Ground state phase diagram of an $S = \frac{1}{2}$ two-leg Heisenberg spin ladder system with negative four-spin interaction

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We investigate the ground-state phase diagram and critical properties of the $S = 1/2$ two-leg Heisenberg spin ladder system with a negative four-spin interaction using a numerical exact diagonalization method. Using the perturbation theory in the strong negative rung-coupling limit, we derive an $S = 1$ bilinear-biquadratic chain as an effective model. We discuss the ground-state phase diagram in this limit. Next we numerically determine a phase boundary between the rung singlet phase and the columnar dimer (CD) phase by the phenomenological renormalization group method, and one between the CD phase and the Haldane phase by the twisted boundary condition method. We confirm that the phase transition between the CD phase and the Haldane phase is of second order and this universality class is described by the $k = 2$ $SU(2)$ Wess-Zumino-Novikov-Witten nonlinear σ model, calculating the central charge and scaling dimensions.

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I. INTRODUCTION

Quantum phase transitions and quantum critical phenomena are very interesting subjects in condensed matter, statistical, and mathematical physics.[1] Low-dimensional quantum systems need not have ordered ground states because of the effects of quantum fluctuations. Spin chains and spin ladders are typical systems having such ground states. In particular, quantum spin ladders have been studied from both theoretical and experimental points of view.[2] Spin-ladder systems have rich physics related to the Haldane conjecture,[3] high-pressure-induced high-T$_c$ superconductivity,[4] and spin-gap problems.[5]

In recent years, multiple spin exchange interactions have attracted attention. It is well known that these types of interaction have played an important role for magnetism in solid ^{3}He for a long time.[6–8] And it is expected that these interactions play a significant role in other systems, for example, ^{3}He absorbed on graphite,[9] and Wigner crystal.[10]

These multispin interactions are derived from several origins, for example, the direct exchange process in solid ^{3}He, higher-order perturbation in the strong-coupling limit of the half-filled Hubbard model,[11,12] the effects of phonons,[13] orbital degeneracy,[14] and effective models for higher spin systems using composite spins.[15] The three-body cyclic exchange interactions can be rewritten as a summation of two-body interactions. Thus, the smallest-order many-body interactions that we note are four-body terms. The existence of four-spin (cyclic) exchange interactions is reported in inelastic neutron scattering and Raman scattering experiments for several copper oxides,[16–23] for example, a two-dimensional square lattice La_2CuO_4, which is a high-T$_c$ superconductor parent compound, and a spin ladder compound, $La_6Ca_8Cu_{24}O_{41}$.

In general, because general multiple (ring) spin exchange terms have complex forms represented by many spin operators, it is difficult to understand their effects. Therefore, it is better to investigate a simpler Hamiltonian first. In this paper, we study an $S = \frac{1}{2}$ two-leg Heisenberg spin ladder system with a four-spin exchange interaction which is described as the following Hamiltonian:

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

where $\mathbf{S}_{\alpha,j}$ is an $S = \frac{1}{2}$ spin operator at a site (α, j), where α is the index of spin chains (1 or 2), j is a site number and we set $J_{\rm leg} = 1$ and $J_4 \leqslant 0$, and L is the length of the ladder in the leg direction. This is one of the simplest models, which has four spin interactions (see Fig. 1).

Previously, a ground-state phase diagram and criticalities in a $J_{\rm rung} > 0$ and $J_4 > 0$ regime, for the case of not large $J_{\rm rung}, J_4$, were discussed.[24] In this regime there are two phases; one is a rung-singlet (RS) phase which has a unique gapped ground state, and the other is a staggered dimer (SD) ordered phase which has twofold degenerate gapped ground states. We determined the phase boundary using the twisted boundary condition method and confirmed the universality class of this second-order transition calculating the central charge $c \simeq \frac{3}{2}$ and scaling dimensions $x \simeq \frac{3}{8}, 1$ numerically. The phase transition between these phases is of second order, which is described by the $k = 2$ $SU(2)$ Wess-Zumino-Novikov-Witten nonlinear σ model (WZNW model) in the weak-coupling regime and of first order in the relatively strong-coupling regime.

There has been some research for some models with $J_4 > 0$ and other types of four-spin exchange terms related to the ring exchange,[25–29] spin-orbital model,[30] and exact solvable models.[31–33] On the other hand, negative J_4 cases have hardly been studied. We can get these negative four-spin interactions to consider effects of optical phonons and a Hubbard ladder with additional π flux in each plaquette. Nersesyan and Tsvelik predicted that the dimerization occurs in the $J_4 < 0$ regime.[13] Recently, Takayoshi and Sato discussed a phase diagram of Eq. (1) in the weak-coupling regime using the bosonization technique.[34] They proposed that there are four phases in the

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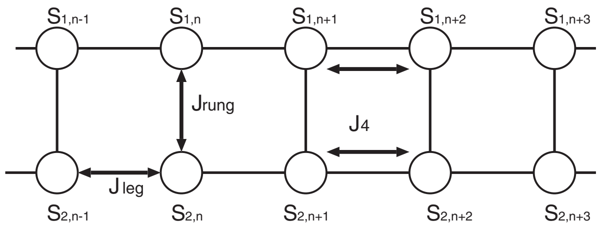

FIG. 1. Schematic structure of the $S = \frac{1}{2}$ two-leg spin ladder system with a four-spin interaction in Eq. (1).

$|J_{\mathrm{rung}}|,|J_4| \ll 1$ regime: the RS phase, the columnar dimer (CD) phase, the SD ordered phase, and the Haldane phase. In their proposal, the phase transitions between the RS and the CD phases and between the CD and the Haldane phases are of second order and belong to the two-dimensional Ising universality class. And a transition between the RS and the SD ordered phases and between the Haldane and the CD phases are of first- or second order and are described by $c = \frac{3}{2}$ conformal field theory (CFT).

