] Usually, a universality class is classified by a set of critical exponents (scaling dimensions). In the CFT, scaling dimensions x_i are related to the excitation energy of the finite-size system with the PBC,[31]

$$\Delta E_i = E_i - E_g \simeq \frac{2\pi v}{L}x_i, \qquad (12)$$

where x_i is the scaling dimension and i is an index characterizing the excitation state. Unfortunately, there are logarithmic corrections from marginal operators.[44,49] The leading logarithmic correction term in the SU(2) WZW model is the following:

$$\Delta E_i \simeq \frac{2\pi v}{L}\left[x_i - \frac{1}{2}\frac{S(S+1) - s_{\rm R}(s_{\rm R}+1) - s_{\rm L}(s_{\rm L}+1)}{\ln L}\right]. \qquad (13)$$

Using this formula, we can remove logarithmic corrections selecting appropriate excitations which depend on the spin. After we remove logarithmic corrections, we need to consider finite-size corrections from the $x=4$ irrelevant fields $L_{-2}\bar{L}_{-2}\mathbf{1}$, $L_{-4}\mathbf{1}$, and $\bar{L}_{-4}\mathbf{1}$.[31–33] Considering these fields, we can obtain an extrapolation formula,

$$x_i(L) = x_i + a\frac{1}{L^2} + b\frac{1}{L^4} + \cdots, \qquad (14)$$

where a and b are nonuniversal coefficients, and neglecting higher order terms.

For $x=3/8$ case with momentum $q=\pi$ and spin $S=0,1$, we obtain

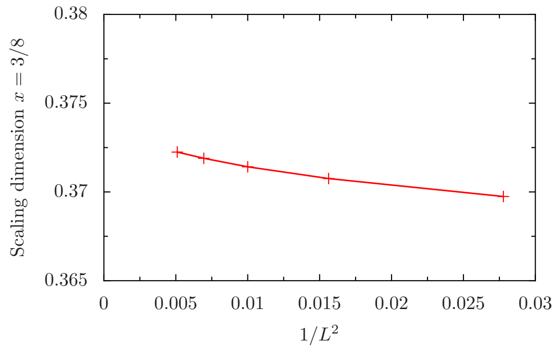

FIG. 8. (Color online) The size dependence of the scaling dimension $x=3/8$ at $J_{\mathrm{rung}}=1.0$ after logarithmic corrections removed. Extrapolated value is $x\sim 0.3726$.

$$\Delta E_i(S=1) \simeq \frac{2\pi v}{L}\left(x_i - \frac{1}{4}\frac{1}{\ln L}\right) \tag{15}$$

and

$$\Delta E_i(S=0) \simeq \frac{2\pi v}{L}\left(x_i + \frac{3}{4}\frac{1}{\ln L}\right). \tag{16}$$

Thus we can remove logarithmic corrections,

$$x_i \simeq \frac{L}{8\pi v}[3\Delta E_i(S=1) + \Delta E_i(S=0)]. \tag{17}$$

In Fig. 8, we show the size dependence of the scaling dimension, removing logarithmic corrections with Eq. (17) at the fixed $J_{\mathrm{rung}}=1.0$. Furthermore, extrapolating them using Eq. (14), we show the resulting scaling dimension in Fig. 7 on the phase boundary. Thus, we confirm $x\simeq 3/8$ in the weak-coupling region ($J_{\mathrm{rung}}<1.5$).

For $x=1$ case with momentum $q=0$ and spin $S=0,1,2$, we obtain

$$\Delta E_i(S=2) \simeq \frac{2\pi v}{L}\left(x_i - \frac{1}{\ln L}\right), \tag{18}$$

and

$$\Delta E_i(S=1) \simeq \frac{2\pi v}{L}\left(x_i + \frac{1}{\ln L}\right), \tag{19}$$

and

$$\Delta E_i(S=0) \simeq \frac{2\pi v}{L}\left(x_i + 2\frac{1}{\ln L}\right). \tag{20}$$

Thus we can remove logarithmic corrections,

$$x_i \simeq \frac{L}{4\pi v}[\Delta E_i(S=2) + \Delta E_i(S=1)]. \tag{21}$$

As before, in Fig. 9, we show the size dependence of the scaling dimension, removing logarithmic corrections with Eq. (21) at the fixed $J_{\mathrm{rung}}=1.0$. Extrapolating them using Eq. (14), we show the resulting scaling dimension in Fig. 7 on the phase boundary. We confirm $x\simeq 1$ in the weak-coupling region ($J_{\mathrm{rung}}<1.5$).

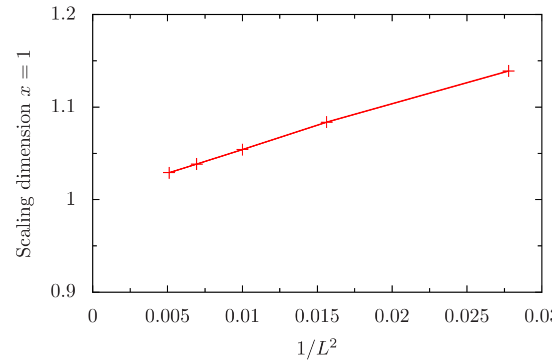

FIG. 9. (Color online) The size dependence of the scaling dimension $x=1$ at $J_{\mathrm{rung}}=1.0$ after logarithmic corrections removed. Extrapolated value is $x\sim 1.0052$.

IV. SUMMARY AND CONCLUSIONS

In this paper, we have studied the $S=\frac{1}{2}$ two-leg spin ladder systems with four-spin interactions. We numerically determined the phase boundary between the rung-singlet phase and the staggered dimer ordered phase using the twisted boundary-condition method. And we confirmed the universality class of this phase transition combining the CFT and the numerical diagonalization.

Calculating the effective central charge $\tilde{c}$, we found $\tilde{c}\simeq 3/2$ for small J_{rung} and small J_4, and $\tilde{c}\simeq 0$ for large J_{rung} and large J_4. This means that the second-order phase transition occurs in the weak-coupling region and that the first-order phase transition occurs in the strong-coupling region.

And we calculated scaling dimensions x since we cannot decide a universality class from the central charge only. Since this model has the SU(2) symmetry, there are logarithmic corrections. Removing the logarithmic corrections, we obtained $x\simeq 3/8$ and $x\simeq 1$ in the weak-coupling region numerically. As a result, we conclude that the phase transition between the rung-singlet phase and the staggered dimer phase in the weak-coupling region is of the second order which is described by the $k=2$ SU(2) WZW model. This is consistent with Gritsev's prediction from an effective-field theoretical approach.[22] This universality class belongs to the same universality class as Takhtajan-Babujian point of $S=1$ one dimensional bilinear-biquadratic model.[50–53] And this has been found in a $S=\frac{1}{2}$ two-leg ladder system with four-spin cyclic exchange interactions.[41,54]

It is a future task to study what happens in the region where the interaction is sufficiently strong, and to determine the global phase diagram.

ACKNOWLEDGMENTS

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