

# Numerical diagonalization study of an $S = \frac{1}{2}$ ladder model with open boundary conditions

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(Received 11 January 1994; revised manuscript received 16 May 1994)

Low-lying energy states of an  $S = \frac{1}{2}$  ladder model are investigated by applying the numerical diagonalization method to finite clusters. This model has the antiferromagnetic intrachain coupling  $J$  ( $J > 0$ ) and the ferromagnetic interchain one  $-\lambda J$  ( $\lambda > 0$ ). Both the inverse correlation length  $\xi^{-1}(\lambda)$  and an energy gap are shown to be finite at least for  $\lambda \geq 0.05$ , the former of which is shown to approach the same value as that of the  $S = 1$  antiferromagnetic Heisenberg chain with increasing  $\lambda$ . A generation mechanism of the gap is also discussed in terms of a simple model by using the Lieb-Mattis theorem.

## I. INTRODUCTION

Haldane predicted that the antiferromagnetic (AF) Heisenberg chain with integer spins has a finite energy gap (Haldane gap) above the singlet ground state (Haldane state) and that the ground-state correlation functions decay exponentially with respect to the spatial distance, while the AF Heisenberg chain with half-odd-integer spins has no energy gap above the singlet ground state and the ground-state correlation functions exhibit a power-law decay with respect to the spatial distance.<sup>1,2</sup> His prediction has been supported by a number of numerical, experimental, and theoretical works.<sup>3-21</sup> In the last few years, various double-chain models with  $S = \frac{1}{2}$  spins have been investigated<sup>22-30</sup> in relation to the Haldane gap problem of the chain with  $S = 1$  spins. We have investigated an  $S = \frac{1}{2}$  ladder model as one of them. This model has an AF intrachain coupling  $J$  ( $J > 0$ ) and a ferromagnetic interchain coupling  $-\lambda J$  ( $\lambda > 0$ ) and is schematically shown in Fig. 1.

Letting  $J$  be the unit of energy, the Hamiltonian is written as

$$H = H_\sigma + H_\tau + H_{\sigma\tau}, \tag{1}$$

where

$$H_\sigma = \sum_{i=1}^N \sigma_i \cdot \sigma_{i+1}, \tag{2}$$

$$H_\tau = \sum_{i=1}^N \tau_i \cdot \tau_{i+1}, \tag{3}$$

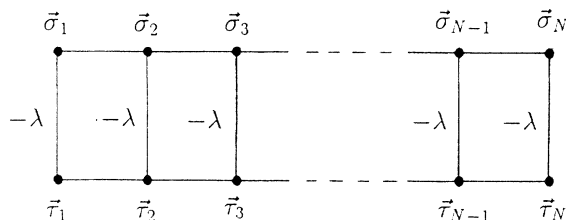


FIG. 1. The quantum spin ladder with  $S = \frac{1}{2}$  spins. The spin operator on site  $i$  ( $\sigma_i$  and  $\tau_i$ ) is coupled with  $-\lambda$  for all  $i$ .

$$H_{\sigma\tau} = -\lambda \sum_{i=1}^N \sigma_i \cdot \tau_i, \tag{4}$$

with  $\sigma_{N+1} = \sigma_1$  and  $\tau_{N+1} = \tau_1$  if we select periodic boundary conditions for the ladder with the length  $N$ . This model is fitted to study properties of the Haldane systems since we can prove that the model is reduced to an  $S = 1$  AF Heisenberg chain of which exchange couplings are  $\frac{1}{2}$  in the limit  $\lambda \rightarrow \infty$ .<sup>31</sup> Hida obtained the following results using the numerical diagonalization method, the projector Monte Carlo method, and a perturbational theory.<sup>26</sup>

(1) A finite energy gap appears when  $\lambda$  is large enough.

(2) With the decrease of  $\lambda$ , the energy gap decreases rapidly between  $\lambda = 1.0$  and  $0.6$  and it is undetectably small for  $\lambda < 0.6$ .

(3) The gap for small  $\lambda$  is, if it exists, of higher order in  $\lambda$  or essentially singular at  $\lambda = 0$ .

Further, Hida mapped the model with spin-space anisotropies to a coupled nonlinear  $\sigma$  model in a semiclassical limit and accordingly argued that  $\lambda_C$ , at which an excitation gap opens, might be finite in a vortex gas picture of the nonlinear  $\sigma$  model even if we approach the isotropic limit.<sup>27</sup> Takada and the author transformed the model with open boundary conditions to a ferromagnetic model with  $Z_2 \times Z_2$  symmetry using the Kennedy-Tasaki transformation,<sup>32,33</sup> and consequently showed that the ground state is fourfold degenerate in a whole region  $\lambda > 0$  with using a mean-field-type variational wave function,<sup>29</sup> the degeneracy of which ground state is due to an edge effect of the Haldane state<sup>21</sup> and is accompanied with a finite value of a string order parameter proposed by den Nijs and Rommelse<sup>34</sup> and by Tasaki.<sup>35</sup> The author, Nomura, and Takada applied Wilson's renormalization-group method to the bosonized Hamiltonian of the model and thereby concluded as follows.<sup>30</sup>

(1)  $\lambda_C = 0$ .

(2) An inverse correlation length increases gradually with the increase of  $\lambda$  as that does above  $T_C$  of the Kosterlitz-Thouless transition.<sup>36</sup>

(3) The string order parameter is finite for  $\lambda > 0$ .