In the $J_4 = 0$ case, the model (1) becomes a simple two-leg spin ladder Hamiltonian. We well know the ground-state phase diagram. The ground state is the RS phase for $J_{\mathrm{rung}} > 0$, and it is the Haldane phase for $J_{\mathrm{rung}} < 0$. Each phase is unique and gapful. We can distinguish these phases by the hidden $Z_2 \times Z_2$ symmetry. The phase transition at $J_{\mathrm{rung}} = 0$ is the Gaussian transition with the central charge $c = 2(=1+1)$ because the system consists of two decoupled spin chains.[35,36] From these previous results, we expect that there are three phases for the $J_4 < 0$ case: the RS phase (see Fig. 2), the CD phase (see Fig. 3), and the Haldane phase.

The aim of this paper is to determine the ground-state phase diagram of Eq. (1) and to discuss critical properties for a negative J_4 regime using numerical calculations and the perturbation theory.

The organization of this paper is as follows. In the next section, we discuss the strong negative rung-coupling limit $J_{\mathrm{rung}} \to -\infty$. We derive an $\hat{S} = 1$ bilinear-biquadratic model as an effective model. We briefly review this effective model and discuss a ground-state phase diagram in this limit. In Sec. III, we determine the phase boundary between the RS phase and the CD phase using the phenomenological renormalization group (PRG) method. Next we determine a phase boundary between the CD phase and the Haldane phase using the twisted boundary condition method, and we study the critical properties of the CD-Haldane transition using the CFT with the numerical diagonalization analysis. The last section is the summary and discussion.

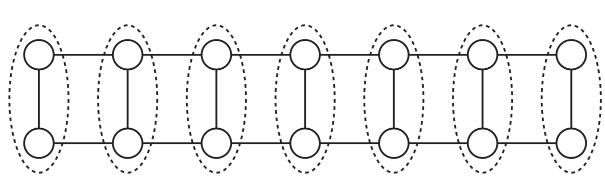

FIG. 2. A schematic picture of the rung-singlet state. Two spins enclosed by a dotted line represent a singlet state $\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$.

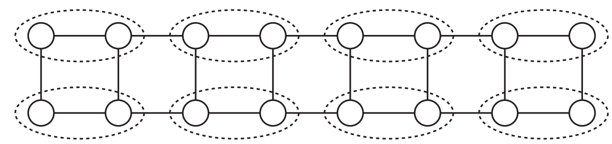

FIG. 3. A schematic picture of the columnar-dimer state. Two spins enclosed by a dotted line represent a singlet state.

II. PERTURBATION THEORY FROM THE STRONG NEGATIVE RUNG-COUPLING LIMIT

Here we investigate the strong negative rung-coupling limit $J_{\mathrm{rung}} \to -\infty$. There are two spins on each rung, coupled as $J_{\mathrm{rung}}\mathbf{S}_{1,j} \cdot \mathbf{S}_{2,j}$. In the $J_{\mathrm{rung}} \to -\infty$ limit, we can consider that there are $\hat{S} = 1$ pseudospins on each rung, $\hat{\mathbf{S}}_j = \mathbf{S}_{1,j} + \mathbf{S}_{2,j}$. This pseudospin basis $(|1\rangle,|0\rangle,|-1\rangle)$ is a triplet in the original $S = \frac{1}{2}$ basis $(|\uparrow\rangle_1|\uparrow\rangle_2,\ \frac{1}{\sqrt{2}}(|\uparrow\rangle_1|\downarrow\rangle_2 - |\downarrow\rangle_1|\uparrow\rangle_2),\ |\downarrow\rangle_1|\downarrow\rangle_2)$. Using this basis, we can derive an effective $\hat{S} = 1$ Hamiltonian from the first-order perturbation theory. This $\hat{S} = 1$ effective Hamiltonian is the following:

$$\hat{\mathcal{H}} = \left(\frac{1}{2} + \frac{1}{8}J_4\right)\sum_{j=1}^{L}\hat{\mathbf{S}}_j \cdot \hat{\mathbf{S}}_{j+1} + \frac{1}{4}J_4\sum_{j=1}^{L}(\hat{\mathbf{S}}_j \cdot \hat{\mathbf{S}}_{j+1})^2 + \frac{5}{16}J_4 L, \tag{2}$$

where a first $1/2$ term arises from the J_{leg} term. This Hamiltonian is known as the $\hat{S} = 1$ bilinear-biquadratic model. This is traditionally parametrized as follows:

$$\mathcal{H} = \cos\theta\sum_{j=1}^{L}\hat{\mathbf{S}}_j \cdot \hat{\mathbf{S}}_{j+1} + \sin\theta\sum_{j=1}^{L}(\hat{\mathbf{S}}_j \cdot \hat{\mathbf{S}}_{j+1})^2. \tag{3}$$

The ground-state phase diagram of this model is well known, and there are some exact solvable points. There are four phases as follows. The dimer phase is in $-3\pi/4 < \theta < -\pi/4$, which is gapful and twofold degenerate. This degeneracy is related to the spontaneously one-site translational symmetry breaking. The Haldane phase is in $-\pi/4 < \theta < \pi/4$, which is gapful and a unique ground state which is called the valence-bond-solid (VBS) state.[3,37] The trimerized massless phase is in $\pi/4 < \theta < \pi/2$.[38] The ferromagnetic phase is in $\pi/2 < \theta < 3\pi/2$. There are some exact solvable points in this model. At $\theta = \pi/4$, this model is solved by the Bethe ansatz.[39] This point is massless, and the soft modes appear at wave numbers $q = 0,\pm 2\pi/3$. This model has an $SU(3)$ symmetry on this point and is described by the $k = 1$ $SU(3)$ WZNW model.[40]

At $\theta = \arctan(\frac{1}{3})$, this model has an exact VBS state as the ground state.[37] It is proved that the system has a finite excitation gap at this point. At $\theta = -\pi/4$, this model is solved by the Bethe ansatz.[41] This point is massless, and the soft modes appear at wave numbers $q = 0,\pi$. Thus, the phase transition between the Haldane phase and the dimer phase is of second order, which is described by $c = \frac{3}{2}$ CFT, as the $k = 2$ $SU(2)$ WZNW model.[40,42] This has been confirmed by the Bethe ansatz.[43] At $\theta = 3\pi/4$, this model is solved by Haldane.[44] This point is in the ferromagnetic phase. At $\theta = -\pi/2$, this model is solved by Barber, Batchelor, and Klümper using the Bethe ansatz.[45,46] On this point the ground state is gapful and twofold degenerate and has an $SU(3)$ symmetry.[40] This ground state is the dimer state.

