Quantum phase transitions of the asymmetric three-leg spin tube

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We investigate quantum phase transitions of the $S=\frac{1}{2}$ three-leg antiferromagnetic spin tube with asymmetric interchain (rung) exchange interactions. On the basis of the electron tube system, we propose a useful effective theory to give the global phase diagram of the asymmetric spin tube. In addition, using other effective theories we raise the reliability of the phase diagram. The density-matrix renormalization-group and the numerical diagonalization analyses show that the finite spin gap appears in a narrow region around the rung-symmetric line, in contrast to a recent paper by Nishimoto and Arikawa, [Phys. Rev. B **78**, 054421 (2008)]. The numerical calculations indicate that this global phase diagram obtained by use of the effective theories is qualitatively correct. In the gapless phase on the phase diagram, the numerical data are fitted by a finite-size scaling in the $c=1$ conformal field theory. We argue that all the phase transitions between the gapful and gapless phases belong to the Berezinskii-Kosterlitz-Thouless universality class.

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I. INTRODUCTION

The spin tube,[1–16] i.e., the spin ladder with the periodic boundary condition along the interchain (rung) direction, is one of interesting magnetic systems which is expected to exhibit some exotic phenomena due to special topology such as the carbon nanotube and the magnetic frustration. Actually, several theoretical works[6,8,9,11,12] have shown that the $S=\frac{1}{2}$ three-leg antiferromagnetic spin tube has a spin gap, in contrast to the corresponding three-leg spin ladder with the open boundary condition along the rung. Moreover, it has been predicted in the field theoretical method[13,14] that both the gapless and gapful vector-chiral long-range orders emerge in certain parameter regions of the three-leg tube in a magnetic field. Recently some candidates for the spin nanotubes have been synthesized; a three-leg tube $[(CuCl_2\,tachH)_3Cl]Cl_2$ (Ref. 1), a nine-leg tube $Na_2V_3O_7$ (Ref. 2), and a four-leg tube $Cu_2Cl_4\cdot D_8C_4SO_2$ (Refs. 3 and 4). It is therefore expected that novel, intriguing phenomena will be detected in these materials.

Let us here focus on the $S=\frac{1}{2}$ three-leg antiferromagnetic spin tube that is the simplest tube with geometrical frustration. Since the unit cell consists of three spins with $S=\frac{1}{2}$ in this tube, the Lieb-Schultz-Mattis theorem[17] suggests that the spin gap must be accompanied with at least doubly degenerate ground states. In fact, previous numerical analyses[6,11,12] have confirmed such doubly degenerate $S=0$ ground states due to the spontaneous breaking of the translational symmetry along the leg direction. The ground states have a valence-bond-type (superposition of spin-singlet pairs) order.[6,12] Here if one of the three rung coupling constants is changed, the following two models are reproduced as limiting cases: the three-leg spin ladder and the decoupled system of a single chain and a two-leg ladder. These two systems are believed to possess a gapless excitation. Therefore, the $S=\frac{1}{2}$ three-leg system, where one of the three rung couplings is varied, would undergo a quantum phase transition from the gapless state to the gapful symmetry-broken one. A recent numerical work[11] has suggested that the gapful phase is extended to a finite (although narrow) region when the rung-coupling asymmetry is introduced. Unfortunately, however, the feature of the transition was not so clarified because the system size used in Ref. 11 was too small. On the other hand, a recent density-matrix renormalization-group (DMRG) approach,[12] assuming a special power-law form of the finite-size correction, has concluded that the transition is of the first order and the system is always gapless except for the symmetric three-leg spin tube. Such a discontinuous transition, however, has not been reported so far in any realistic systems. In addition, from the viewpoint of the effective theory, the occurrence of such a transition must require a highly fine tuning of parameters. Thus the phase diagram and the critical properties of the quantum phase transitions in the three-leg spin systems are still controversial.

Motivated by the above situation, in this paper, we study the wide ground-state phase diagram and the universality classes of the quantum phase transitions in $S=\frac{1}{2}$ three-leg antiferromagnetic spin tube with the rung-coupling asymmetry. We first propose a simple effective theory to explain the quantum phase transitions between gapful and gapless phases on the basis of the Hubbard model on the tube lattice and the non-Abelian bosonization.[18–20] This effective theory enables us to draw a global phase diagram by counting the number of Fermi points. We find one gapful phase and three gapless phases in the phase diagram, and predict that the gapless phases are all described by a level-1 SU(2) Wess-Zumino-Witten (WZW) field theory,[18–20] which is a $c=1$ conformal field theory (CFT). Besides this effective theory, using other analytical strategies, we consider the strong-rung-coupling regime and the weak-rung-coupling regime

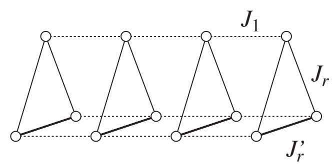

FIG. 1. Structure of the three-leg asymmetric spin tube (1).

with a strong rung distortion (i.e., asymmetry) in the phase diagram. In the former regime, two of three gapless phases are predicted by using a known effective theory.[12] In the latter regime, we prove that a finite gapless phase definitely exists.

We subsequently perform the numerical diagonalization and the DMRG calculation combined with some finite-size scaling analyses on the basis of the above effective theories. Applying the CFT approach[21–23] to our numerical data, we argue that the quantum phase transitions belong to the Berezinskii-Kosterlitz-Thouless (BKT) universality class.[24,25] A numerically quantitative phase diagram is presented and is consistent with that of the effective theories.

This paper is organized as follows. In Sec. II, we define the Hamiltonian of an asymmetric three-leg spin tube model. In Sec. III, we draw a qualitative but global ground-state phase diagram by means of an effective theory based on the half-filled Hubbard model on the tube lattice. Employing another approach based on the non-Abelian bosonization, we precisely show the existence of a gapless phase in the weak-rung-coupling regime with a strong asymmetry. Moreover, we discuss the gapful phase in the strong-rung-coupling regime. Section IV is devoted to the numerical analyses for the spin tube. We plot a scaled gap calculated by the DMRG method to confirm the phase diagram obtained by the effective theories. We further analyze the numerical data obtained in the exact diagonalization on the basis of the finite-size scaling in the $c=1$ CFT. We provide the summary and short discussions in Sec. V.

II. MODEL

We consider the $S=\frac{1}{2}$ asymmetric three-leg spin tube, shown in Fig. 1, described by the Hamiltonian

$$H = J_1\sum_{i=1}^{3}\sum_{j=1}^{L}\vec{S}_{i,j}\cdot\vec{S}_{i,j+1} + J_r\sum_{i=1}^{2}\sum_{j=1}^{L}\vec{S}_{i,j}\cdot\vec{S}_{i+1,j} + J_r'\sum_{j=1}^{L}\vec{S}_{3,j}\cdot\vec{S}_{1,j}, \tag{1}$$

where $\vec{S}_{i,j}$ is the spin-$\frac{1}{2}$ operator and L is the length of the tube in the leg direction. The exchange coupling constant J_1 is for the neighboring spin pairs along the legs, while J_r and J_r' are the rung coupling constants. All the exchange interactions are supposed to be antiferromagnetic (namely, positive). The ratio $\alpha = J_r'/J_r$ stands for the degree of the asymmetry of the rung couplings. We will vary α and J_1 to investigate the quantum phase transitions. Throughout this paper, we fix J_r to one.

The present model includes three typical models as limiting cases; (a) $\alpha=0$: the three-leg spin ladder, (b) $\alpha=1$: the symmetric spin tube, and (c) $\alpha\to\infty$: the single chain plus rung dimers. Since the system is gapless in the cases (a) and (c), while gapful in the case (b), at least two quantum phase transitions should occur with increasing α from 0 to infinity. As we already mentioned, the one-site translational symmetry along the leg ($\vec{S}_{i,j}\to\vec{S}_{i,j+1}$) is spontaneously broken in the symmetric spin tube at least in the strong-rung-coupling regime.[6,12]

III. EFFECTIVE THEORIES

In this section, we study the spin tube (1) by constructing its low-energy effective theories. In Sec. III A, we draw a phase diagram in the whole coupling-constant space (α, J_1). To this end, we develop a simple effective theory for the spin tube from the corresponding Hubbard model on the tube lattice, where the SU(2) spin-rotational symmetry is preserved automatically. This effective theory allows us to find three gapless phases and one extended gapful phase. Next, utilizing other theoretical schemes, we carefully investigate two special regimes $J_r \ll J_r' \ll J_1$ and $J_r \gg J_1$, respectively, in Secs. III B and III C.