As for the case in which the interchain couplings are antiferromagnetic ( $\lambda < 0$ ), Barnes *et al.* showed existence

of a finite energy gap, the  $\lambda$  dependence of which gap does not obey the function  $E_{\text{gap}} \approx c_1 \lambda + c_2 \lambda^2$  near  $\lambda=0$  using the Monte Carlo method with a guiding-random-walk algorithm.<sup>37</sup> In the limit  $N \rightarrow \infty$ , the linear coefficient  $c_1$  is finite and negative, and the quadratic coefficient  $c_2$  diverges linearly with  $N$ . In that case, Hsu *et al.* concluded that the interchain couplings are relevant with numerically examining level distributions of finite clusters.<sup>38</sup> Their results seem to support our previous results since we can show that the Kosterlitz-Thouless-like behavior near  $\lambda=0$  also occurs even if we apply our bosonization technique to this case.<sup>39</sup> Further, Hida's argument is not conclusive since the vortex gas picture applied by him does not hold in the isotropic limit. Our argument is, however, neither conclusive since we neglected the intrachain umklapp terms in bosonizing the Hamiltonian, although Schulz succeeded in explaining the ground-state phase diagram of the  $S=1$  AF Heisenberg chain with a single-ion anisotropy in the same approximation.<sup>23</sup> In conclusion, further studies are necessary to determine whether  $\lambda_C=0$  or not.

A ladder lattice system is realized in the laboratory by the vanadyl pyrophosphate,  $(\text{VO})_2\text{P}_2\text{O}_7$ , and was experimentally studied by Johnston *et al.*<sup>40</sup> Although the lattice structure is a ladder, they reported that both the magnitude and the temperature dependence of its magnetic susceptibility accurately agree with those predicted by Bonner *et al.*<sup>41</sup> for an  $S=\frac{1}{2}$  bond-alternating AF Heisenberg chain of which alternation ratio  $J_2/J_1$  ( $\equiv \alpha$ ) is 0.6. The bond-alternating chain is reduced to the  $S=1$  AF Heisenberg chain in the limit  $\alpha \rightarrow -\infty$ . The point  $\alpha=0.6$  is located in the Haldane-phase region in the ground-state phase diagram of the bond-alternating chain according to Hida.<sup>42</sup> The temperature dependence of the susceptibility of the material further resembles that of the typical Haldane gap material, NENP  $[\text{Ni}(\text{C}_2\text{H}_8\text{N}_2)_2\text{NO}_2(\text{ClO}_4)]$ . These facts suggest that  $(\text{VO})_2\text{P}_2\text{O}_7$  is one of the Haldane gap systems although we cannot exclude the possibility that an energy gap arises from another mechanism.

In this paper, we investigate low-lying states of the  $S=\frac{1}{2}$  ladder model for  $\lambda > 0$  with open boundary conditions and show evidence suggesting  $\lambda_C=0$ . We further intend to clarify a gap-generation mechanism of the ladder model for  $\lambda > 0$  in terms of a simple model with some defect using the Lieb-Mattis theorem.<sup>43</sup>

In Sec. II, we estimate values of an inverse correlation length for several values of  $\lambda$  using the numerical diagonalization method. It is shown that the inverse correlation length approaches that of the  $S=1$  AF Heisenberg chain in increasing  $\lambda$  and that  $\lambda_C$  is less than 0.05. Our results also suggest that an energy gap opens for  $\lambda \geq 0.05$ . Section III is devoted to discussion.

## II. NUMERICAL RESULTS

We show low-lying states of the ladder models with  $N=6$  and 5 in Figs. 2 and 3, respectively. The energies are calculated within the subspace in which the total number of the  $Z$  components of the spins are zero, and

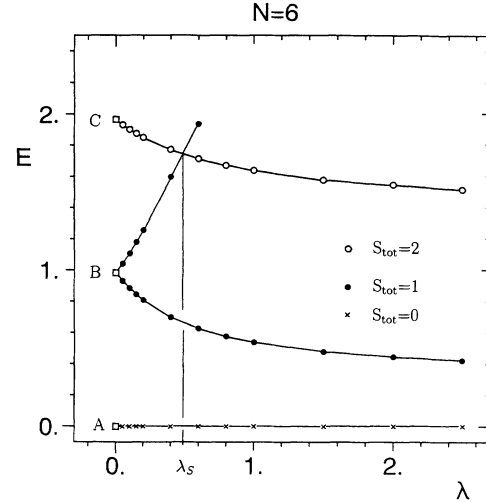


FIG. 2. Low-lying levels measured from the lowest one for  $N=6$ . The solid dots, open dots, and crosses are used according to  $S_{\text{tot}}=1, 2$ , and 0, respectively.

are measured from the lowest energy. We show the energies with different symbols according to  $S_{\text{tot}}$ , which is defined by  $\{\sum_i (\sigma_i + \tau_i)\}^2 = S_{\text{tot}}(S_{\text{tot}} + 1)$ . The solid dots, open dots, and crosses denote the state with  $S_{\text{tot}}=1, 2$ , and 0, respectively. We use the open squares at points A, B, and C to show low-lying states for  $\lambda=0$ . For  $N=6$ , the lowest state is a singlet, which is proved with the Lieb-Mattis theorem. The second lowest state is a triplet and is connected to the point B in decreasing  $\lambda$ . The third and fourth lowest states cross at  $\lambda_S$ , one of which states is the triplet connected to the point B in decreasing  $\lambda$  and the other is the quintuplet connected to the point C in decreasing  $\lambda$ . It is further found that the energy difference between the points A and B is numerically equal to that between the points B and C. A similar feature is observed for the other even  $N$  ( $N=4, 8$ , and 10), and we thus discuss the case of  $N=6$  as an example of general even  $N$ 's. We are interested particularly in