In this effective model (2), the ground-state phase diagram is simple. The correspondence between θ and J_4 is as follows: $J_4 = \infty \leftrightarrow \theta = \arctan(2)$, $J_4 = 0 \leftrightarrow \theta = 0$, and $J_4 = -\infty \leftrightarrow \theta = \arctan(-2)$. So the trimerized massless phase is in $J_4 > 4$, the Haldane phase is in $-\frac{4}{3} < J_4 < 4$, and the dimer phase is in $J_4 < -\frac{4}{3}$. Now we pay attention to the $J_4 < 0$ case. In this case, two phases appear: the Haldane phase in $-\frac{4}{3} < J_4$ and the dimer phase in $J_4 < -\frac{4}{3}$. A phase transition between the Haldane and the dimer phases occurs at $J_4 = -\frac{4}{3}$, which is an exact solvable point. This is a second-order phase transition which is described by $c = \frac{3}{2}$ CFT as the $k = 2$ $SU(2)$ WZNW model. There exists another exact solvable point at $\theta = -\pi/2$ which corresponds to the $J_4 = -4$ case. The ground state at this point is the dimer state in the $\hat{S} = 1$ case, which smoothly connects to the CD state in the original $S = \frac{1}{2}$ case. On this point, the original ladder Hamiltonian has an additional symmetry. We can show that a staggered rung dimer operator $\sum_j (-1)^j \mathbf{S}_{1,j} \cdot \mathbf{S}_{2,j}$ commutes with the Hamiltonian (1) with $J_{\text{leg}} = 1$, $J_{\text{rung}} = 0$, and $J_4 = -4$.

Then we can obtain the ground-state phase diagram of the original spin ladder system in the strong negative rung-coupling limit as follows. The Haldane phase is in $-\frac{4}{3} < J_4 < 0$ and the CD phase is in $J_4 < -\frac{4}{3}$, and this phase transition at $J_4 = -\frac{4}{3}$ is of second order.

III. NUMERICAL ANALYSIS

In this section, we determine transition points and the universality class. We numerically analyze the $S = \frac{1}{2}$ two-leg Heisenberg spin ladder system with a negative four-spin interaction (1). We use results by the numerical exact diagonalization up to $L = 16$ (the number of sites, $N = 32$) with the periodic boundary condition (PBC) and the twisted boundary condition (TBC).

A. Haldane–columnar dimer transition

In this section, we study the phase transition between the Haldane phase and the CD phase. This CD phase is smoothly connected to the $\hat{S} = 1$ dimer phase in the $\hat{S} = 1$ bilinear-biquadratic model (2). So we expect that a direct transition occurs in a (J_{rung}, J_4) parameter space. Because of the bosonization study for the weak-coupling limit[34] and discussions of the strong negative J_{rung} limit in Sec. II, this phase boundary starts from $(J_{\text{rung}}, J_4) = (0,0)$ to $(J_{\text{rung}}, J_4) = (-\infty, -\frac{4}{3})$ in the $J_{\text{rung}} \leqslant 0$ and $J_4 \leqslant 0$ region. The start point and the end point are gapless. And the phase transition for the corresponding effective $\hat{S} = 1$ model is the integrable Takhtajan-Babujian model,[41] which is described by the $k = 2$ $SU(2)$ WZNW model.[40,42,43] So we expect that this Haldane-CD phase transition belongs to the same universality class. Then we can use the TBC method[47,48] in order to determine this phase boundary. The TBC is as follows:

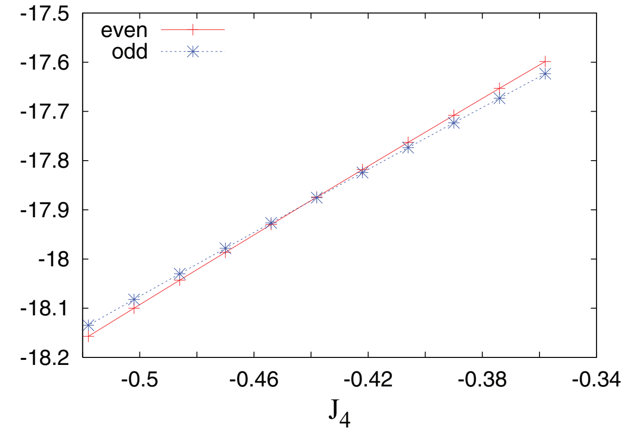

FIG. 4. (Color online) Level crossing in the system under the twisted boundary condition for $L = 16$ ($N = 32$) at $J_{\text{rung}} = -1.0$ with the absolute unit $J_{\text{leg}} = 1$. The symbol $+$ is the lowest energy with $S_T^z = 0$, $P_l^* = 1$, and $P_r^* = 1$. The symbol $*$ is the lowest energy with $S_T^z = 0$, $P_l^* = -1$, and $P_r^* = 1$.

$$S^{\pm}_{\alpha,j+L} = -S^{\pm}_{\alpha,j}, \quad S^z_{\alpha,j+L} = S^z_{\alpha,j}, \tag{4}$$

where $\alpha = 1,2$ denotes the chain index and $L(=N/2)$ is the system size. Here we define quantum numbers under this TBC. We define a leg parity P_1^* which is related to the inversion symmetry along the leg direction $S^{\beta}_{\alpha,j} \leftrightarrow S^{\beta}_{\alpha,L-j+1}$ where $\alpha = 1,2$ and $\beta = x,y,z$. Next we define a rung parity P_r which is related to the inversion symmetry along the rung direction $S^{\beta}_{1,j} \leftrightarrow S^{\beta}_{2,j}$. The TBC does not affect this rung parity. We define $S_T^z \equiv \sum_{\alpha,j} S^z_{\alpha,j}$ as a total magnetization. The TBC does not affect the total magnetization.