A. Global phase diagram derived from the Hubbard model on the tube lattice

Here, we provide a systematic method to draw global phase diagrams of one-dimensional antiferromagnetic quantum spin systems. It is well known that any $S=\frac{1}{2}$ Heisenberg model is obtained from the corresponding half-filled Hubbard model in the limit of strong on-site Coulomb interactions. In one dimension, the spin configurations of the low-energy states in the Heisenberg model qualitatively agree with those in the half-filled Hubbard model even with a weak Coulomb interaction. Furthermore, the phases in the weak Coulomb regime often smoothly connect to those in the strong Coulomb regime in one-dimensional electron systems. Relying on these arguments, we construct the low-energy effective theory for the spin tube (1) from the corresponding Hubbard model. To discuss the wider parameter space, first we diagonalize the kinetic parts of the Hubbard Hamiltonian including both the leg and rung hopping terms.[26–28] Then, we take account of the on-site Coulomb interaction as the perturbation, with the help of the non-Abelian bosonization and CFT. As one will see later, the number of Fermi points is essential to determine whether or not the Coulomb interaction open a spin gap.

Since we consider the electron tube instead of the original spin tube, our results in this subsection should be regarded as a qualitative argument. However, the approach from the electron tube can be applicable to the wide parameter space (α, J_1), in contrast to the other conventional methods. For example, the nonlinear sigma model is not usually reliable for frustrated magnets including the present spin tube. It is dangerous to apply the Abelian bosonization to any SU(2)-symmetric magnets.[29] Moreover, a standard non-Abelian bosonization method, taking into account rung couplings perturbatively (we will use it in Sec. III B), is of course valid only in the weak-rung-coupling regime.

Now, let us begin with the definition of the Hubbard model on the three-leg tube lattice. The Hamiltonian,

$$H = H_{\text{hop}} + H_{\text{int}}, \tag{2}$$

consists of the hopping part

$$H_{\text{hop}} = \sum_{n=1}^{L}\sum_{i=1}^{3}\sum_{\sigma=\uparrow,\downarrow}(tc^{\dagger}_{n+1,i,\sigma}c_{n,i,\sigma} + s_{i+1,i}c^{\dagger}_{n,i+1,\sigma}c_{n,i,\sigma} + \text{H.c.}), \tag{3}$$

and the on-site interaction part

$$H_{\text{int}} = U\sum_{n=1}^{L}\sum_{i=1}^{3} n_{n,i,\uparrow}n_{n,i,\downarrow}, \tag{4}$$

where $n_{n,i,\sigma}=c^{\dagger}_{n,i,\sigma}c_{n,i,\sigma}$ and $U>0$ is the repulsive coupling constant. The electron operators $c_{n,i,\sigma}$ and $c^{\dagger}_{n,i,\sigma}$ satisfy the periodic boundary conditions for both the leg and the rung directions,

$$c_{n+L,i,\sigma} = c_{n,i,\sigma}, \quad c_{n,i+3,\sigma} = c_{n,i,\sigma},$$

and anticommutation relations,

$$\{c_{m,i,\sigma}, c^{\dagger}_{n,j,\tau}\} = \delta_{m,n}\delta_{i,j}\delta_{\sigma,\tau},$$

$$\{c_{m,i,\sigma}, c_{n,j,\tau}\} = 0, \quad \{c^{\dagger}_{m,i,\sigma}, c^{\dagger}_{n,j,\tau}\} = 0.$$

The hopping parameters are given by $t>0$, $s_{1,2}=s_{2,3}=s>0$, and $s_{3,1}=\beta s>0$. The strong coupling expansion shows that this model at the half-filling case is reduced to the Heisenberg model with $J_1=4t^2/U$, $J_r=4s^2/U$, and $\alpha=\beta^2$.

By performing the suitable unitary transformation, the hopping Hamiltonian can be mapped to the following diagonal form:

$$H_{\text{hop}} = \sum_{k}\sum_{i=1}^{3}\sum_{\sigma=\uparrow,\downarrow} E_i(k) d^{\dagger}_{k,i,\sigma}d_{k,i,\sigma}, \tag{5}$$

where the wave number k is summed over $\frac{2\pi}{L}\le k\le 2\pi$. The operators $d_{k,i,\sigma}$ and $d^{\dagger}_{k,i,\sigma}$ are defined by

$$d_{k,i,\sigma} = \frac{1}{\sqrt{L}}\sum_{n=1}^{L}\sum_{j=1}^{3} e^{-\imath kn}O_{ij}c_{n,j,\sigma}, \tag{6a}$$

$$d^{\dagger}_{k,i,\sigma} = \frac{1}{\sqrt{L}}\sum_{n=1}^{L}\sum_{j=1}^{3} e^{\imath kn}O_{ij}c^{\dagger}_{n,j,\sigma}, \tag{6b}$$

which satisfy the standard anticommutation relations

$$\{d_{k,i,\sigma}, d^{\dagger}_{l,j,\tau}\} = \delta_{k,l}\delta_{i,j}\delta_{\sigma,\tau},$$

$$\{d_{k,i,\sigma}, d_{l,j,\tau}\} = 0, \quad \{d^{\dagger}_{k,i,\sigma}, d^{\dagger}_{l,j,\tau}\} = 0. \tag{7}$$

The explicit form of the orthogonal matrix is

$$O = \begin{pmatrix} -\frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ u_+ & v_+ & u_+ \\ u_- & v_- & u_- \end{pmatrix},$$

where the matrix elements are given by

$$u_{\pm} = \frac{1}{n_{\pm}}, \quad v_{\pm} = \frac{c_{\pm}}{n_{\pm}}, \quad n_{\pm} = \sqrt{2 + c_{\pm}^2},$$

$$c_{\pm} = \frac{3\beta \pm \sqrt{\beta^2+8}}{\beta^2 + 2 \pm \beta\sqrt{\beta^2+8}}. \tag{8}$$

The energy eigenvalues of the one-electron states are

$$E_1(k) = -\beta s + 2t\cos k, \tag{9a}$$

$$E_2(k) = \frac{1}{2}(\beta s - s\sqrt{\beta^2+8} + 4t\cos k), \tag{9b}$$

$$E_3(k) = \frac{1}{2}(\beta s + s\sqrt{\beta^2+8} + 4t\cos k). \tag{9c}$$

Note that a degeneracy $E_1(k)=E_2(k)$ appears at $\beta=1$ due to the translational ($\vec{S}_{i,j}\to\vec{S}_{i+1,j}$) and the parity ($\vec{S}_{1,j}\leftrightarrow\vec{S}_{3,j}$) symmetries along the rung direction.

For the half-filled case, $3L$ one-electron states should be occupied by electrons with up and down spins. As a result, the ground state of the hopping Hamiltonian has one, two or three pairs of the Fermi points $(k_j,\bar{k}_j)$ just on the Fermi sea, depending on the parameters s/t and β. Since the low-energy excitations are given by the particle-hole creations around these Fermi points, they may be represented by using the Dirac fermions, the left mover $\psi_{j,\sigma}(x)$ and the right one $\bar{\psi}_{j,\sigma}(x)$, which are defined from the electrons around the jth pair of Fermi points. If the jth band has no Fermi points in the half-filled case, we should neglect $\psi_{j,\sigma}(x)$ and $\bar{\psi}_{j,\sigma}(x)$. On this understanding, we approximate the original electron operators in terms of the Dirac fermions as follows:

$$c_{n,i,\sigma} \sim \sqrt{a}\sum_{j=1}^{3} O^{-1}_{ij}[e^{\imath k_j x/a}\psi_{j,\sigma}(x) + e^{\imath \bar{k}_j x/a}\bar{\psi}_{j,\sigma}(x)], \tag{10}$$

where a is the lattice spacing with dimension of length and $x=an$ is the continuous position coordinate.

For this free Dirac fermion system, we take into account the effects of the on-site Coulomb interaction (4) as the perturbation and we use the non-Abelian bosonization techniques. Following naively the field-theory argument in Ref. 30, one can expect that when the number of Fermi-point pairs is odd (even), the spin excitations are gapless (gapped) in the half-filled Hubbard tube. In particular, in the cases of one or two Fermi-point pairs, we can explicitly determine whether or not a spin gap exists as follows.

