Phase diagram of the $S=\frac{1}{2}$ two-leg spin ladder with staggered bond alternation

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The ground state of the $S=1/2$ two-leg ladder with the staggered bond alternations is investigated. We have determined the precise phase diagram on the δ-J' plane (δ and J' are the magnitudes of the bond alternation and the rung interaction, respectively), employing the level spectroscopic analysis of the numerical diagonalization data obtained by the Lanczos algorithm with the twisted boundary condition. The phase boundary between the leg-dimer state and the rung-dimer state near $(\delta,J')=(0,0)$ is of the form $J'\propto\delta^{0.69}$, which is consistent with the prediction $J'\propto\delta^{2/3}$ by Martín-Delgado, Duleksky, and Sierra, and also by Wang and Nersesyan, but not with $J'\propto\delta^2$ by Cabra and Grynberg.

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I. INTRODUCTION

In recent years the spin systems with the excitation gaps have been extensively studied theoretically, numerically, and experimentally. In this report we study the ground-state phase diagram of the $S=1/2$ two-leg ladder with the staggered bond alternations, which is sketched in Fig. 1. The Hamiltonian of our model is given by

$$H=\sum_j \sum_{\alpha=1,2} [1+(-1)^{j+\alpha}\delta]\boldsymbol{S}_{\alpha,j}\cdot\boldsymbol{S}_{\alpha,j+1}+J'\sum_j \boldsymbol{S}_{1,j}\cdot\boldsymbol{S}_{2,j}, \tag{1}$$

where α labels the leg, and δ and J' are the magnitudes of the bond alternation and the rung interaction, respectively. We can set $\delta>0$ without loss of generality. All the interactions are assumed to be antiferromagnetic.

As is well known, both the bond alternation and the rung interaction bring about the spin gap due to the formation of the effective singlet pairs. First we consider the case near $(\delta,J')=(0,0)$. When $J'=0$, our model is reduced to two independent bond alternating chains, where two spins connected by $1+\delta$ interactions effectively form a singlet pair (leg-dimer state). For the $\delta=0$ case, on the other hand, the effective singlet pair is composed of two spins connected by the rung interactions (rung-dimer state). Next let us consider the $\delta=1$ case where the $1-\delta$ interactions (thick lines in Fig. 2) vanish. In this case, our model is reduced to the usual $S=1/2$ chain with the bond alternation. The ground state is the leg-dimer state when $J'<2$, the rung-dimer state when $J'>2$, and the spin-fluid state when $J'=2$.

From the above limiting cases, we see that the ground-state phase diagram is composed of the leg-dimer state and the rung-dimer state. On the phase boundary of these states the spin-fluid state (gapless) is realized. This fact was originally suggested by Martín-Delgado, Shankar, and Sierra[1] (MSS) through use of the nonlinear σ model approach. The boundary between these two state will start at $(\delta,J')=(0,0)$ and end at $(\delta,J')=(1,2)$. Martín-Delgado, Duleksky, and Sierra[2] (MDS) stated that the phase boundary near $(\delta,J')=(0,0)$ is of the form $J'\propto\delta^{2/3}$. MDS have considerated the following. The gap due to the bond alteration is proportional to[3] $\delta^{2/3}$ when $J'=0$, and that due to the rung interaction is proportional to[4] J' when $\delta=0$. Then the phase boundary is determined by the equation $J'\sim\delta^{2/3}$, where two gap-generating mechanisms cancel each other. Later Wang and Nersesyan[5] (WN) obtained the same conclusion $J'\sim\delta^{2/3}$, by use of the Majorana fermion method, and also pointed out that the criticality of the present problem is essentially the same as that of the $S=1$ bilinear and biquadratic chain with the bond alternation near the Takhtajan[6] and Babujian[7,8] point which is discussed by Kitazawa and Nomura.[9] On the other hand, Cabra and Grynberg[10,11] (CG) discussed this problem by use of the bosonization technique and concluded that the phase boundary is of the form $J'\propto\delta^2$. Kotov, Oitmaa, and Wielhong[12] (KOW) studied this problem by use of the dimer series expansion and the diagrammatic analysis of an effective Hamiltonian. Although MDA, CG, and KOW performed the numerical diagonalization of this model, these groups could not determine the precise phase diagram because of the numerical errors coming from the extrapolation procedure of the gap data which becomes more severe as the point $(\delta,J')=(0,0)$ is approached. Thus the form of the phase boundary remains an unsolved problem.

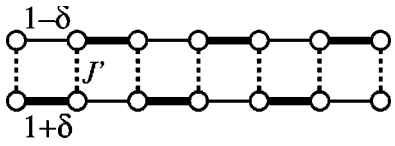

FIG. 1. $S=1/2$ two-leg ladder with the staggered bond alternations. Thick lines represent the stronger leg interactions $1+\delta$, thin lines the weaker leg interactions $1-\delta$, and the dotted lines the rung interactions J'.