We can detect phase-transition points using level crossing points between two lowest energy eigenvalues with quantum numbers $S_T^z = 0$, $P_1^* = 1$, $P_r = 1$ with the TBC and the lowest one with $S_T^z = 0$, $P_1^* = -1$, $P_r = 1$ with the TBC.[47,48] We show numerical results for $L = 6,8,10,12,16$ ($N = 12,16,20,24,28,32$) using the exact diagonalization. In Fig. 4, we show the level crossing for $L = 16$ and $J_{\text{rung}} = -1.0$. These crossing points depend on the system size. In Fig. 5, we show the size dependence of crossing points for $J_{\text{rung}} = -1.0$. Because there are finite size corrections from the irrelevant field, we need to extrapolate crossing points. These leading corrections come from the irrelevant field with the scaling dimension $x = 4$ such as $L_{-2}\bar{L}_{-2}\mathbf{1}$, $L_{-2}^2\mathbf{1}$, and $\bar{L}_{-2}^2\mathbf{1}$,[50,51] where $L_{-n}, \bar{L}_{-n}$ are generators of the conformal transformation.[52] These fields are related to the lattice effect not included in the continuum theory. We extrapolate crossing points as follows:

$$J_4^{\text{cross}}(L) = J_4^{\text{cross}} + a\frac{1}{L^2} + b\frac{1}{L^4} + (\text{higher-order terms}), \tag{5}$$

where we neglect higher-order terms. We present the phase boundary (level crossing points) in Fig. 6.

Next we confirm the universality class of this Haldane-CD transition, and we justify this type of level crossing method with the TBC to determine this phase boundary.

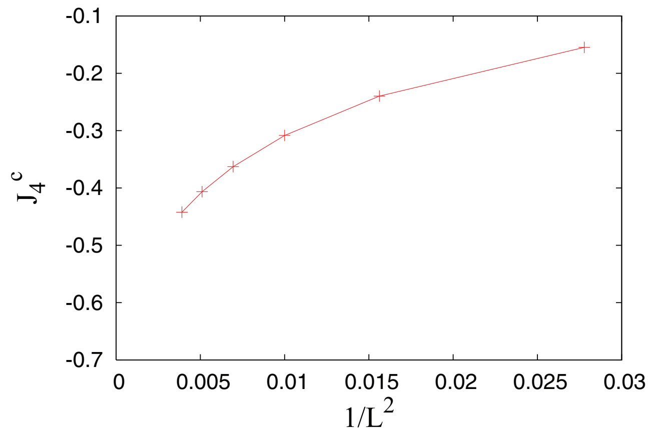

FIG. 5. (Color online) Size dependence of crossing points for $J_{\mathrm{rung}} = -1.0$ as a function of $1/L^2$ with the absolute unit $J_{\mathrm{leg}} = 1$.

This phase transition is expected to be of second order. Because it is believed that ground states of one-dimensional quantum systems on critical points are invariant for conformal transformations, we can determine the universality class using the CFT.[52]

In the CFT, the leading finite size correction of the ground-state energy on a critical point with the PBC has the following form:

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

where L is the system size, $E_g(L)$ is the ground-state energy for a finite system size, ε is the energy per unit length in the infinite system limit, v is the velocity of the system, and c is the cental charge.[42,53] By the way, we can obtain this central charge from the entropy profile of finite systems.[54] However, we need very large systems in order to obtain accurate values from the entropy numerically.[55] So we obtain the central charge from Eq. (6).

Unfortunately, there are logarithmic corrections for the ground-state energy of finite size systems on critical points because of the marginally irrelevant field as follows:

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

where b is constant. Fortunately, it is proved that there are no $O(\frac{1}{\ln L})$, $O(\frac{1}{(\ln L)^2})$ terms.[56–58] In this paper, we neglect $O(\frac{1}{(\ln L)^3})$ and higher-order terms, since these corrections are expected to be small enough.

To obtain the central charge, we need the value of the velocity. We can determine the velocity v by the current field with the scaling dimension $x = 1$ and the wave number $q = 2\pi/L$,

$$v = \lim_{L\to\infty} \frac{L}{2\pi}\left(E\left(q = \frac{2\pi}{L}\right) - E_g\right). \tag{8}$$

The finite system velocity is

$$v(L) = \frac{L}{2\pi}\left[E\left(q = \frac{2\pi}{L}\right) - E_g\right]. \tag{9}$$

Since there are no logarithmic corrections in a current-current correlation,[59] we can extrapolate the velocity as follows:

$$v(L) = v + a\frac{1}{L^2} + b\frac{1}{L^4} + \text{higher-order terms}, \tag{10}$$

where a and b are fitting parameters. In Fig. 7, we show the central charge on the crossing line obtained with the TBC. We can see the central charge decreasing from $c = 2$ to $c = \frac{3}{2}$. At $(J_{\mathrm{rung}}, J_4) = (0,0)$, the system consists of two independent antiferromagnetic Heisenberg chains and has $SU(2) \times SU(2)$ symmetry. In this case, we know the exact solution by Bethe ansatz. This system is described by the two independent Tomonaga-Luttinger (TL) liquids. One TL

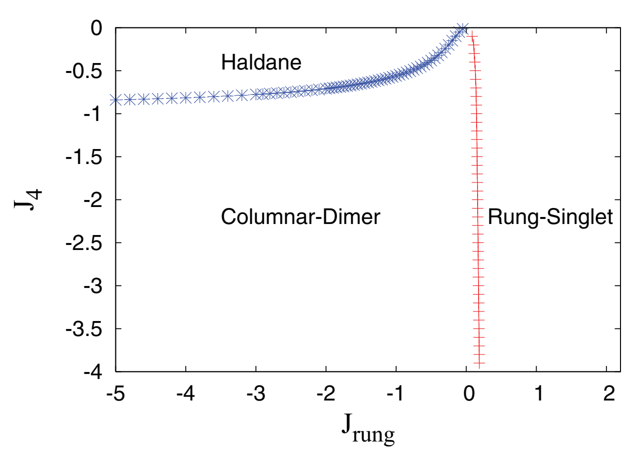

FIG. 6. (Color online) The ground-state phase diagram of the spin ladder system (1) for $J_4 < 0$ with the absolute unit $J_{\mathrm{leg}} = 1$, which is obtained from $L = 6,8,10,12,14,16$. The phase boundary between the rung-singlet phase and the columnar-dimer phase is determined by the PRG method and this is a second-order phase transition which belongs to the two-dimensional Ising universality class. The phase boundary between the Haldane phase and the columnar-dimer phase is determined by the twisted boundary condition method and is a second-order phase transition which is described by $c = \frac{3}{2}$ CFT.