First, we consider the case of one pair of Fermi points $k_1=\frac{3\pi}{2}$ and $\bar{k}_1=\frac{\pi}{2}$. In this case, interaction (4) is approximated as the sum of an Umklapp interaction and two marginal ones,

$$H_{\rm int} \sim \int dx[g_1\Theta_1(x) - g_2\Theta_2(x) - g_3\Theta_3(x) + \cdots],$$

where $g_{1,2,3}$ are positive coupling constants proportional to U. The Umklapp term is expressed as

$$\Theta_1(x) = \psi_{1,\uparrow}(x)^\dagger\psi_{1,\downarrow}(x)^\dagger\bar{\psi}_{1,\uparrow}(x)\bar{\psi}_{1,\downarrow}(x), \tag{11}$$

and the marginal interaction between the U(1) charge currents is given by

$$\Theta_2(x) = \psi_1(x)^\dagger\psi_1(x)\bar{\psi}_1(x)^\dagger\bar{\psi}_1(x),$$

where $\psi_1 = {}^t(\psi_{1,\uparrow},\psi_{1,\downarrow})$. It is known that the bosonized form of $\Theta_{1,2}$ contains only the charge degrees of freedom and they open a charge gap when g_2 is positive. Then, the remaining spin degrees of freedom are described by the gapless level-1 SU(2) WZW theory.[18–20] This phenomenon, i.e., the charge-spin separation, is well known in the single Hubbard chain model. For this WZW theory, the third interaction,

$$\Theta_3(x) = \psi_1(x)^\dagger\frac{\vec{\sigma}}{2}\psi_1(x)\cdot\bar{\psi}_1(x)^\dagger\frac{\vec{\sigma}}{2}\bar{\psi}_1(x), \tag{12}$$

is known to be marginally irrelevant if $g_3>0$. The coupling constant g_3 is hence renormalized to be zero in the low-energy limit. Except for the above interactions $\Theta_{1,2,3}(x)$, there is no relevant operator with the invariance under the one-site translation along the leg,

$$\psi_{1,\sigma}(x) \to e^{\imath k_1}\psi_{1,\sigma}(x), \quad \bar{\psi}_{1,\sigma}(x) \to e^{\imath \bar{k}_1}\bar{\psi}_{1,\sigma}(x), \tag{13}$$

as in the case of the Heisenberg chain. The spin excitations, therefore, remain gapless.

On the other hand, when there exist two pairs of the Fermi points, $(k_1,\bar{k}_1)$ and $(k_2,\bar{k}_2)$, the fate of the spin excitations is different from the above scenario. In this case, the spin sector in the hopping part of the Hubbard tube is described by a level-2 SU(2) WZW theory, which is derived from two decoupled Dirac fermions.[31] The Coulomb interaction yields several perturbations for this theory. For example, applying the non-Abelian bosonization rule,[18] we find that an interaction derived from Eq. (4),

$$\psi_{1,\uparrow}(x)^\dagger\bar{\psi}_{2,\uparrow}(x)\bar{\psi}_{1,\downarrow}(x)^\dagger\psi_{2,\downarrow}(x), \tag{14}$$

contains a relevant perturbation for the level-2 WZW model, and it is invariant under the translational operation

$$\psi_{j,\sigma}(x) \to e^{\imath k_j}\psi_{j,\sigma}(x), \quad \bar{\psi}_{j,\sigma}(x) \to e^{\imath \bar{k}_j}\bar{\psi}_{j,\sigma}(x). \tag{15}$$

Particularly for $\beta=1$, the number of possible relevant operators with the translational invariance is increased, because of the coincident Fermi points $k_1=k_2$ and $\bar{k}_1=\bar{k}_2$. Therefore, we conclude that any gapless spin excitation generally has no chance to survive except particularly rare cases [e.g., when the coupling constant of Eq. (14) is zero].

Since for the case of three Fermi-point pairs, the interactions among three Dirac fermions, generated from Eq. (4), are fairly complicated, it is difficult to analyze them and judge whether or not the spin excitation can survive as gapless. However, as we already stated, it can be expected from Ref. 30 that the spin excitation is presumably gapless in this case of three Fermi-point pairs.

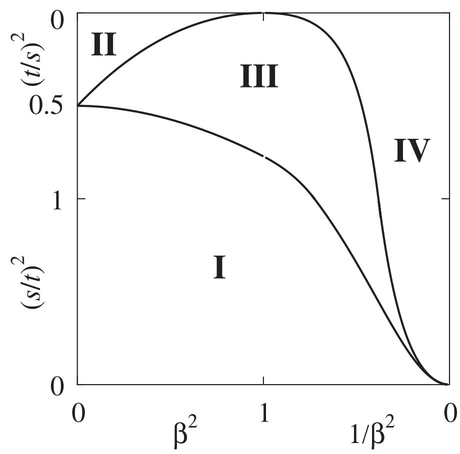

FIG. 2. Phase diagram obtained from the effective Hubbard model (2). In the strong-coupling limit $(U/t, U/s \gg 1)$, the horizontal axis β^2 and vertical one $(s/t)^2$ can be regarded as α and J_r/J_1, respectively. The effective theory claims that the phases (II) and (IV) are gapless and the phase (III) is gapful. The phase (I) is possibly gapless.

From these arguments, we can draw the ground-state phase diagram of the half-filled Hubbard tube as shown in Fig. 2. The phase (I) has three pairs of the Fermi points, the phases (II) and (IV) have one pair, and the central phase (III) has two pairs. Therefore, we can predict that the phases (II) and (IV) have gapless spin excitations, whereas the phase (III) possesses a spin gap. If $(s/t)^2$ and β^2 are, respectively, replaced with the coupling ratio J_1/J_r and the asymmetric parameter α in Fig. 2, one may interpret the phase diagram as that of the $S=\frac{1}{2}$ three-leg spin tube (1). Although we have treated the on-site interaction (4) perturbatively, we have assumed that the weakly interacting case $(U/t, U/s \ll 1)$ is smoothly linked to the strongly interacting one, which is nothing but the spin tube (1).

We here note that the gapful phase (III) is predicted to be extended around the line $\beta=1$ for a finite s/t. In the limit $s/t\to\infty$, both the left- and right-side phase boundaries of the region (III) converge to $\beta=1$. This narrowing of the phase (III) is consistent with the numerical results[11,12] in the strong-rung-coupling limit $J_r/J_1\to\infty$. We will discuss this limit in more detail in Sec. III C.

Finally, we briefly argue the universality classes of the phase transitions at two phase boundaries, (II)-(III) and (III)-(IV). For the level-1 SU(2) WZW model in the phases (II) and (IV), the most relevant perturbation is the marginal current-current interaction,[18–20] Eq. (12), which is invariant under the translational and spin-rotational operations. Since it possibly becomes marginally "relevant" when parameters are finely tuned and then g_3 becomes negative, we speculate that the transition from the phases (II) or (IV) to (III) is caused by this marginal term. Therefore, the transitions are expected to be in the BKT universality class. This speculation may be naturally accepted if we recall the following two known results of the $S=\frac{1}{2}$ zigzag Heisenberg chain, namely, the spin chain with the nearest- and the next-nearest-neighbor interactions:[32] (i) When the next-nearest-neighbor hopping is sufficiently small in the half-filled electron system on zigzag lattice, one obtains one pair of Fermi points. The spin excitations are therefore described by a level-1 SU(2) WZW model, like the phases (II) and (IV). (ii) It has been numerically shown[32] that when the next-nearest-neighbor interaction is increased in the zigzag spin chain, the BKT transition takes place and the ground state changes into a dimerized state from a Tomonaga-Luttinger liquid described by a level-1 SU(2) WZW model. On the basis of this speculation, we numerically analyze the phase transitions between (II)-(III) and (III)-(IV) in Sec. IV.

B. Gapless phase for $J_r \ll J_r' \ll J_1$

In Sec. III A, we have obtained a qualitative phase diagram of the spin tube (1) as shown in Fig. 2. However, some subtle points still remain, and particularly it is doubtful whether or not there is the gapless phase (I). To partially resolve these issues, we here focus on the extreme situation $J_r \ll J_r' \ll J_1$, $(\alpha = J_r'/J_r \gg 1)$, which corresponds to the right lower regime in Fig. 2. In this regime, we prove the existence of the gapless phase (I) and discuss the phase transition between the gapless phase (I) and the gapful phase (III).

Before embarking on our analysis, we sketch the scenario of this subsection. We introduce three level-1 SU(2) WZW theories for the three decoupled Heisenberg chains,[18–20] and then we treat their rung couplings as the perturbation, because the weak-rung-coupling regime $J_r, J_r' \ll J_1$ is considered now. The first and the third chains are coupled to each other with J_r' which is much stronger than two remaining couplings J_r. It is well known that the J_r' coupling involves a relevant interaction with conformal dimensions $(\frac{1}{2},\frac{1}{2})$ in the two coupled WZW models [see Eq. (20)], and it produces an energy gap.[33] On the other hand, like the case of one Fermi-point pair in Sec. III A, the WZW model for the second chain has the marginal irrelevant current-current interaction,

$$\lambda_2 \Phi_2, \tag{16}$$

with a finite negative coupling constant $\lambda_2 < 0$. The operator Φ_2 is equivalent to Eq. (12), if we use the Dirac fermions $(\psi_{1,\sigma}, \bar{\psi}_{1,\sigma})$ to describe the second chain. The negative sign makes Eq. (16) irrelevant and the second chain is gapless. A weak rung coupling J_r between this WZW model and the massive theory for the two coupled chains must give a correction to the coupling constant λ_2. If J_r is sufficiently small, the sign of $\lambda_2 < 0$ would not change and the gapless excitation is preserved. These arguments convince us that the gapless phase (I) definitely exists. Furthermore, we expect the phase transition from the gapless phase (I) to the gapful phase (III). Namely, if J_r exceeds a critical value, the coupling constant λ_2 might change to be positive. In this case, the marginal operator (16) becomes relevant, which produces an excitation gap. This transition between the phases (I) and (III) is nothing but of the BKT type,[24,25] as in the zigzag Heisenberg chain.[32]