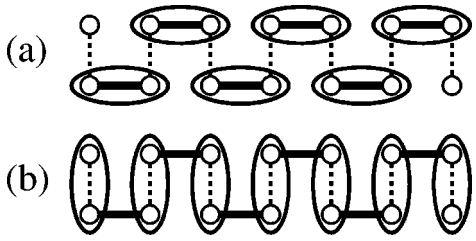

FIG. 2. The ground states when $\delta=1$. (a) the $J'<2$ case, and (b) the $J'>2$ case. Ellipses denote the effective singlet pair.

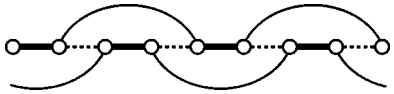

FIG. 3. Linear chain representation of our model. Thick lines represent $1+\delta$ interactions, thin lines $1-\delta$ interactions, and the dotted lines J' interactions.

In this report we determine the precise phase diagram from the numerical diagonalization data by use of the level spectroscopy[13,14] with the twisted boundary condition developed by Kitazawa.[15] Our result supports the form $J' \propto \delta^{2/3}$ predicted by MDS and WN.

II. NUMERICAL ANALYSIS

If we redraw the model into the single-chain form (Fig. 3), the transition between the leg-dimer state and the rung-dimer state is interpreted as the different configuration of the dimers. Namely, the dimers exist on the thick lines in the leg-dimer state, and on the dotted lines in the rung-dimer state. Kitazawa[15] proposed the twisted boundary condition (TBC) method for this kind of transition. In his method, the leg-dimer state and the rung-dimer state are distinguished by the parity $P=\pm 1$ for the space inversion transformation $\boldsymbol{S}_j \rightarrow \boldsymbol{S}_{L-j+1}$ where L is the number of spins. The transition point can be known from crossing the energies of the lowest states with $P=\pm 1$. We have done the numerical diagonalization by the Lanczos method up to 24 spins. We show an example of the crossing in Fig. 4.

We can determine the final transition point by the $L\rightarrow\infty$ extrapolation of the crossing data $\delta_c(J',L)$. Thus we obtain the phase diagram in Fig. 5. From the log-log plot [Fig. 5(b)], we see that the phase boundary near $(\delta,J')=(0,0)$ is expressed by

$$J'_c = 1.9\delta^{0.69} \quad [\text{near } (\delta,J')=(0,0)], \tag{2}$$

which is consistent with the prediction $J' \propto \delta^{2/3}$ by MSS and WN. We note that the estimated error for the exponent 0.69 is less than 0.01. Similar log-log plot near $(\delta,J')=(1,2)$ shown in Fig. 5(c) leads to

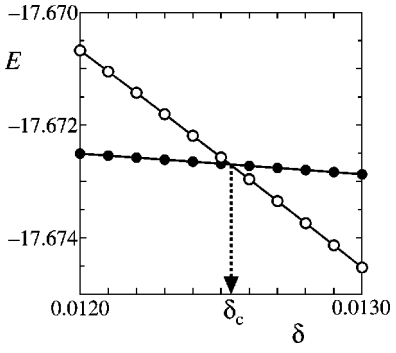

FIG. 4. Crossing of the energies of the lowest states with the different parity when $J'=0.1$ and $L=20$. Open circles denote the energies with $P=1$, and closed circles those with $P=-1$. From the crossing point we can estimate $\delta_c(J'=0.1,L=20)=0.012\,53$ as indicated by the arrow.

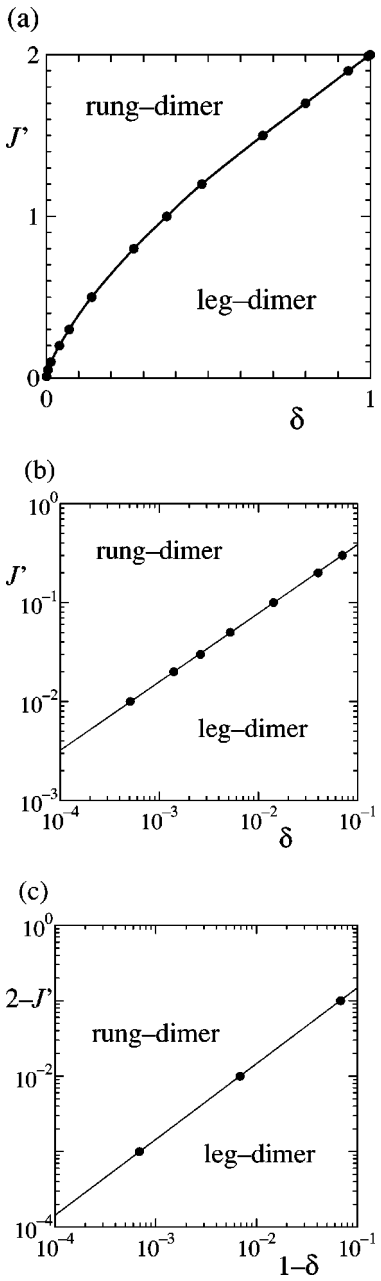

FIG. 5. (a) Phase diagram of the present model. (b) The log-log plot of the phase boundary near $(\delta,J')=(0,0)$. which can be fitted by $J'=1.9\delta^{0.69}$. (c) The log-log plot of the phase boundary near $(\delta,J')=(1,2)$, which can be fitted by $2-J'=1.50(1-\delta)$. The estimated errors are less than the size of marks for (a), (b), and (c).