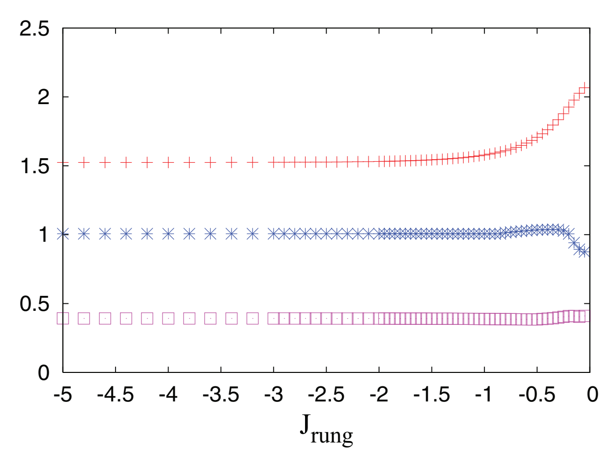

FIG. 7. (Color online) The central charge (+) and scaling dimensions (×), (□) on the phase transition line. Scaling dimensions are extrapolated after logarithmic corrections removed. ∗ denotes the scaling dimension $x = 1$ for a $q = 0$ mode; □ denotes the scaling dimension $x = \frac{3}{8}$ for a $q = \pi$ mode. Here we set the absolute unit $J_{\mathrm{leg}} = 1$.

liquid has the central charge $c = 1$, so this system has $c = 2(=1+1)$. This point is a multicritical point among the RS phase, the SD phase, the Haldane phase, and the CD phase. Now the central charge is expected to be $c = \frac{3}{2}$ on the transition line between the Haldane phase and the CD phase. At the end point $(J_{\text{rung}}, J_4) = (-\infty, -\frac{4}{3})$, we know the central charge $c = \frac{3}{2}$ from the $\hat{S} = 1$ effective model, which is the exact solvable model, called the Takhtajan-Babujian model.[41] We can expect that the Haldane-CD transition connects to the strong-coupling limit continuously. It is consistent with Zamolodchikov's c theorem[60] that the central charge decreases.

Unfortunately, we cannot completely determine the universality class of the phase transition only by the central charge. Using non-Abelian bosonization,[61,62] we can obtain a relation between the central charge and the topological coupling constant k, called the level, of the $SU(2)$ WZNW model as follows:

$$c = \frac{3k}{k+2}. \tag{11}$$

Combining the symmetry of this system and this relation, this phase transition with the central charge $c = \frac{3}{2}$ is described by the $k = 2$ $SU(2)$ WZNW model.[40,42]

Usually, the universality class is classified by the set of critical exponents. Here we consider scaling dimensions which are related to energy gaps of the finite size system, because scaling dimensions are related to critical exponents. The scaling dimension x of a primary field in the Kac-Moody algebra can be completely classified by the left and right spins $s_L = s_R = 0, 1/2, \ldots, k/2$,

$$x = \frac{2s_L(s_L+1)}{k+2}, \tag{12}$$

where k is a level of the WZNW model.[62] Now we have $s_L = s_R = 0, \frac{1}{2}, 1$ because of $k = 2$. Thus, the $k = 2$ $SU(2)$ WZNW model has two relevant primary fields. One has $s_L = s_R = \frac{1}{2}$; then the scaling dimension is $x = \frac{3}{8}$ with the total spin $S = 0,1$. Since the operators with the half odd integer s_L are odd under one-site translation, they correspond to states with momentum $q = \pi$. Another has $s_L = s_R = 1$; then the scaling dimension is $x = 1$ with the total spin $S = 0,1,2$. Since the operators with the integer s_L are even under one-site translation, they correspond to states with momentum $q = 0$.[58] In the CFT, scaling dimensions are related to excitation energy in the finite size system with the PBC,[49]

$$\Delta E_i = E_i - E_g \simeq \frac{2\pi v}{L} x_i, \tag{13}$$

where E_i is the excitation energy, x_i is the scaling dimension, and i is an index characterizing the excitation state. Unfortunately, there exist logarithmic corrections because of marginal operators.[58,63] A leading logarithmic correction in the $k = 2$ $SU(2)$ WZNW model is the following form:[58]

$$\Delta E_i \simeq \frac{2\pi v}{L}\left(x_i - \frac{1}{2}\frac{S(S+1) - s_R(s_R+1) - s_L(s_L+1)}{\ln L}\right). \tag{14}$$

Using this formula, we can remove leading logarithmic corrections by selecting excitations with appropriate quantum numbers. After we remove logarithmic corrections, there are other finite size corrections from the irrelevant field with $x = 4$, $L_{-2}\bar{L}_{-2}\mathbf{1}$, $L_{-2}^2\mathbf{1}$, and $\bar{L}_{-2}^2\mathbf{1}$.[50,51] To remove effects of this irrelevant field, we can use the following extrapolation formula:

$$x_i(L) = x_i + a\frac{1}{L^2} + b\frac{1}{L^4} + \text{higher-order terms}, \tag{15}$$

where a and b are nonuniversal coefficients, and we neglect higher-order correction terms here.