Now, let us calculate the correction to λ_2 in an explicit way to confirm the above sketch. We represent the partition function of the three coupled WZW models through the path integral formalism. Note that the SU(2) spin-rotational symmetry is conserved automatically in the language of the WZW models, i.e., the non-Abelian bosonization. The three WZW models can be represented in six Dirac fermions $\Psi_{i,\alpha}(z,\bar{z})$ $[i=1,2,3$ and $\alpha=\uparrow,\downarrow]$ and three ghost bosons $\varphi_i(z,\bar{z})[i=1,2,3]$. Here, $z=v\tau+\imath x$ and $\bar{z}=v\tau-\imath x$ are the chiral coordinates (τ: imaginary time) and the index i denotes the chain number of the spin tube (1). We employ this free-field representation.[34–36] The Lagrangian density for the decoupled three chains is given by

$$\mathcal{L}_0(z,\bar{z}) = 2\sum_{i=1}^{3}\left[\sum_{\alpha=\uparrow,\downarrow}(\bar{\Psi}_{i,\alpha}^{\dagger}\,\partial\,\bar{\Psi}_{i,\alpha} + \Psi_{i,\alpha}^{\dagger}\bar{\partial}\Psi_{i,\alpha}) - \partial\varphi_i\bar{\partial}\varphi_i\right], \tag{17}$$

where we have decomposed the Dirac fermions into the linear combination of the left mover $\Psi_{i,\alpha}(z)$ and the right mover $\bar{\Psi}_{i,\alpha}(\bar{z})$ as $\Psi_{i,\alpha}(z,\bar{z}) = \Psi_{i,\alpha}(z) + \bar{\Psi}_{i,\alpha}(\bar{z})$.[37] The nonvanishing two-point correlation functions of these fields, calculated from this free Lagrangian (17), are

$$\langle \Psi_{i,\alpha}(z)^{\dagger}\Psi_{j,\beta}(w)\rangle = \frac{\delta_{ij}\delta_{\alpha\beta}}{z-w}, \tag{18a}$$

$$\langle \bar{\Psi}_{i,\alpha}(\bar{z})^{\dagger}\bar{\Psi}_{j,\beta}(\bar{w})\rangle = \frac{\delta_{ij}\delta_{\alpha\beta}}{\bar{z}-\bar{w}}, \tag{18b}$$

$$\langle e^{\imath\varphi_i(z,\bar{z})}e^{-\imath\varphi_i(w,\bar{w})}\rangle = \delta_{ij}|z-w|. \tag{18c}$$

The anomalous correlation of the ghost bosons should be noted. These ghost fields kill the charge degrees of freedom and extract the gapless spin degrees of freedom in the Dirac fermions. The primary field $g^i_{\alpha\beta}(z,\bar{z})$ with the conformal dimension $(\frac{1}{4},\frac{1}{4})$ in the ith level-1 SU(2) WZW theory is represented in terms of these free fields:

$$g^i_{\alpha\beta}(z,\bar{z}) = \Psi_{i,\alpha}(z)^{\dagger}\bar{\Psi}_{i,\beta}(\bar{z})e^{\imath\varphi_i(z,\bar{z})}.$$

Furthermore, the spin operators are represented as

$$\vec{S}_{i,n}/a \approx \vec{J}_i(z,\bar{z}) + (-1)^n\vec{N}_i(z,\bar{z}),$$

in which the smooth and the staggered parts are given by

$$\vec{J}_i(z,\bar{z}) = \Psi_i^{\dagger}\frac{\vec{\sigma}}{2}\Psi_i + \bar{\Psi}_i^{\dagger}\frac{\vec{\sigma}}{2}\bar{\Psi}_i, \tag{19a}$$

$$\vec{N}_i(z,\bar{z}) = C_0\left(\Psi_i^{\dagger}\frac{\vec{\sigma}}{2}\bar{\Psi}_i e^{\imath\varphi_i} + \text{H.c.}\right), \tag{19b}$$

with $\Psi_i = {}^t(\Psi_{i,\uparrow},\Psi_{i,\downarrow})$. Here C_0 is a nonuniversal constant. Applying Eqs. (18a)–(18c), one can evaluate the asymptotic forms of several correlation functions for the field $g^i_{\alpha\beta}$ and the spins $\vec{S}_{i,n}$. Among the spin-rotational and the translational-symmetric operators, the most relevant coupling between the ith and the jth WZW models is

$$\Phi_{ij}(z,\bar{z}) = \vec{N}_i(z,\bar{z})\cdot\vec{N}_j(z,\bar{z}), \tag{20}$$

with the conformal dimensions $(\frac{1}{2},\frac{1}{2})$. As we already mentioned, this relevant term $\Phi_{31}(z,\bar{z})$ produces the energy gap in the two strongly coupled WZW models. The WZW model for the second chain interacts with these coupled WZW models via the weak rung coupling $\Phi_{12}(z,\bar{z})$ and $\Phi_{23}(z,\bar{z})$. The explicit form of the marginal operator (16) of the second WZW model is

$$\Phi_2(z,\bar{z}) = \Psi_2^\dagger \frac{\vec{\sigma}}{2}\Psi_2 \cdot \bar{\Psi}_2^\dagger \frac{\vec{\sigma}}{2}\bar{\Psi}_2. \tag{21}$$

From these materials, the total Lagrangian density for the asymmetric spin tube under the condition $J_r \ll J_r' \ll J_1$ is written as

$$\mathcal{L}(z,\bar{z}) = \mathcal{L}_0(z,\bar{z}) + \lambda_{31}\Phi_{31}(z,\bar{z}) + \lambda_{12}\Phi_{12}(z,\bar{z}) + \lambda_{23}\Phi_{23}(z,\bar{z}) + \lambda_2\Phi_2(z,\bar{z}) + \cdots, \tag{22}$$

where the coupling constants are $\lambda_{31} \propto J_r'$, $\lambda_{12}=\lambda_{23}\propto J_r$, and $\lambda_2 < 0$. Therefore, the partition function is written in the path integral over Grassmann and boson fields as

$$Z = \int \prod_{i,\alpha} \mathcal{D}\bar{\Psi}_{i,\alpha}\mathcal{D}\bar{\Psi}_{i,\alpha}^\dagger \mathcal{D}\Psi_{i,\alpha}\mathcal{D}\Psi_{i,\alpha}^\dagger \mathcal{D}\varphi_i \times \exp\left[-\int \frac{d^2z}{2\pi}\mathcal{L}(z,\bar{z})\right].$$

Under the condition $J_r \ll J_r' \ll J_1$, the low-energy physics must be governed by the second chain weakly coupled to the other two chains. To obtain its effective theory, we may integrate out the massive degrees of freedom $\Psi_{i,\alpha}(z,\bar{z})$ and $\varphi_i(z,\bar{z})$ with $i=1,3$. To calculate the correction to the coupling constant λ_2, we regard the relevant term $\Phi_{31}(z,\bar{z})$ as an unperturbed Lagrangian and expand the partition function in all the other operators $\mathcal{L}_0$, $\Phi_{12}(z,\bar{z})$, $\Phi_{23}(z,\bar{z}),\ldots$. This expansion can be performed by a lattice regularization of two-dimensional Euclidean spacetime. In this regularization, the partition function is represented as the following multiple integration over countable variables:

$$Z = \int \prod_{n\in N}\prod_{i\in I}\prod_{\alpha\in S}\left\{ a^2 d\bar{\Psi}_{i,\alpha}(\bar{z}_n) d\bar{\Psi}_{i,\alpha}^\dagger(\bar{z}_n) d\Psi_{i,\alpha}(z_n) d\Psi_{i,\alpha}^\dagger(z_n) \times d\varphi_i(z_n,\bar{z}_n)\exp\left[-\frac{a^2}{2\pi}\mathcal{L}(z_n,\bar{z}_n)\right]\right\}, \tag{23}$$

where $I=\{1,2,3\}$, $S=\{\uparrow,\downarrow\}$, and $N=\{(n_1,n_2)\in\mathbb{Z}^2 | 1\le n_1,n_2 \le L\}$ is a finite set of integer pairs with a large number of elements. For an integer pair $n=(n_1,n_2)\in N$, we define discretized coordinates $(z_n,\bar{z}_n)=a(n_1+\imath n_2, n_1-\imath n_2)$ for $(z,\bar{z})$ with a lattice spacing parameter a. For a finite number of Grassmann variables, the Taylor expansion is reduced to a finite summation,

$$\exp\left[-\frac{a^2}{2\pi}\mathcal{L}(z_n,\bar{z}_n)\right] = \sum_{k=1}^{K}\frac{1}{k!}\left[-\frac{a^2}{2\pi}\mathcal{L}(z_n,\bar{z}_n)\right]^k,$$

with a certain positive integer $K \le 12|N|$, due to the nilpotency of the Grassmann variables

$$\Psi_{i,\alpha}(z_n)^2 = 0, \quad \bar{\Psi}_{i,\alpha}(\bar{z}_n)^2 = 0,$$

$$\Psi_{i,\alpha}^\dagger(z_n)^2 = 0, \quad \bar{\Psi}_{i,\alpha}^\dagger(\bar{z}_n)^2 = 0.$$