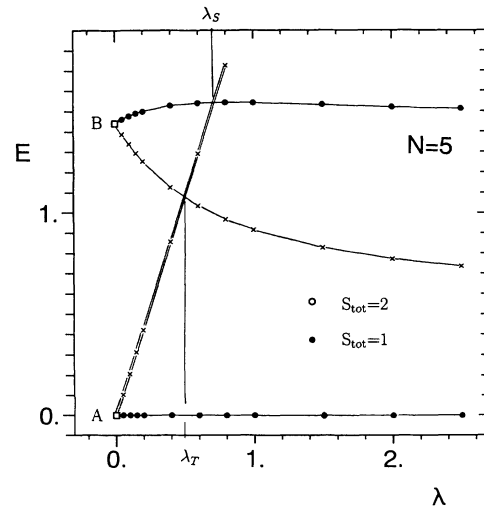


FIG. 3. Low-lying levels measured from the lowest one for  $N=5$ . The solid dots, open dots, and crosses are used according to  $S_{\text{tot}}=1, 2$ , and 0, respectively.

how these spectra change in increasing  $N$ . At the first step, note that there are the two open AF Heisenberg chains with  $N$  spins of  $S = \frac{1}{2}$  when  $\lambda = 0$ . The eigenstate associated with point  $A$  is a singlet ( $S_{\text{tot}} = 0$ ) since this state is composed of the two lowest states ( $S = 0$ ) of both chains. Point  $B$  is the junction of two triplets ( $S_{\text{tot}} = 1$ ), which reflects the eigenstates associated with this point are composed of the lowest state ( $S = 0$ ) of one chain and the second-lowest one ( $S = 1$ ) of the other chain. Point  $C$  is the junction of another singlet ( $S_{\text{tot}} = 0$ ), another triplet ( $S_{\text{tot}} = 1$ ), and the quintuplet ( $S_{\text{tot}} = 2$ ), but both the singlet and the triplet will be ignored in this argument. This situation reflects that the eigenstates associated with point  $C$  are composed of the two second-lowest states ( $S = 1$ ) of both chains. [Here, the difference between the lowest and the third-lowest energies of the chain is larger than  $2\Delta_1(N)$  for even  $N$ , where  $\Delta_1(N)$  denotes the difference between the lowest and the second-lowest energies of the chain.] At the second step, let us define  $\Delta_1(N, \lambda)$  and  $\Delta'_1(N, \lambda)$  for even  $N$  as the differences between the second-lowest and the lowest states and between the quintuplet and the second-lowest ones, respectively. The difference  $\Delta_1(N, \lambda)$  is expected to approach zero in increasing  $N$ , according to  $\Delta_1(N, \lambda) \propto \exp[-N/\xi(\lambda)]$  for  $\lambda > 0$ , where  $\xi(\lambda)$  diverges in the limit  $\lambda \rightarrow 0$ . If  $\lambda_S$  approaches zero in increasing  $N$ , then we expect

$$\Delta(\lambda) = \lim_{N \rightarrow \infty} [\Delta'_1(N, \lambda) - \Delta_1(N, \lambda)]_{N=\text{even}}$$

as an energy gap in the limit  $N \rightarrow \infty$  for  $\lambda > 0$ , since the quintuplet approaches the lowest excited state in increasing  $N$ . If  $\lambda_S$  was finite in the limit  $N \rightarrow \infty$ , then a crossover of the gap generation might occur at  $\lambda_S$  in varying  $\lambda$ , as seen in Fig. 4(a).

However, Fig. 5 showing  $\lambda_S$  against  $N^{-1}$  makes us expect  $\lambda_S = 0$  in the limit  $N \rightarrow \infty$ . In Fig. 6, we show  $\Delta'_1(N, \lambda) - \Delta_1(N, \lambda)$  for even  $N$ . The energy gap in the limit  $N \rightarrow \infty$  looks to open for  $\lambda \geq 0.05$ , since in increasing  $N$  the gap shows no  $N$  dependence at  $\lambda = 0.05$ .

Let us examine the odd- $N$  case. See Fig. 3 for  $N = 5$ . The lowest state is a triplet, which is proved with the Lieb-Mattis theorem. Two singlets cross at  $\lambda_T$ , one state of which is connected with point  $A$  in decreasing  $\lambda$  and the other is connected to point  $B$  in decreasing  $\lambda$ . The singlet state connected to point  $A$ , further, crosses over the triplet state connected to point  $B$  at  $\lambda_S$  in increasing  $\lambda$ . A similar feature is detected for  $N = 7, 9$ , and  $11$ , and we thus argue the case  $N = 5$  as an example of general odd  $N$ 's. We are interested particularly in how these spectra change in increasing  $N$ . At the first step, note that there are the two open AF Heisenberg chains with  $N$  spins of  $S = \frac{1}{2}$ , when  $\lambda = 0$ . Point  $A$  is the junction of the lowest state ( $S = 1$ ) and a singlet ( $S = 0$ ), which reflects that the eigenstates associated with this point are composed of the two lowest states ( $S = \frac{1}{2}$ ) of both chains. On the other hand, point  $B$  is the junction of the upper triplet ( $S_{\text{tot}} = 1$ ) and the other singlet ( $S_{\text{tot}} = 0$ ), which reflects that the eigenstates associated with this point are composed of the lowest state ( $S = \frac{1}{2}$ ) of one chain and the