$$2-J'_c = 1.50(1-\delta) \quad [\text{near } (\delta,J')=(1,2)]. \tag{3}$$

III. DISCUSSION

We have obtained the boundary equation $J'_c=1.9\delta^{0.69}$ near $(\delta,J')=(0,0)$, which is consistent with the prediction $J' \propto \delta^{2/3}$ by MSS and WN. Our exponent, 0.69, is slightly larger than the predicted value 2/3. This can be explained as follows. For the bond alternating chain, the dimer gap behaves as $\delta^{2/3}/\sqrt{|\ln\delta|}$ when we take into account the margin-

ally irrelevant operator that generates the Néel gap, as pointed out by Black and Emery.[16] Thus the apparent dimer gap exponent will be somewhat larger than 2/3 due to the logarithmic correction effect, if we estimate it from the numerical data assuming the pure power law.[17,18] MSS conjectured that the preceding numerical factor is 2 (our value is 1.9), because $J_c'=2\delta^{2/3}$ is satisfied even when $(\delta,J')=(1,2)$. However, this is not justified since the form $J_c' \propto \delta^{2/3}$ will be valid only near $(\delta,J')=(0,0)$.

CG have discussed the phase boundary near $(\delta,J')=(0,0)$ by use of the bosonization method. They bosonized the single-chain Hamiltonian using the phase variables ϕ_1 and ϕ_2, which are hybridized with each other by the introduction of the interchain rung couplings. They first made a linear transformation of these two phase variables to diagonalize the harmonic part of the bosonized Hamiltonian, and treated the bond alternation effect perturbationally. In their treatment, it seems that the effect of the bond alternation was considered after that the spin gap is established due to the interchain rung couplings. In such a case the noninteger exponent will not appear, because the perturbation with respect to δ will be valid as far as δ is small. Since the present Hamiltonian is symmetric under the transformation $\delta \Leftrightarrow -\delta$, the perturbational expansion begins with δ^2. Thus the conclusion of CG was $J' \propto \delta^2$.

Near $(\delta,J')=(1,2)$ we have obtained

$$2-J_c' \propto 1-\delta. \tag{4}$$

If we neglect the $1-\delta$ interactions (thin lines in Fig. 3), the phase boundary near $(\delta,J')=(1,2)$ clearly has the form $2-J_c'=1-\delta$, because the interactions of the thick lines are $2-(2-J')$ and those of the dotted lines are $2-(1-\delta)$. The thin line interactions $1-\delta$ are the third-neighbor interactions in the linear chain representation of Fig. 3, which may modify only the coefficient of the relation, resulting in $2-J_c' \propto 1-\delta$.

Very recently Wang, Essler, Fabrizio, and Nersesyan[19] (WEFN) discussed the competition between the rung interaction and the staggered magnetic field in $S=1/2$ two-leg ladder. Namely, instead of the bond alternation of our model, there exists the staggered magnetic field

$$h\sum_j \sum_{\alpha=1,2} (-1)^j S_j^z \tag{5}$$

in their model. The rung interactions are going to form a singlet dimer pair at the rung, whereas the staggered field will form a $\uparrow\uparrow$ or $\downarrow\downarrow$ pair at the rung. They treated this competition problem between these two states by use of the bosonization method and the Majonara fermion method. Their phase boundary was $J' \propto h^{2/3}$, which is the same form as our Eq. (2). In one chain problem, the effects of the bond alternation and the staggered magnetic field are expressed as very similar mass-generating terms in the language of the bosonized Hamiltonian. We think that our level spectroscopy method of analyzing the numerical data can be also applied to this staggered field problem.

In conclusion, we have numerically determined the phase diagram of the $S=1/2$ two-leg ladder with the staggered bond alternations [Fig. 1 and Eq. (1)]. Our phase boundary is consistent with that predicted by Martín-Delgado, Shankar, and Sierra,[2] and also by Wang and Nersesyan,[5] but not with that by Cabra and Grynberg.[10,11] We believe that our work gives the definite conclusion on the phase boundary form of the present model.

Note added in proof. After this work was completed, I was informed that M. Nakamura, T. Yamamoto, and K. Ide investigated the same model (to be published in J. Phys. Soc. Jpn.). Their conclusion is essentially the same as that in this paper.

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