The following integration formula of Grassmann variables,

$$\int \prod_{n\in N}\prod_{i\in I}\prod_{\alpha\in S}(a^2 d\bar{\Psi}_{i,\alpha}(\bar{z}_n) d\bar{\Psi}_{i,\alpha}^\dagger(\bar{z}_n) d\Psi_{i,\alpha}(z_n) d\Psi_{i,\alpha}^\dagger(z_n)) \times \prod_{n\in M}\prod_{i\in J}\prod_{\alpha\in T}(a^2\Psi_{i,\alpha}^\dagger(z_n)\Psi_{i,\alpha}(z_n)\bar{\Psi}_{i,\alpha}^\dagger(\bar{z}_n)\bar{\Psi}_{i,\alpha}(\bar{z}_n)) = \begin{cases} 1: & M=N, J=I, T=S \\ 0: & \text{otherwise,}\end{cases} \tag{24}$$

is important to calculate this expansion. In addition, using an equality for two Grassmann variables,

$$\Psi_\alpha\Psi_\beta = \imath\sigma^2_{\alpha\beta}\Psi_\uparrow\Psi_\downarrow, \quad (\sigma^{1,2,3}=\sigma^{x,y,z}),$$

and a trace formula of the Pauli matrices

$$\mathrm{tr}[\sigma^a\sigma^{2t}\sigma^b\sigma^2] = \sum_{\alpha,\beta,\gamma,\delta}\sigma^a_{\alpha\beta}\sigma^2_{\beta\gamma}\sigma^b_{\delta\gamma}\sigma^2_{\delta\alpha} = -2\delta^{ab},$$

one can reduce products of Pauli matrices and Grassmann variables to the following single term:

$$\prod_i \Psi_i^\dagger\frac{\sigma^a}{2}\bar{\Psi}_i\Psi_i^\dagger\frac{\sigma^b}{2}\bar{\Psi}_i\Psi_i^\dagger\frac{\sigma^c}{2}\Psi_i\bar{\Psi}_i^\dagger\frac{\sigma^d}{2}\Psi_i = \prod_i \Psi_{i,\uparrow}^\dagger\Psi_{i,\downarrow}^\dagger\Psi_{i,\uparrow}\Psi_{i,\downarrow}\bar{\Psi}_{i,\uparrow}^\dagger\bar{\Psi}_{i,\downarrow}^\dagger\bar{\Psi}_{i,\uparrow}\bar{\Psi}_{i,\downarrow}\frac{\delta^{ab}}{2}\frac{\delta^{cd}}{2}. \tag{25}$$

These formulas (24) and (25) make it easier to calculate the expansion of the partition function (23). As a result, we obtain

$$Z = \int \prod_{n\in N}\prod_{\alpha\in S}[a^2 d\bar{\Psi}_{2,\alpha}(\bar{z}_n) d\bar{\Psi}_{2,\alpha}^\dagger(\bar{z}_n) d\Psi_{2,\alpha}(z_n) d\Psi_{2,\alpha}^\dagger(z_n) d\varphi_2(z_n,\bar{z}_n)] \times \prod_{n\in N}\left\{\exp\left[-\frac{a^2\lambda_2}{2\pi}\Phi_2(z_n,\bar{z}_n)+\cdots\right]\left[\frac{15}{32}\frac{\lambda_{31}^4}{(2\pi)^4} - \frac{5}{16}\frac{\lambda_{31}^3\lambda_{12}\lambda_{23}}{(2\pi)^5}\Phi_2(z_n,\bar{z}_n)+\cdots\right]\right\}$$
$$\sim \int \prod_\alpha \mathcal{D}\bar{\Psi}_{2,\alpha}\mathcal{D}\bar{\Psi}_{2,\alpha}^\dagger\mathcal{D}\Psi_{2,\alpha}\mathcal{D}\Psi_{2,\alpha}^\dagger\mathcal{D}\varphi_2 \exp\left[-\int\frac{d^2z}{2\pi}\left(\lambda_2+\frac{2\lambda_{12}\lambda_{23}}{3\lambda_{31}}\right)\Phi_2(z,\bar{z})\int + \cdots\right]. \tag{26}$$

Here, we have neglected several terms of charge degrees of freedom. The final expression in Eq. (26) clearly indicates that the correction to λ_2 is $2\lambda_{12}\lambda_{23}/(3\lambda_{31})=2J_r/(3\alpha)$, and the phase boundary between (I) and (III) is given by

$$J_r = -\frac{3}{2}\lambda_2\alpha, \quad (\lambda_2 < 0). \tag{27}$$

Thus, the gapless excitation in the second chain is preserved and the gapless phase is expanded under the condition $J_r \ll J'_r \ll J_1$. Namely, we have proved that the phase (I) is exactly present at least in the region $J_r \ll J'_r \ll J_1$. Furthermore, we find that if J_r is large enough to change the sign of $\lambda_2 + \frac{2J_r}{3\alpha}$, $\Phi_2(z,\bar{z})$ becomes relevant and an energy gap appears. Since this phase transition is induced by the marginal operator $\Phi_2(z,\bar{z})$, it belongs to the BKT universality class, as in the $S=\frac{1}{2}$ zigzag Heisenberg chain. This gapped state must correspond to the phase (III) in Fig. 2. In the gapful region under $J_r \ll J'_r \ll J_1$, the second chain must be dimerized. On the other hand, as we have often mentioned, the gapful phase in the vicinity of the symmetric line $\alpha=1$ has the valence-bond order. Since both the orders break the same translational symmetry, the state with the dimerized second chain would smoothly change into the valence-bond ordered state when we vary α from a large value to unity in the gapful phase (III).

Finally, we notice that in the prediction (27), the gapless phase (I) becomes wider for larger α, contrary to the phase diagram, Fig. 2. Two reasons for this contradiction are immediately found. First, we should not precisely trust the location of the phase boundaries in Fig. 2, which are drawn just by counting the number of Fermi points. The argument in Sec. III A is only qualitatively correct to determine the phase boundaries. Particularly, since the gapful phase (III) sandwiched by two gapless phases (I) and (IV) is quite narrow for large α in Fig. 2, then we cannot claim the existence of the gapful phase (III) for $\alpha \gg 1$ by using Fig. 2. Therefore, the phases (I) and (IV) might be smoothly connected in the large-α region. For such a case, the transition between two regions (III) and (IV) is expected to be also of the BKT type. Second, the three Dirac fermions in the region (I) do not always imply the gapless phase,[27,28] as discussed in Sec. III A. The coupled three Dirac fermions possibly produce an energy gap by the strong frustration, if α approaches the symmetric point $\alpha=1$. The result (27) also shows this tendency.

C. Energy gap for $J_r \gg J_1$ and $J_r \sim J'_r$

In this subsection, we discuss the existence of an energy gap for a sufficiently strong rung coupling $J_r \gg J_1$ and a sufficiently weak asymmetry $|\alpha-1| \ll 1$ except at $J_1=0$. Namely, we explain that the phase (III) has a finite width along the line $J_r/J_1=\text{const} \gg 1$.

As we mentioned before, Kawano and Takahashi[6] have obtained the spin-orbital-type model as an effective theory for the symmetric ($\alpha=1$) spin tube with a strong rung coupling. The Hamiltonian is written as

$$H_{\text{eff}}^{\text{sym}} = \frac{J_1}{3J_r}\sum_{j=1}^{L} \vec{S}_j \cdot \vec{S}_{j+1}[1 + 4(\tau_j^+\tau_{j+1}^- + \tau_j^-\tau_{j+1}^+)], \tag{28}$$

which is the result of the first-order expansion in J_1/J_r. The orbital Pauli matrices τ_i^ν ($\nu=x,y,z$) are defined for the states with respect to the left- and right-handed spin configurations on each rung (see Refs. 6 and 12). From this theory (28), Kawano and Takahashi have shown that the ground state has a valence-bond order with the translational symmetry ($\vec{S}_{i,j} \to \vec{S}_{i,j+1}$) spontaneously broken, and a finite excitation gap exists. It is believed that the energy gap is generated by the strong coupling between the spin and orbital degrees of freedom in the effective Hamiltonian (28). Obviously, either of them becomes gapless if the other is frozen.