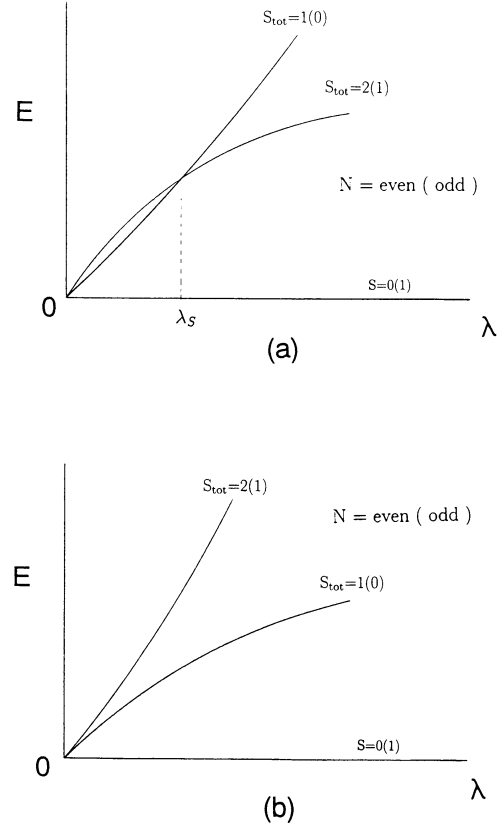


FIG. 4. The expected spectrums of the infinite volume ladder model with  $S = \frac{1}{2}$  spins are shown in (a) and (b) when  $\lambda_S$  is finite and zero, respectively.

second-lowest state ( $S = \frac{1}{2}$ ) of the other chain. At the second step, let us define  $\Delta_1(N, \lambda)$  and  $\Delta'_1(N, \lambda)$  for odd  $N$  as the differences between the singlet state connected to point  $B$  and the lowest state and between the upper triplet and the lowest states, respectively. The difference

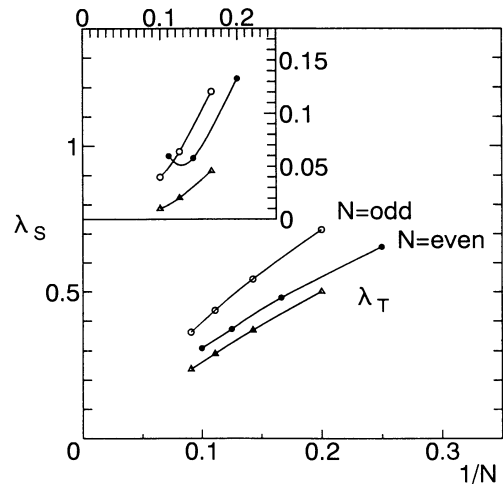


FIG. 5. The extrapolation of  $\lambda_S$  and  $\lambda_T$  in terms of  $N^{-1}$ . The inset shows  $\lambda_S(N)$  and  $\lambda_T(N)$  redefined by fitting  $\lambda_S(N-1)$  and  $\lambda_S(N+1)$  linearly and fitting  $\lambda_T(N-1)$  and  $\lambda_T(N+1)$  linearly, respectively.

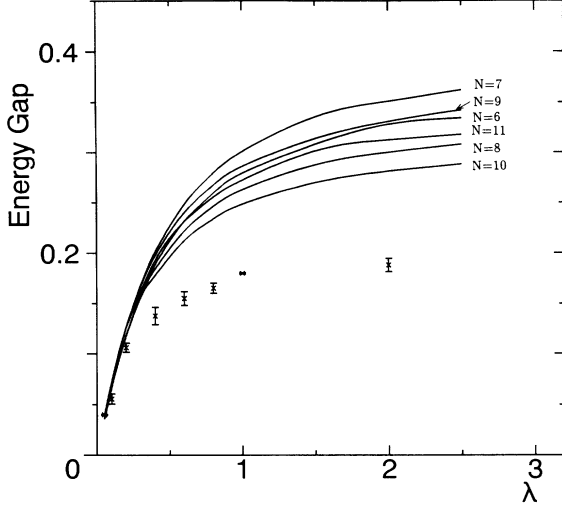


FIG. 6. The energy gap against  $\lambda$ . The crosses display the energy gap of the infinite volume ladder.

$\Delta_1(N, \lambda)$  is expected to approach zero in increasing  $N$ , according to  $\Delta_1(N, \lambda) \propto \exp[-N/\xi(\lambda)]$  for  $\lambda > 0$ . Since both  $\lambda_T$  and  $\lambda_S$  approach zero in increasing  $N$ , as seen in Fig. 5, we expect

$$\Delta(\lambda) = \lim_{N \rightarrow \infty} [\Delta'_1(N, \lambda) - \Delta_1(N, \lambda)]_{N=\text{odd}}$$

as the energy gap in the limit  $N \rightarrow \infty$ . This means that the upper triplet connected to point  $B$  approaches the lowest excited state as  $N$  increases. In Fig. 6, we show  $\Delta'_1(N, \lambda) - \Delta_1(N, \lambda)$  for odd  $N$ . Since it shows no  $N$  dependence at  $\lambda = 0.05$  in increasing  $N$ , the energy gap looks to open for  $\lambda \geq 0.05$ .