For the $x = \frac{3}{8}$ case with momentum $q = \pi$ and spin $s = 0,1$, we obtain the following excitation energies from Eq. (14):

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

and

$$\Delta E_i(S=0) \simeq \frac{2\pi v}{L}\left(x_i + \frac{3}{4}\frac{1}{\ln L}\right). \tag{17}$$

Using these formulas, we can remove the leading logarithmic corrections as follows:

$$x_i \simeq \frac{L}{8\pi v}[3\Delta E_i(S=1) + \Delta E_i(S=0)]. \tag{18}$$

In Fig. 7, we show the scaling dimension $x \simeq \frac{3}{8}$ on the phase transition points after extrapolation by Eq. (15).

Next for the $x = 1$ case with momentum $q = 0$ and spin $s = 0,1,2$, we obtain the following excitation energies from Eq. (14):

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

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

and

$$\Delta E_i(S=0) \simeq \frac{2\pi v}{L}\left(x_i + 2\frac{1}{\ln L}\right). \tag{21}$$

Using these formulas, we can remove the leading logarithmic corrections as follows:

$$x_i \simeq \frac{L}{4\pi v}[\Delta E_i(S=2) + \Delta E_i(S=1)]. \tag{22}$$

In Fig. 7, we show the scaling dimension $x \simeq 1$ on the phase transition points after extrapolation by Eq. (15). We confirm good agreement with $c = \frac{3}{2}$, $x = \frac{3}{8}$, and $x = 1$ on the transition line.

B. Rung singlet–columnar dimer transition

In this section, we study the phase transition between the RS phase and the CD phase. In the CD phase, ground states are gapful and twofold degenerate because of the spontaneously broken Z_2 symmetry which is related to the one-site translational symmetry. In the RS phase, the ground state is unique and gapful. So this phase transition is expected to be of second order and belongs to the two-dimensional Ising universality class.[34] We can determine this type of phase transition point using the PRG method.[64] In this method, we

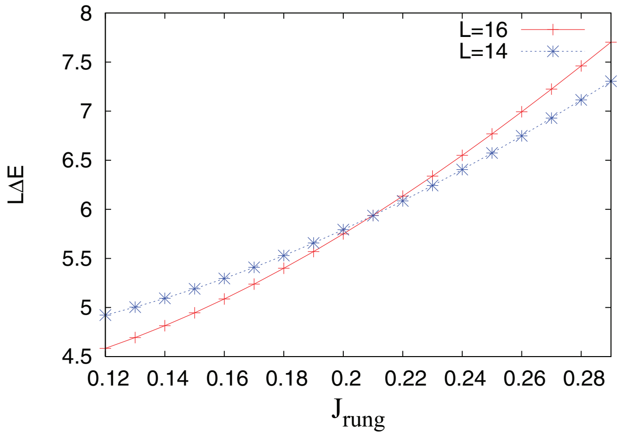

FIG. 8. (Color online) The level crossing of the scaled gap $L\Delta E$ with $J_4 = -1.1$ between $L = 14$ and $L = 16$ with the absolute unit $J_{\mathrm{leg}} = 1$.

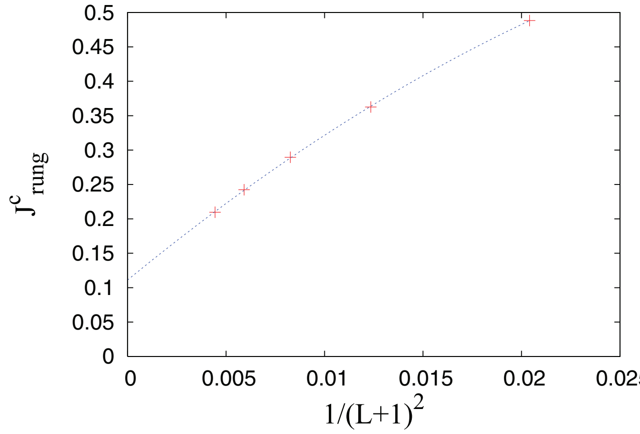

FIG. 9. (Color online) Size dependence of crossing points of the scaled gap for $J_4 = -1.1$ as a function of $1/(L+1)^2$ with the absolute unit $J_{\mathrm{leg}} = 1$.

see the scaled gap $L\Delta E(L)$, for which the excited state is degenerate to the ground state in the thermodynamic limit. This energy gap for finite systems behaves as $\Delta E \propto \exp[-L/\xi]$ for $L \to \infty$ in the CD phase, where ξ is a correlation length. On the other hand, in the RS phase, ΔE remains finite in the thermodynamic limit. Thus, this scaled gap $L\Delta E(L)$ increases with the system size L in the RS phase ($J_{\mathrm{rung}} > J^c_{\mathrm{rung}}$) and decreases in the CD phase ($J_{\mathrm{rung}} < J^c_{\mathrm{rung}}$), where J^c_{rung} means the critical value of J_{rung} at the RS-CD transition. We use the following equation to determine the RS-CD transition point:

$$
\begin{aligned}
&L\Delta E\big(L, J^c_{\mathrm{rung}}(L,L+2), J_4\big)\\
&\quad = (L+2)\Delta E\big(L+2, J^c_{\mathrm{rung}}(L,L+2), J_4\big).
\end{aligned} \tag{23}
$$

We show scaled gaps for $J_4 = -1.1$ and $L = 14,16$ in Fig. 8. These crossing points depend on the system size. So we need to extrapolate crossing points of scale gaps in the following equation:

$$
\begin{aligned}
&J^c_{\mathrm{rung}}(L,L+2)\\
&\quad = J^c_{\mathrm{rung}} + a\frac{1}{(L+1)^2} + b\frac{1}{(L+1)^4} + \text{higher order},
\end{aligned} \tag{24}
$$

where we neglect higher-order terms. Here we show the size dependence of crossing points for $J_4 = -1.1$ in Fig. 9. We can apply the same procedure for each J_4. Then we can obtain the phase boundary between the RS phase and the CD phase. This phase boundary is shown in Fig. 6.

IV. SUMMARY AND DISCUSSION

In this paper, we have studied the $S = \frac{1}{2}$ two-leg spin ladder systems with the negative four-spin interaction. The expected phases are the RS, the CD, and the Haldane phases. We have determined the ground-state phase diagram using the TBC method and the PRG method numerically.