Quite recently, Nishimoto and Arikawa[12] have extended the effective theory to the asymmetric case as follows:

$$H_{\text{eff}}^{\text{asym}} = H_{\text{eff}}^{\text{sym}} + (\alpha-1)\sum_{j=1}^{L} \tau_j^x. \tag{29}$$

For simplicity, we have redefined the orbital Pauli matrices τ_i^ν through a unitary transformation. Remarkably, the asymmetry induces a transverse external field coupled to the orbital spins. A sufficiently strong asymmetry $|\alpha-1| \gg 1$ hence yields the saturated polarization of the orbital spins. In this case, the effective Hamiltonian (29) is reduced to that of the antiferromagnetic Heisenberg chain. The spin degree thus survives as a gapless excitation. Next, let us focus on the region around the symmetric line $\alpha \sim 1$. In the limit $J_1/J_r \to 0$, the ground state has a saturated orbital spin at any asymmetric point $\alpha \neq 1$. For a finite J_1/J_r, however, we expect an extended gapful phase around $\alpha=1$, if the energy gap exists at $\alpha=1$ due to the coupling between the spin and the orbital degrees of freedom. The finite energy gap does not vanish by an infinitesimal external field $\alpha-1$. In other words, the magnetization process of the orbital spins should show a zero-magnetization plateau. Therefore an energy gap would also be present for sufficiently weak asymmetry $|\alpha-1| \ll 1$.

From these arguments, we find that the gapful phase surely exists in a finite region under the conditions $J_r \gg J_1$ and $J_r \sim J'_r$, and its width becomes smaller with decreasing J_1/J_r. This is consistent with the result obtained in Sec. III A.

IV. NUMERICAL ANALYSIS

In this section, we numerically analyze the asymmetric spin tube (1), taking into account the results in the preceding Sec. III. We show that the arguments based on the effective theories are in good agreement with the results of the numerical calculations. We will use results of the numerical diagonalization up to $L=10$ for the periodic boundary system, and those of the DMRG up to $L=128$ for the open boundary system.

A. Phenomenological renormalization

A useful order parameter to determine the phase boundaries between the gapless and the gapful phases in Fig. 2 is the spin gap Δ, which is the energy gap between the singlet

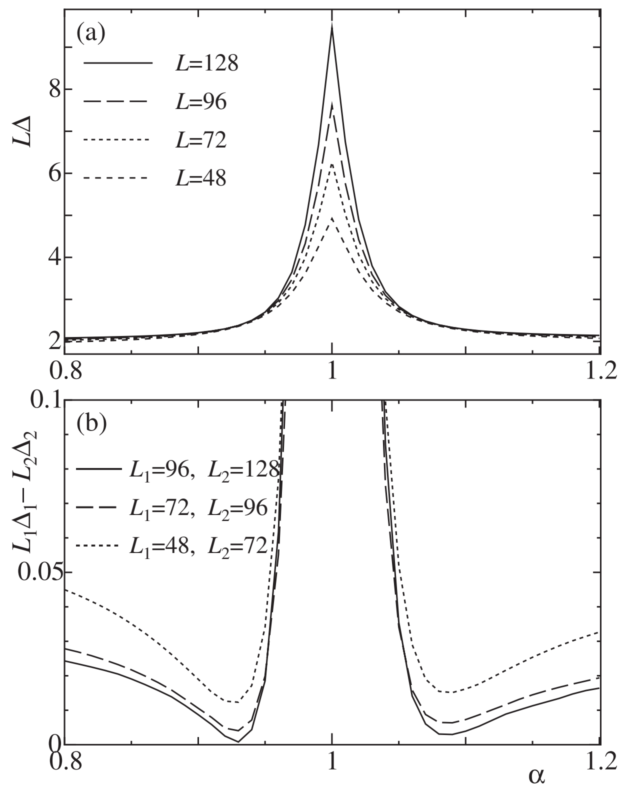

FIG. 3. (a) Scaled gap calculated by DMRG for $J_1=0.5$. (b) Difference of the scaled gaps between two systems with sizes L_1 and L_2.

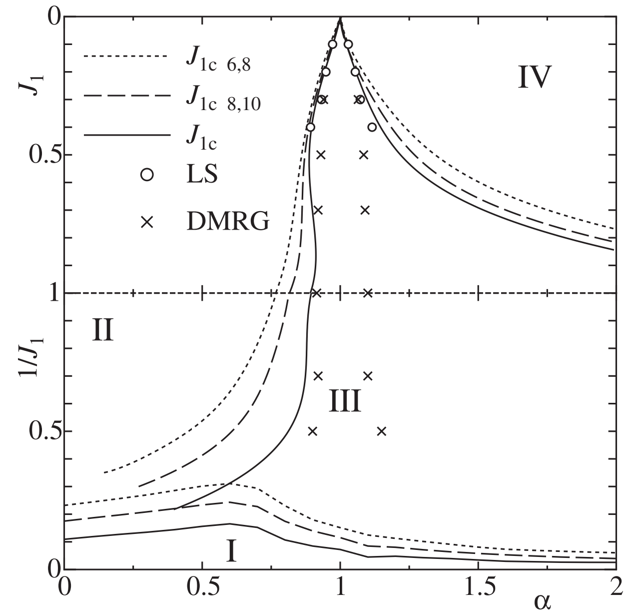

FIG. 4. Ground-state phase diagram of the asymmetric three-leg spin tube (1), derived from the numerical analysis. The phases (I)–(IV) correspond to those in Fig. 2. The cross points are determined by the DMRG. The three kinds of lines are done by the numerical diagonalization. The circle points are obtained from the level-spectroscopy method in Sec. IV C.

ground state and the triplet excited state in the finite but large system. We calculate it by means of the DMRG up to $L=128$, where we do not see such a significant open boundary effect as local edge excitation. In actual DMRG computation, the number of retained bases is up to $m=300$, within which well convergence is achieved for the scaled gap. In Fig. 3(a), the scaled gap $L\Delta$ is plotted versus α for $J_1=0.5$. It indicates that the spin gap is just open in a tiny region $\alpha\sim 1$ and it rapidly vanishes away from $\alpha=1$. Thus we find two critical points α_{c1} and α_{c2} ($\alpha_{c1}<1<\alpha_{c2}$), which are expected to be of the BKT type because of the wide gapless regions outside the gapful phase and the discussion in Sec. III.

In order to determine a phase boundary of the usual second-order phase transition, the phenomenological renormalization equation $L_1\Delta_{L_1}(\alpha_c)=L_2\Delta_{L_2}(\alpha_c)$ is often used effectively. For the present critical point α_c, however, this type of phenomenological renormalization has no clear crossing point. It seems from Fig. 3(a) that the scaled gap $L\Delta$ increases with increasing L in both gapless and gapful phases. This is because the scaled gap is an increasing function with respect to L not only in the gapful phase but also in the gapless phase, since the finite-size gap must have the logarithmic size correction term $\sim -1/\log L$. Here, we should recall that the logarithmic correction normally vanishes just at α_c due to the SU(2) symmetry in the $c=1$ CFT.[32] Therefore, instead of using the crossing point of the scaled gaps, we can estimate α_c as a point where the size correction is minimized. The difference of the scaled gap between two system sizes L_1 and L_2 is plotted versus α for $J_1=0.5$ in Fig. 3(b). The minimum of the difference $L_1\Delta_{L_1}-L_2\Delta_{L_2}$ has a very small L dependence. Note that the minimum value $L_1\Delta_{L_1}-L_2\Delta_{L_2}$ decreases as the size increases. This phenomenon and the assumption of the BKT-type transition suggest that this minimal value approaches zero as the system size increases. This is quite reasonable if we suppose the most important finite-size correction to the scaled gap $L\Delta$ next to $1/\log L$ term is order of $1/L^2$.[32,38,39] We thus determine α_c from the minima for two large systems with $L_1=96$ and $L_2=128$ for $J_1<2$. The estimated α_{c1} and α_{c2} are shown as crosses in Fig. 4. They correspond to the phase boundary between two regions (II) and (III) and that between (III) and (IV), respectively. At least these boundaries for the strong-rung-coupling regime $J_1\leq 2$ are precise enough to justify that a finite gapful phase (III) exists. However, it is difficult to obtain α_c for $J_1>2$ because the DMRG calculation is not well converged there.