We summarize both results for odd and even  $N$  as follows. Figure 4(b) shows an expected energy spectrum in the limit  $N \rightarrow \infty$ . Here, it has been assumed that the ground state becomes fourfold degenerate in the limit  $N \rightarrow \infty$  since the lowest state with  $S_{\text{tot}} = 0$  (1) and the second-lowest state with  $S_{\text{tot}} = 1$  (the singlet connected to point  $B$ ) are mixed when  $N$  is even (odd). The total spin of the lowest excited state in the limit  $N \rightarrow \infty$  is two (one) for even (odd)  $N$ . Figure 6 suggests that  $\lambda_C$  is less than 0.05 even in the limit  $N \rightarrow \infty$ . In this figure, the crosses depict the energy gap in the thermodynamic limit, the gap of which is given as follows. We have fitted  $\Delta(N, \lambda)$  defined as  $\Delta'_1(N, \lambda) - \Delta_1(N, \lambda)$  with the formula<sup>26</sup>

$$\Delta(N, \lambda) = \Delta(\infty, \lambda) + \delta\Delta(\lambda) N^{\alpha(\lambda)} e^{-N/\xi(\lambda)}, \quad (5)$$

in a least-squares fit for even and odd  $N$ , respectively. At that time,  $\alpha(\lambda)$  was chosen by hand in order to make the difference of  $\Delta(\infty, \lambda)$  for even and odd  $N$  as small as we can. We regarded the mean value and the difference of  $\Delta(\infty, \lambda)$  for even and odd  $N$  as the extrapolated energy gaps and the error bars for several values of  $\lambda$ , respectively.

Let us define a variable approaching the inverse correlation length,  $\xi_N^{-1}(\lambda)$ , in the limit  $N \rightarrow \infty$ :

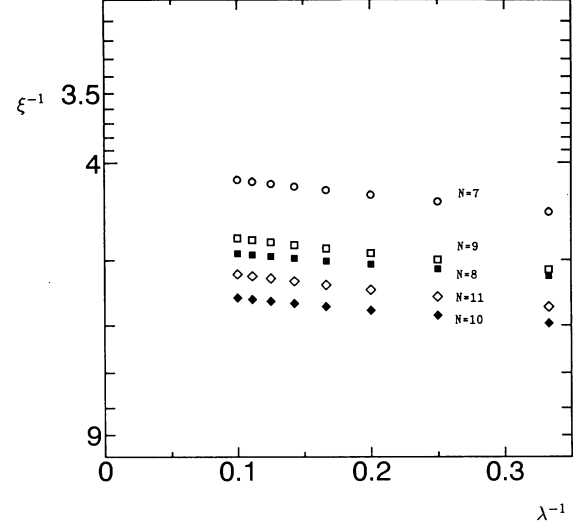


FIG. 7.  $\xi_N^{-1}(\lambda)$  from  $N=7$  to 11 against  $\lambda^{-1}$ . The open dots, solid squares, open squares, solid diamonds, and open diamonds display the data for  $N=7, 8, 9, 10$ , and 11, respectively.

$$\xi_N^{-1}(\lambda) = \frac{1}{2} \ln \left[ \frac{\Delta_1(N-2, \lambda)}{\Delta_1(N, \lambda)} \right]. \quad (6)$$

Figure 7 shows extrapolations of  $\xi_N^{-1}(\lambda)$  in terms of  $\lambda^{-1}$ . We can fit the data linearly and estimate  $\xi_N = 4.0, 4.8, 4.6, 5.4$ , and 5.0 for  $N=7-11$ , respectively.

These values roughly agree with those of the  $S=1$  AF Heisenberg chain calculated by Kennedy.<sup>21</sup> This fact reflects that the  $S=\frac{1}{2}$  ladder model is reduced to the  $S=1$  AF Heisenberg chain in the limit  $\lambda \rightarrow \infty$ .<sup>31</sup> On the other hand, we extrapolate  $\xi_N^{-1}(\lambda)$  in terms of  $N^{-1}$  in a region of small  $\lambda$  in Fig. 8 and show  $\xi^{-1}(\lambda)$  in Fig. 9 for

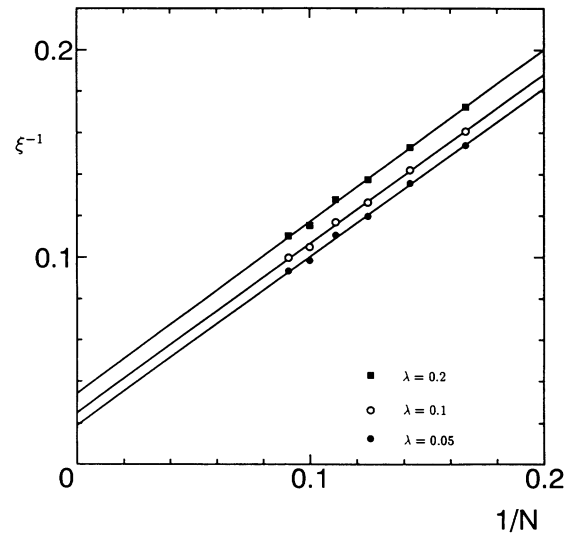


FIG. 8.  $\xi_N^{-1}(\lambda)$  defined in the text. The data for  $\lambda=0.20, 0.10$ , and 0.05 are shown by the solid squares, open dots, and solid dots, respectively. The line shows the linear fit in terms of  $N^{-1}$ .

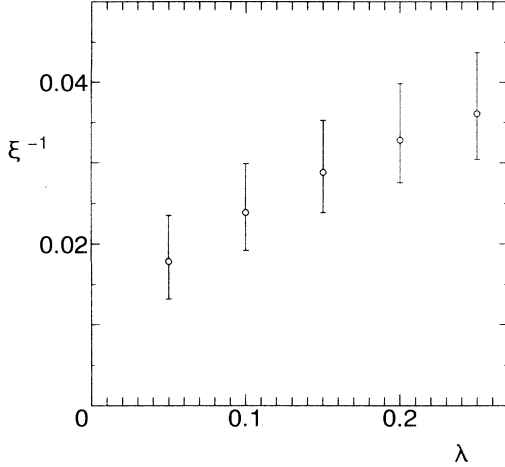


FIG. 9. The extrapolated inverse correlation length for small  $\lambda$ . The error bars show differences between the maximum and the minimum values obtained by fitting  $\xi_N^{-1}(\lambda)$  and  $\xi_{N-2}^{-1}(\lambda)$  linearly.