First, we considered the strong negative rung-coupling limit. We derived the $\hat{S} = 1$ effective model. Then we obtained a part of the phase diagram. In this limit, there are the Haldane phase and the $\hat{S} = 1$ dimer phase, which corresponds to the $S = \frac{1}{2}$ CD phase. The phase transition between these two phases is of second order, which is described by the $k = 2$ $SU(2)$ WZNW model.

We numerically determined the phase boundary between the Haldane phase and the CD phase using the twisted boundary condition method. And we confirmed the universality class of this phase transition by combining the CFT and the numerical diagonalization. We obtained the central charge $c \simeq 2$ at $(J_{\mathrm{rung}}, J_4) = (0,0)$ and $c \simeq \frac{3}{2}$ on this transition line. This means that the phase transition is of second order between these two phases in this ladder system, and this phase transition connects from $(J_{\mathrm{rung}}, J_4) = (0,0)$ to $(J_{\mathrm{rung}}, J_4) = (-\infty, -\frac{4}{3})$ smoothly.

And we numerically calculated scaling dimensions x because we cannot completely determine the universality class from the central charge only. We expected that this universality class would be the $k = 2$ WZNW model. This universality class has logarithmic corrections, because this model has $SU(2)$ symmetry. Assuming this universality class, we removed logarithmic corrections. We obtained $x \simeq \frac{3}{8}$ and $x \simeq 1$ on this transition line. As a result, we conclude that this phase transition is of second order, which is described by the $k = 2$ $SU(2)$ WZNW model. This is consistent to Takayoshi and Sato's prediction by a bosonization approach.[34] Our results suggest that this phase transition smoothly connects to the strong negative rung-coupling limit which is the Takhtajan-Babujian point of the $S = 1$ bilinear-biquadratic chain.