In order to determine the phase boundaries for the weak-rung-coupling regime $J_1>2$, we use the minimum points of $L_1\Delta_{L_1}-L_2\Delta_{L_2}$ calculated by the numerical diagonalization up to $L=10$ under the periodic boundary condition. The estimated phase boundaries for $(L_1,L_2)=(6,8)$ and (8,10) are plotted as long-dashed and dashed curves, respectively, in Fig. 4. In addition, the infinite-L curves extrapolated assuming the size correction is proportional to $1/L^2$ in both directions of J_1 and α are also shown as solid curves in Fig. 4. At least the phase boundaries (II)-(III) and (III)-(IV) are consistent with the DMRG results for $J_1\ll 1$. The boundary (III)-(IV) is, however, significantly deviated from the DMRG estimation for $J_1\sim 1$. This discrepancy is supposed to be due to the error of extrapolation. This analysis also justifies the existence of the phase (I). However, the error of extrapolation becomes larger as we approach the line $1/J_1=0$ in the case of $\alpha<1$. Thus it is difficult to conclude that the phase (I) really exists for $\alpha<1$ within the present numerical demonstration. The boundary (I)-(III) will be discussed later. It is also difficult to confirm the boundary (I)-(II), and the phase (I) might combine with the phase (II) in a certain regime with $\alpha<1$.

B. Conformal field theory analysis

The numerical analysis based on CFT is generally efficient in investigating the feature of quantum phase transitions in 1+1 dimensional systems. The conformal invariance gives the L dependences of the ground-state energy E_0 and the energy gaps for triplet excitations Δ_t and that for singlet excitations Δ_s as the forms

$$\frac{E_0}{L} \approx \epsilon_\infty - \frac{\pi v_s}{L^2}\frac{c}{6} + \cdots, \tag{30a}$$

$$\Delta_t \approx \frac{\pi v_s}{L}\left(\eta - \frac{\sigma_t}{\log L} + \cdots\right), \tag{30b}$$

$$\Delta_s \approx \frac{\pi v_s}{L}\left(\eta - \frac{\sigma_s}{\log L} + \cdots\right), \tag{30c}$$

where v_s is the spin wave velocity, c is the central charge, and η, σ_t and σ_s are the critical exponents. These exponents η and σ_t appear in the spin correlation function[36,40]

$$\langle S^\nu_{i,0} S^\nu_{i,j}\rangle \sim (-1)^j (\log|j|)^{\sigma_t}|j|^{-\eta}, \quad (\nu = x,y,z),$$

where $|j| \gg 1$. As discussed in Sec. III, the gapless phases (II) and (IV) are predicted to be described by the level-1 SU(2) WZW model. This model indicates the universal constants $c=1$, $\eta=1$, $\sigma_t=\frac{1}{2}$, and $\sigma_s=-\frac{3}{2}$.

The exponent η can be determined from the triplet and singlet excitation gaps in the finite-size system, by using the relations $\eta = L\Delta_t/\pi v_s + \cdots$ and $\eta = L\Delta_s/\pi v_s + \cdots$. Using the results from the numerical diagonalization for $L=8$ and 10, we estimate c, $L\Delta_t/\pi v_s = \eta_t$ and $L\Delta_s/\pi v_s = \eta_s$ independently, shown in Fig. 5 for $J_1=0.3$. Here, we have evaluated the spin wave velocity by $v_s=(E_1-E_0)/k_1$, where E_1 is the lowest energy of the eigenstate with the smallest nonzero wave number $k_1=\frac{2\pi}{L}$. The velocity is generally nonuniversal and depends on the couplings J_1 and J_r.

In Fig. 5, we also depict a special average $(3L\Delta_t/\pi v_s + L\Delta_s/\pi v_s)/4$ of the singlet and the triplet gaps such that the dominant finite-size logarithmic corrections cancel out each other.[41] This average and c seem to be almost unity in the gapless phases in Fig. 5 as observed in the $S=\frac{1}{2}$ antiferromagnetic Heisenberg chain with the next-nearest-neighbor interaction.[32] These results are completely consistent with the expected BKT transition. We therefore conclude that both gapless phases (II) and (IV) are governed by the WZW model and the transition between (II)-(III) and that between (III)-(IV) belong to the BKT universality class.

Now, we note the level crossing between $L\Delta_t/\pi v_s$ and $L\Delta_s/\pi v_s$ around $\alpha=1$ in Fig. 5. This level crossing implies the appearance of another singlet ground state as a reflection

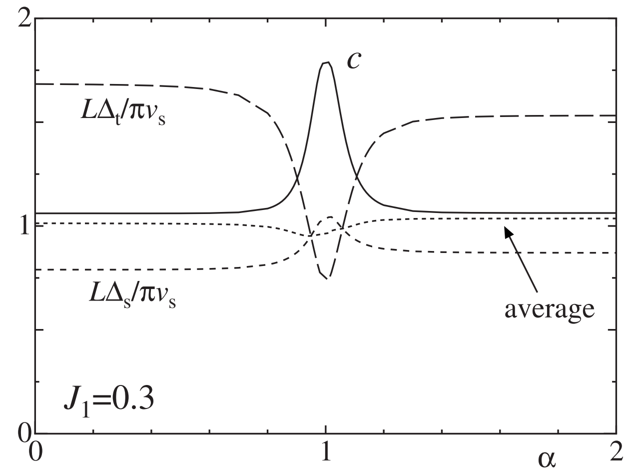

FIG. 5. Central charge c and critical exponents $L\Delta_t/\pi v_s$ and $L\Delta_s/\pi v_s$ including finite-size corrections for $J_1=0.3$. These are estimated from the numerical diagonalization up to $L=10$, based on the size dependence of low-lying energy spectra predicted by the CFT.

of the valence-bond order in the thermodynamic limit. This is a clear numerical evidence of the extended gapful phase (III) predicted by several effective theories. On the contrary, Nishimoto and Arikawa[12] have claimed that the gapless phase is extended everywhere except at the point $\alpha=1$, by means of the DMRG analysis. Our observation does not agree with their claim.

C. Level-spectroscopy method

The level-spectroscopy method[32,42–44] is a very powerful tool to determine the critical point of the BKT transition in one-dimensional quantum systems. For the SU(2)-symmetric cases including the present spin tube, its strategy becomes easier.[32] According to this method, the critical point can be determined as an intersection between the singlet and the triplet excitation gaps, where their logarithmic finite-size corrections vanish. The phase boundaries (II)-(III) and (III)-(IV) estimated by this method are shown in Fig. 6. Here we have applied the results of the numerical diagonalization up to $L=10$ for $J_1=0.2$. The numerical data are well converged to those of the thermodynamic limit by use of the $1/L^2$ extrapolation. The $1/L^2$ extrapolation is justified by considering the most important finite-size correction to the excitation gaps Δ next to the logarithmic term.[32]

Several critical points estimated by the level spectroscopy are plotted by open circles in Fig. 4. We find that at least for $J_1 \ll 1$, the results are in good agreement with the phase boundaries (II)-(III) and (III)-(IV) evaluated in the preceding Sec. IV A.

On the other hand, when we consider the transition between two phases (III) and (I) along the line $\alpha=1$, the finite-size correction to the critical point is too large to determine the precise value of the infinite-length limit, as shown in Fig. 7. The extrapolated value of the critical J_1 results in $1/J_{1c}=0.51\pm0.45$. It is therefore difficult to conclude whether J_{1c} is finite or zero for $\alpha=1$, namely, whether or not the gapless

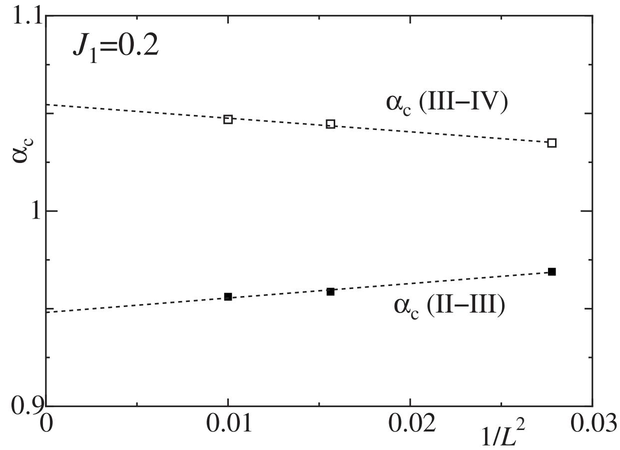

FIG. 6. Critical points α_c evaluated by the level-spectroscopy analysis for $J_1=0.2$, assuming the size correction is proportional to $1/L^2$.

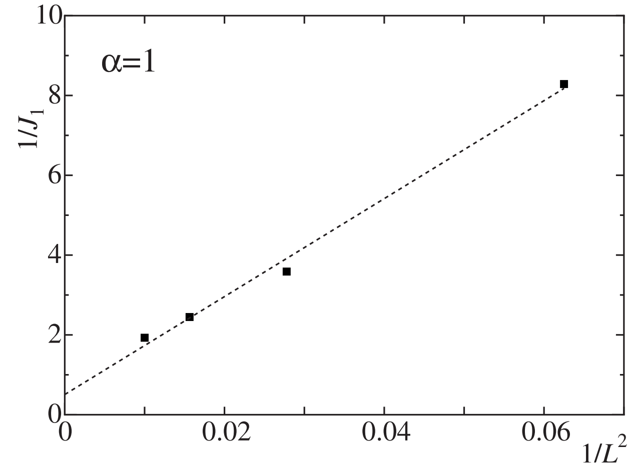

FIG. 7. Critical value of J_1 for the regular triangle spin tube ($\alpha=1$) evaluated by the level-spectroscopy analysis.

phase (I) still survives for small α. [We have already shown the presence of the phase (I) for large $\alpha \gg 1$ in Sec. III B.]