$\lambda = 0.05, 0.10, \dots, 0.25$ .

In Fig. 8, we have succeeded in fitting data of  $\xi_N^{-1}(\lambda)$  linearly for small  $\lambda$  and consequently show that  $\lambda_C$  is less than 0.05 and that  $\xi(\lambda)$  is estimated at nearly 29, 39, and 52 for  $\lambda = 0.2, 0.1$ , and 0.05, respectively. In Fig. 9, we show the shape of  $\xi^{-1}(\lambda)$ , which shape resembles that of the energy gap  $\Delta(\infty, \lambda)$  in Fig. 6.

### III. DISCUSSION

To make sure of the conclusion obtained in the previous section, we discuss the case with a finite  $\lambda_S$ . In that case we unexpectedly reach the idea with different origins for the energy gap for  $\lambda < \lambda_S$  and  $\lambda > \lambda_S$ . [See Fig. 4(a).] For  $\lambda > \lambda_S$ , the quintuplet (the upper triplet) connected to point  $C$  ( $B$ ) approaches the lowest excited state in increasing even (odd)  $N$ . For  $\lambda < \lambda_S$ , the upper triplet (singlet) connected to point  $B$  ( $A$ ) approaches the lowest excited state in increasing even (odd)  $N$ .

At the first step, compared with the quasiparticle proposed as the elementary excitation related to the valence-bond solid state by Knabe,<sup>20</sup> we discuss the quintuplet (the upper triplet) connected to point  $C$  ( $B$ ) for even (odd)  $N$ . Let us regard the ground state for  $\lambda > 0$  as the  $S = 1$  Haldane state, where two  $S = \frac{1}{2}$  spins connected ferromagnetically by an interchain coupling form a triplet pair. In order to propose a candidate of the elementary excitation, we create a quasiparticle on the ground state of the ladder model. We consider  $\mathbf{S}_{M,M+1}$  and  $\tilde{\mathbf{S}}_{M,M+1}$  defined by  $\mathbf{S}_{M,M+1} \equiv \sigma_M + \tau_M + \sigma_{M+1} + \tau_{M+1}$  and  $\tilde{\mathbf{S}}_{M,M+1}(\tilde{\mathbf{S}}_{M,M+1} + 1) \equiv \langle (\mathbf{S}_{M,M+1})^2 \rangle$ , respectively. Since  $\tilde{\mathbf{S}}_{M,M+1} = 0$  or 1 in the VBS state for all  $M$ , we expect that two AF couplings between the sites  $M$  and  $M+1$  are cracked to form the  $\tilde{\mathbf{S}}_{M,M+1} = 2$  state. We depict such an artificial  $S = 2$  quasiparticle by the solid square in Fig. 10.

Note that we can select  $N - 1$  values of  $M$  from  $M = 1$  to  $M = N - 1$ . We assume that the state with the  $S = 2$

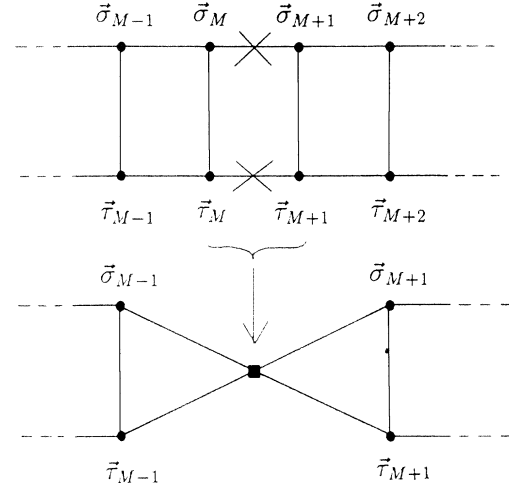


FIG. 10. The ladder model with the  $S = 2$  quasiparticle. This quasiparticle is regarded as an artificial particle with  $S = 2$  and is depicted by the solid square. The solid dots depict the  $S = \frac{1}{2}$  spins.

quasiparticle is approximated by a superposition of the ground states of  $N - 1$  different ladder models with  $S = 2$  quasiparticles. Applying Lieb-Mattis' theorem to this ladder model with the  $S = 2$  quasiparticle, we can prove the following lemma.

- (1) For even  $N$ , the total spin of the ground state of this ladder model is two if the  $S = 2$  quasiparticle stays at sites with  $M$  being odd and is zero if it stays at sites with  $M$  being even.
- (2) For odd  $N$ , the total spin of the ground state of this ladder model is one.

We thereby expect that the  $S = 2$  quasiparticle prefers to stay at sites with  $M$  being odd for even  $N$ . This feature is numerically observed in the quintuplet connected to point  $C$  for  $N = 4, 6, 8$ , and 10. (See Fig. 11 for  $N = 10$ .)