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[1]S. Sachdev, *Quantum Phase Transitions*, 2nd ed. (Cambridge University Press, Cambridge, 2011).
[2]E. Dagotto and T. M. Rice, Science **271**, 618 (1996); E. Dagotto, Rep. Prog. Phys. **62**, 1525 (1999).
[3]F. D. M. Haldane, Phys. Lett. A **93**, 464 (1983); Phys. Rev. Lett. **50**, 1153 (1983).
[4]M. Uehara, T. Nagata, J. Akimitsu, H. Takahashi, N. Môri, and K. Kinoshita, J. Phys. Soc. Jpn. **65**, 2764 (1996).
[5]A. N. Vasilév, M. M. Markina, and E. A. Popova, Low Temp. Phys. **31**, 203 (2005).
[6]D. J. Thouless, Proc. Phys. Soc. London **86**, 893 (1965).
[7]M. Roger, J. H. Hetherington, and J. M. Delrieu, Rev. Mod. Phys. **55**, 1 (1983).
[8]D. D. Osheroff, J. Low. Temp. Phys. **87**, 297 (1992).
[9]H. Fukuyama, J. Phys. Soc. Jpn. **77**, 111013 (2008).
[10]S. Chakravarty, S. Kivelson, C. Nayak, and K. Voelker, Philos. Mag. B **79**, 859 (1999).
[11]M. Takahashi, J. Phys. C: Solid State Phys. **10**, 1289 (1977).
[12]A. H. MacDonald, S. M. Girvin, and D. Yoshioka, Phys. Rev. B **37**, 9753 (1988).
[13]A. A. Nersesyan and A. M. Tsvelik, Phys. Rev. Lett. **78**, 3939 (1997).
[14]I. Kugel and D. I. Khomskii, Zh. Eksp. Teor. Fiz. **64**, 1429 (1973) [Sov. Phys. JETP **37**, 725 (1973)]; Usp. Fiz. Nauk **136**, 621 (1982) [Sov. Phys. Usp. **25**, 231 (1982)].
[15]J. Sólyom and J. Timonen, Phys. Rev. B **34**, 487 (1986); Ö. Legeza, G. Fáth, and J. Sölyom, *ibid*. **55**, 291 (1997).
[16]R. Coldea, S. M. Hayden, G. Aeppli, T. G. Perring, C. D. Frost, T. E. Mason, S.-W. Cheong, and Z. Fisk, Phys. Rev. Lett. **86**, 5377 (2001).
[17]M. Matsuda, K. Katsumata, R. S. Eccleston, S. Brehmer, and H.-J. Mikeska, J. Appl. Phys. **87**, 6271 (2000); Phys. Rev. B **62**, 8903 (2000).
[18]T. S. Nunner, P. Brune, T. Kopp, M. Windt, and M. Grüninger, Phys. Rev. B **66**, 180404(R) (2002).
[19]S. Notbohm, P. Ribeiro, B. Lake, D. A. Tennant, K. P. Schmidt, G. S. Uhrig, C. Hess, R. Klingeler, G. Behr, B. Buchner, M. Reehuis, R. I. Bewley, C. D. Frost, P. Manuel, and R. S. Eccleston, Phys. Rev. Lett. **98**, 027403 (2007).
[20]E. Bordas, C. de Graaf, R. Caballol, and C. J. Calzado, Phys. Rev. B **71**, 045108 (2005).
[21]B. Lake, A. M. Tsvelik, S. Notbohm, D. A. Tennant, T. G. Perring, M. Reehuis, C. Sekar, G. Krabbes, and B. Buchner, Nat. Phys. **6**, 50 (2010).
[22]Y. Mizuno, T. Tohyama, and S. Maekawa, J. Low. Temp. Phys. **117**, 389 (1999).
[23]K. P. Schmidt, A. Gössling, U. Kuhlmann, C. Thomsen, A. Löffert, C. Gross, and W. Assmus, Phys. Rev. B **72**, 094419 (2005).
[24]K. Hijii and K. Nomura, Phys. Rev. B **80**, 014426 (2009).
[25]T. Hikihara, T. Momoi, and X. Hu, Phys. Rev. Lett. **90**, 087204 (2003).
[26]A. Läuchli, G. Schmid, and M. Troyer, Phys. Rev. B **67**, 100409(R) (2003).
[27]K. P. Schmidt, H. Monien, and G. S. Uhrig, Phys. Rev. B **67**, 184413 (2003).
[28]V. Gritsev, B. Normand, and D. Baeriswyl, Phys. Rev. B **69**, 094431 (2004).
[29]K. Totsuka, P. Lecheminant, and S. Capponi, Phys. Rev. B **86**, 014435 (2012).
[30]C. Itoi, S. Qin, and I. Affleck, Phys. Rev. B **61**, 6747 (2000).
[31]A. K. Kolezhuk and H.-J. Mikeska, Int. J. Mod. Phys. B **12**, 2325 (1998); Phys. Rev. Lett. **80**, 2709 (1998).
[32]Y. Wang, Phys. Rev. B. **60**, 9236 (1999).
[33]V. Gritsev and D. Baeriswyl, J. Phys. A: Math. Gen. **36**, 12192 (2003).
[34]S. Takayoshi and M. Sato, Phys. Rev. B **82**, 214420 (2010).
[35]D. G. Shelton, A. A. Nersesyan, and A. M. Tsvelik, Phys. Rev. B **53**, 8521 (1996).
[36]K. Hijii, A. Kitazawa, and K. Nomura, Phys. Rev. B **72**, 014449 (2005).
[37]I. Affleck, T. Kennedy, E. H. Lieb, and H. Tasaki, Phys. Rev. Lett. **59**, 799 (1987); Commun. Math. Phys. **115**, 477 (1988).
[38]J. Sólyom, Phys. Rev. B **36**, 8642 (1987); K. Nomura and S. Takada, J. Phys. Soc. Jpn. **60**, 389 (1991); G. Fáth and J. Sólyom, Phys. Rev. B **44**, 11836 (1991); C. Itoi and M. H. Kato, *ibid*. **55**, 8295 (1997).
[39]G. V. Uimin, JETP Lett. **12**, 225 (1970); C. K. Lai, J. Math. Phys. **15**, 1675 (1974); B. Sutherland, Phys. Rev. B **12**, 3795 (1975).
[40]I. Affleck, Nucl. Phys. B **265**, 409 (1986).
[41]P. P. Kulish, N. Y. Reshetikhin, and E. K. Sklyanin, Lett. Math. Phys. **5**, 393 (1981); L. A. Takhtajan, Phys. Lett. A **87**, 479 (1982); H. M. Babujian, *ibid*. **90**, 479 (1982); Nucl. Phys. B **215**, 317 (1983).
[42]I. Affleck, Phys. Rev. Lett. **56**, 746 (1986).
[43]F. C. Alcaraz and M. J. Martins, J. Phys. A: Math. Gen. **21**, L381 (1988); H. Frahm, N.-C. Yu, and M. Fowler, Nucl. Phys. B **336**, 396 (1990); A. Klümper and M. T. Batchelor, J. Phys. A: Math. Gen. **23**, L189 (1990).
[44]F. D. M. Haldane, J. Phys. C **15**, L1309 (1982).
[45]M. N. Barber and M. T. Batchelor, Phys. Rev. B **40**, 4621 (1989).
[46]A. Klümper, Europhys. Lett. **9**, 815 (1989).
[47]G. Fáth and J. Sólyom, Phys. Rev. B **47**, 872 (1993).
[48]A. Kitazawa and K. Nomura, Phys. Rev. B **59**, 11358 (1999).
[49]J. L. Cardy, J. Phys. A: Math. Gen. **17**, L385 (1984).
[50]J. Cardy, Nucl. Phys. B **270**, 186 (1986).
[51]P. Reinicke, J. Phys. A **20**, 5325 (1987).
[52]P. Di Francesco, P. Mathieu, and D. Senechal, *Conformal Field Theory* (Springer-Verlag, Berlin 1999).
[53]H. W. J. Blöte, J. L. Cardy, and M. P. Nightingale, Phys. Rev. Lett. **56**, 742 (1986).
[54]G. Vidal, J. I. Latorre, E. Rico, and A. Kitaev, Phys. Rev. Lett. **90**, 227902 (2003); J. I. Latorre, E. Rico, and G. Vidal, Quantum Inf. Comp. **4**, 48 (2004); P. Calabrese and J. Cardy, J. Stat. Mech.: Theor. Exp. (2004) P06002.
[55]Ö. Legeza, J. Sólyom, L. Tincani, and R. M. Noack, Phys. Rev. Lett. **99**, 087203 (2007).
[56]J. L. Cardy, J. Phys. A: Math. Gen. **19**, L1093 (1986); **20**, 5039 (1987).
[57]A. W. W. Ludwig and J. L. Cardy, Nucl. Phys. B **285**, 687 (1987).
[58]I. Affleck, D. Gepner, H. J. Schulz, and T. Ziman, J. Phys. A: Math. Gen. **22**, 511 (1989).

[59] K. Totsuka, Y. Nishiyama, N. Hatano, and M. Suzuki, J. Phys.: Condens. Matter **7**, 4895 (1995).

[60] A. B. Zamolodchikov, Pis'ma Zh. Eksp. Teor. Fiz. **43**, 565 (1986) [JETP Lett. **43**, 730 (1986)]; Yad. Fiz. **46**, 1819 (1987) [Sov. J. Nucl. Phys. **46**, 1090 (1987)].

[61] E. Witten, Commun. Math. Phys. **92**, 455 (1984).

[62] V. G. Knizhnik and A. B. Zamolodchikov, Nucl. Phys. B **247**, 83 (1984); A. B. Zamolodchikov and V. A. Fateev, Yad. Fiz. **43**, 1031 (1986); V. G. Knizhnik and A. B. Zamolodchikov, Sov. J. Nucl. Phys. **43**, 657 (1986); D. Gepner and E. Witten, Nucl. Phys. B **278**, 493 (1986).

[63] T. Ziman and H. J. Schulz, Phys. Rev. Lett. **59**, 140 (1987).

[64] M. N. Barber, in *Phase Transition and Critical Phenomena*, edited by C. Domb and J. L. Lebowitz (Academic Press, New York, 1983), Vol. 8.