V. CONCLUSIONS AND DISCUSSIONS

We have studied the ground-state phase diagram and the quantum phase transitions of the $S=\frac{1}{2}$ three-leg asymmetric spin tube models defined by Eq. (1). In Sec. III A, based on the Hubbard model on the tube lattice, we have proposed an effective theory to draw a global phase diagram, Fig. 2, in the parameter space (J_1,α). Three gapless phases (I), (II), and (IV) and one gapful phase (III) are found by counting the Fermi points. This effective theory indicates that the level-1 SU(2) WZW model describes two extended gapless phases (II) and (IV) which are separated by a extended gapful phase (III) around $\alpha=1$. In Sec. III B, applying another analytical strategy based on the non-Abelian bosonization, we have proved that the predicted gapless phase (I) is exactly present at least for weak rung couplings $J_1 \gg J_r$ with a strong asymmetry $\alpha \gg 1$. Furthermore, we have argued that the gapful region (III) is surely extended (although narrow) for the case $J_r \gg J_1$ and $J_r \sim J_r'$ in Sec. III C.

Following these results of effective theories in Sec. III, we have numerically analyzed the quantum phase transitions of the spin tube (1) in Sec. IV. The phenomenological renormalization approach based on the DMRG and the numerical diagonalization has enabled us to draw the global phase diagram. The numerical results are qualitatively in agreement with those of effective theories. In addition, we have raised the validity of the phase diagram by means of the numerical finite-size scaling arguments based on the $c=1$ CFT. We have confirmed that the phase transitions (II)-(III) and (III)-(IV) belong to the BKT universality class quantitatively. Here, we make a comment on that the gapped region estimated in Ref. 12, where an unconventional power-law fitting with respect to L is employed, is well inside of the present phase III. We should, however, recall that the gap near the BKT transition is exponentially small and thus the gap is difficult to be detected by the phenomenological renormalization approach, which usually overestimates the gapless region. This suggests that the gapped region in Ref. 12 becomes smaller than the present phase diagram (Fig. 4), although the DMRG data itself may be consistent with each other.

The semiquantitative phase diagram of the spin tube (1) has been constructed in this study (see Figs. 2 and 4), but some subtle issues are still remaining, e.g., (A) the topology of the phase boundaries along the two lines $\alpha=0$ and $1/\alpha=0$, (B) how widely the gapless phase is extended, etc. In order to resolve these problems, more sophisticated approaches would be necessary.

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[1] J. Schnack, H. Nojiri, P. Kögerler, G. J. T. Cooper, and L. Cronin, Phys. Rev. B **70**, 174420 (2004).
[2] P. Millet, J. Y. Henry, F. Mila, and J. Galy, J. Solid State Chem. **147**, 676 (1999).
[3] V. O. Garlea, A. Zheludev, L.-P. Regnault, J.-H. Chung, Y. Qiu, M. Boehm, K. Habicht, and M. Meissner, Phys. Rev. Lett. **100**, 037206 (2008).
[4] V. O. Garlea, A. Zheludev, K. Habicht, M. Meissner, B. Grenier, L.-P. Regnault, and E. Ressouche, arXiv:0807.1571 (unpublished).
[5] H. J. Schulz, in *Correlated Fermions and Transport in Mesoscopic Systems*, edited by T. Martin, G. Montambaux, and J. Tran Than Van (Editions Frontières, Gif-sur-Yvette, 1996), arXiv:cond-mat/9605075.
[6] K. Kawano and M. Takahashi, J. Phys. Soc. Jpn. **66**, 4001 (1997).
[7] D. C. Cabra, A. Honecker, and P. Pujol, Phys. Rev. B **58**, 6241 (1998).
[8] A. Luscher, R. M. Noack, G. Misguich, V. N. Kotov, and F. Mila, Phys. Rev. B **70**, 060405 (2004).
[9] J. B. Fouet, A. Läuchli, S. Pilgram, R. M. Noack, and F. Mila, Phys. Rev. B **73**, 014409 (2006).
[10] K. Okunishi, S. Yoshikawa, T. Sakai, and S. Miyashita, Prog. Theor. Phys. **159**, 297 (2005).
[11] T. Sakai, M. Matsumoto, K. Okunishi, K. Okamoto, and M. Sato, Physica E (Amsterdam) **29**, 633 (2005).
[12] S. Nishimoto and M. Arikawa, Phys. Rev. B **78**, 054421 (2008).
[13] M. Sato and T. Sakai, Phys. Rev. B **75**, 014411 (2007).
[14] M. Sato, Phys. Rev. B **75**, 174407 (2007).
[15] M. Sato, Phys. Rev. B **72**, 104438 (2005).
[16] M. Sato and M. Oshikawa, Phys. Rev. B **75**, 014404 (2007).
[17] E. Lieb, T. Schultz, and D. Mattis, Ann. Phys. (N.Y.) **16**, 407 (1961).
[18] I. Affleck, in *Fields, Strings and Critical Phenomena*, Les Houches Lecture Notes, 1988, edited by E. Brézin and J. Zinn-Justin (Elsevier, Amsterdam, 1989), p. 564.
[19] A. O. Gogolin, A. A. Nersesyan, and A. M. Tsvelik, *Bosonization and Strongly Correlated Systems* (Cambridge University Press, United Kingdom, 1998).
[20] A. M. Tsvelik, *Quantum Field Theory in Condensed Matter Physics*, 2nd ed. (Cambridge University Press, United Kingdom, 2003).
[21] J. L. Cardy, J. Phys. A **17**, L385 (1984).
[22] H. W. J. Blöte, J. L. Cardy, and M. P. Nightingale, Phys. Rev. Lett. **56**, 742 (1986).
[23] I. Affleck, Phys. Rev. Lett. **56**, 746 (1986).
[24] Z. L. Berezinskii, Zh. Eksp. Teor. Fiz. **59**, 907 (1970) [Sov. Phys. JETP **32**, 493 (1971)].
[25] J. M. Kosterlitz and D. J. Thouless, J. Phys. C **6**, 1181 (1973).
[26] L. Balents and M. P. A. Fisher, Phys. Rev. B **53**, 12133 (1996).
[27] E. Arrigoni, Phys. Lett. A **215**, 91 (1996).
[28] H. H. Lin, L. Balents, and M. P. A. Fisher, Phys. Rev. B **56**, 6569 (1997).
[29] M. Sato (unpublished).
[30] I. Affleck and F. D. M. Haldane, Phys. Rev. B **36**, 5291 (1987).
[31] We have neglected the difference between the Fermi velocities of the first and second bands.
[32] K. Okamoto and K. Nomura, Phys. Lett. A **169**, 433 (1992).
[33] D. G. Shelton, A. A. Nersesyan, and A. M. Tsvelik, Phys. Rev. B **53**, 8521 (1996).
[34] A. M. Polyakov, in *Two Dimensional Quantum Gravity: Superconductivity at High Tc*, Les Houches Lecture Notes, 1988, edited by E. Brézin and J. Zinn-Justin (North-Holland, Amsterdam, 1990), p. 305.
[35] C. Itoi and H. Mukaida, J. Phys. A **27**, 4695 (1994).
[36] C. Itoi and M.-H. Kato, Phys. Rev. B **55**, 8295 (1997).
[37] Note that the Dirac fermions $(\Psi_{i,\alpha},\bar{\Psi}_{i,\alpha})$ are used to describe the level-1 SU(2) WZW model as the effective theory of each decoupled Heisenberg chain, while the fermions $(\psi_{i,\sigma},\bar{\psi}_{i,\sigma})$ in Sec. III A represent electrons in the Hubbard tube. The physical meanings of these two kinds of fermions are different.
[38] J. L. Cardy, J. Phys. A **19**, L1093 (1986).
[39] J. L. Cardy, J. Phys. A **20**, 5039 (1987).
[40] T. Giamarchi and H. J. Schulz, Phys. Rev. B **39**, 4620 (1989).
[41] T. Ziman and H. J. Schulz, Phys. Rev. Lett. **59**, 140 (1987).
[42] K. Nomura and K. Okamoto, J. Phys. A **27**, 5773 (1994).
[43] K. Okamoto, Prog. Theor. Phys. **145**, 113 (2002).
[44] K. Nomura and A. Kitazawa, in Proceedings of the French-Japanese Symposium on Quantum Properties of Low-Dimensional Antiferromagnets, edited by Y. Ajiro and J.-P. Boucher (Kyushuu University Press, Fukuoka, 2002), arXiv:cond-mat/0201072.