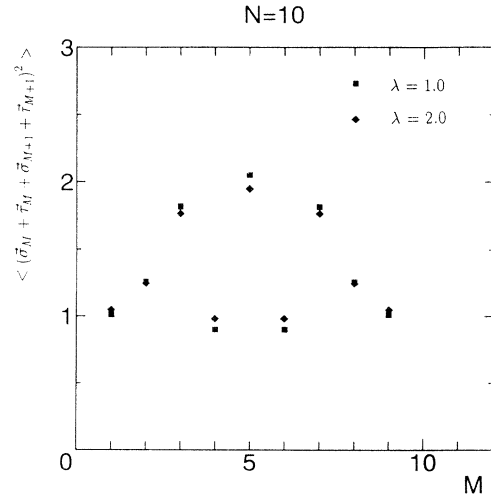


FIG. 11.  $\langle \mathbf{S}_{M,M+1}^2 \rangle$  are plotted against  $M$  ( $1 \leq M \leq N - 1$ ) for  $N = 10$ . The solid squares and solid diamonds depict the data calculated in the third-lowest state for  $\lambda = 1.0$  and 2.0, respectively. These states are in the quintuplet connected to point  $C$ .

Since  $\langle \mathbf{S}_{1,2}^2 \rangle$  and  $\langle \mathbf{S}_{N-1,N}^2 \rangle$  are less than  $\langle \mathbf{S}_{M,M+1}^2 \rangle$  for  $M$  in the middle of the chain, as seen in Fig. 11, it is seemed that the  $S=2$  quasiparticle tends to avoid both edges. It may be caused by the effect of a local staggered order, which is a characteristic of the  $S=1$  Haldane state.<sup>45</sup> For odd  $N$ , the numerical result obtained shows that  $\langle \mathbf{S}_{M,M+1}^2 \rangle$  is larger in the upper triplet connected to point  $B$  than in the singlet connected to point  $B$ . We therefore found that the  $S=2$  quasiparticle appears in the quintuplet (upper triplet) connected to point  $C$  ( $B$ ) for even (odd)  $N$ .

At the second step, we discuss the upper triplet (singlet) connected to point  $B$  ( $A$ ) for even (odd)  $N$ . As a candidate of the excitation in the state, we create some defect on the ground state. We consider  $\mathbf{S}_M$  and  $\tilde{S}_M$  defined by  $\mathbf{S}_M = \sigma_M + \tau_M$  and  $\tilde{S}_M(\tilde{S}_M + 1) = \langle (\mathbf{S}_M)^2 \rangle$ , respectively. Compared with the  $S=2$  quasiparticle, we expect that a triplet pair of  $\sigma_M$  and  $\tau_M$  is cracked to form a singlet pair with  $\tilde{S}_M=0$ . We depict such an artificial spin-0 particle by the solid triangle in Fig. 12.

Note that we can select  $N$  values of  $M$  from  $M=1$  to  $M=N$ . We assume that the state with  $S=0$  quasiparticle is approximated by a superposition of the ground states of  $N$  different ladder models with  $S=0$  quasiparticles. We expect that  $\tilde{S}_M$  is approximately zero, and then apply Lieb-Mattis' theorem to the ladder model with the  $S=0$  quasiparticle. We can thereby derive the following remarks.

- (1) For even  $N$ , the total spin of the ground state of the ladder model with the  $S=0$  quasiparticle is one.
- (2) For odd  $N$ , the total spin of the ground state of the ladder model with the  $S=0$  quasiparticle is two if the  $S=0$  quasiparticle stays at an even site and zero if it stays at an odd site.

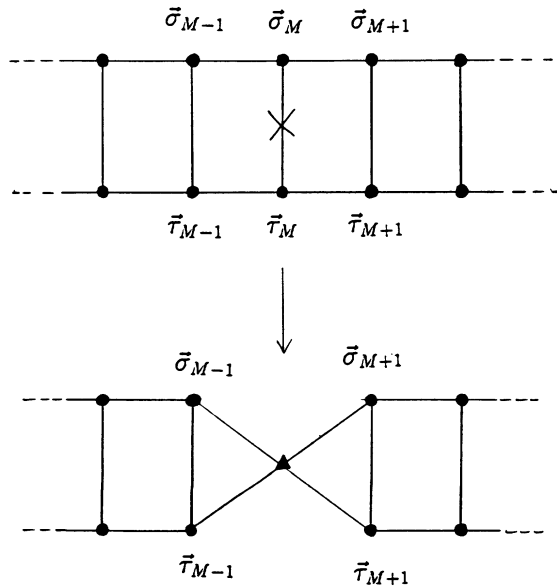


FIG. 12. The ladder model with the  $S=0$  quasiparticle. This quasiparticle is regarded as an artificial spinless particle and is depicted by the solid triangle. The solid dots depict the  $S=\frac{1}{2}$  spins.

For odd  $N$ , it therefore turns out that if the  $S=0$  quasiparticle appears in the singlet connected to point  $A$ , then it prefers to stay at odd sites. This features is actually observed in numerical results for  $N=5, 7, 9$ , and  $11$ . (See Fig. 13 for  $N=11$ .)

In this figure,  $\tilde{S}_M$  which is defined as  $\frac{3}{4} + \langle \sigma_M \cdot \tau_M \rangle$ , is calculated in the singlet connected to point  $A$  and is thus found to be lower for odd  $M$  than for even  $M$ . For even  $N$ , our numerical data show that  $\tilde{S}_M$  is less in the upper triplet connected to point  $B$  than in the lower triplet connected to point  $B$ . In the upper triplet, both  $\tilde{S}_M$  and  $\tilde{S}_{N-M+1}$  are less for odd  $M$  than for even  $M$  for  $M \leq \frac{1}{2}N$ . These features reflect that the  $S=0$  quasiparticle appears in the singlet (upper triplet) connected to point  $A$  ( $B$ ) for odd (even)  $N$ , which state crosses over the state with the  $S=2$  quasiparticle at  $\lambda_S$  as  $\lambda$  is increased.

We have further calculated the energy of the  $S=0$  quasiparticle for small  $\lambda$  as follows. First, a quantity  $\Delta_\lambda(N)$  is defined as the energy difference between the upper triplet connected to point  $B$  and the second-lowest states (between the singlet state connected to point  $A$  and the lowest state) for even (odd)  $N$ . Next, we applied Eq. (5) with  $\alpha(\lambda)$  chosen by hand to  $\Delta_\lambda(N)$  vs  $N^{-1}$  for even and odd  $N$ , respectively and found that  $\Delta_\lambda(\infty)$  are roughly same for even and odd  $N$  for a value of  $\alpha(\lambda)$ . Then, we regard  $\Delta_\lambda(\infty)$  for the value of  $\alpha(\lambda)$  as the energy of the  $S=0$  quasiparticle. For small  $\lambda$ , the energy  $\Delta_\lambda(\infty)$  is larger than the energy of the  $S=2$  quasiparticle we have calculated using  $\Delta'_1(N, \lambda) - \Delta_1(N, \lambda)$  in the text. This situation suggests that  $\lambda_S$  approaches 0 in increasing  $N$ .

Finally, we summarize the concluding remarks. We showed a finite energy gap for  $\lambda \geq 0.05$  and thus concluded that  $\lambda_C$  must be less than 0.05, the gap of which was obtained as  $\Delta'_1(N, \lambda) - \Delta_1(N, \lambda)$  by numerical calculations of finite clusters we have used. For small  $\lambda$ , we extrapolated  $\xi_N(\lambda)$  calculated with Eq. (6) in terms of  $N^{-1}$  and found that the inverse correlation length  $\xi^{-1}(\lambda)$  is finite

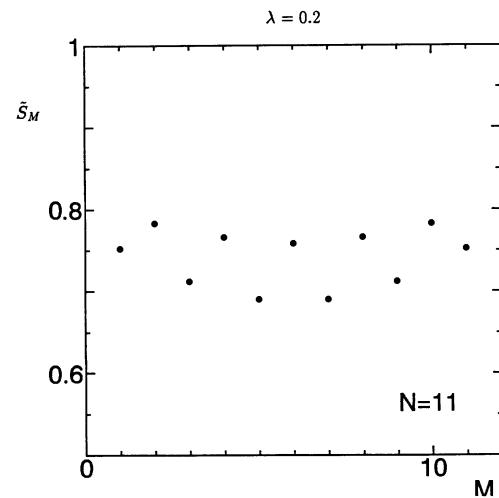


FIG. 13.  $\tilde{S}_M$  against  $M$  ( $0 \leq M \leq N$ ) for odd  $N$  and  $\lambda=0.2$  in the singlet state connected to point  $A$ .

for  $\lambda \geq 0.05$ . However, we cannot have found a Kosterlitz-Thouless-like behavior of  $\xi^{-1}(\lambda)$  for small  $\lambda$ , the behavior of which is predicted by the author and others using a bosonized Hamiltonian. [It is noted that Sólyom and Timonen suggest the absence of the behavior in a vicinity of the massless point ( $\lambda=0$ ) using another type of double-chain system.<sup>44</sup>] This contradiction of the ladder model for small  $\lambda$  may be, if the behavior exists, due to the fact that  $\Delta_1(N, \lambda)$ , which is the finite-size correction to the energy, is too large, compared with  $\Delta'_1(N, \lambda) - \Delta_1(N, \lambda)$ . It is further shown that the elementary excitation of the ladder model is similar to the quasiparticle proposed by Knabe.<sup>20</sup>

## ACKNOWLEDGMENTS

The author would like to thank Professor K. Kubo, Professor S. Takada, and Professor J. Sólyom for helpful and stimulating discussions. He also thanks Dr. D. Hirashima, Dr. K. Nomura, Dr. M. Hagiwara, Dr. H. Kikuchi, Dr. T. Nakamura, and K. Hukushima for useful discussions. The numerical calculation has been accomplished by utilizing TITPACK ver.2 coded and supplied by Professor H. Nishimori. Professor T. Barnes drew the author's attention to Ref. 37. This work was supported by a Grant-in-Aid for Scientific Research on Priority Areas by the Ministry of Education, Science and Culture.

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<sup>31</sup>Let us consider the Hamiltonian, which is seen in Eqs. (1)–(4), of the ladder model in the subspace where all the interchain couplings form the  $S=1$  states. We thus ignore  $H_{\sigma\tau}$  since we can rewrite  $H_{\sigma\tau}$  as  $-\frac{1}{4}\lambda N$  in the subspace. In this case, the wave function is symmetric with respect to  $\sigma_i$  and  $\tau_i$ , so that we can replace  $\sigma_i$  and  $\tau_i$  with  $\frac{1}{2}(\sigma_i + \tau_i)$ . Thus, we obtain
- $$\begin{aligned} H &= H_\sigma + H_\tau \\ &= \frac{1}{2} \sum_{i=1}^N (\tau_i \cdot \sigma_{i+1} + \sigma_i \cdot \tau_{i+1}) + \frac{1}{2} \sum_{i=1}^N (\sigma_i \cdot \sigma_{i+1} + \tau_i \cdot \tau_{i+1}) \\ &= \frac{1}{2} \sum_{i=1}^N \mathbf{S}_i \cdot \mathbf{S}_{i+1}, \end{aligned}$$

where  $\mathbf{S}_i = \sigma_i + \tau_i$ .

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