Ground-state phase diagram of the spin-$\frac{1}{2}$ ferromagnetic-antiferromagnetic alternating Heisenberg chain with anisotropy

Kazuo Hida

Department of Physics, College of Liberal Arts, Saitama University, Urawa, Saitama 338, Japan

(Received 18 February 1992)

The ground state of the ferromagnetic-antiferromagnetic alternating spin-$\frac{1}{2}$ Heisenberg chain is studied with Ising-type anisotropy on the ferromagnetic bond. This model tends to the spin-1 antiferromagnetic Heisenberg chain with on-site anisotropy in the limit of strong ferromagnetic bond. It is found that the Haldane-gap phase, the large-D phase, and the two types of Néel phases appear as the ground state of this model. The duality relations between these four phases are proved for several limiting cases. The string order parameter characterizing the large-D phase is introduced based on these duality relations. The ground-state phase diagram is determined by the numerical diagonalization of the finite-size system.

I. INTRODUCTION

Haldane's conjecture[1,2] opened up an exciting field in the study of quantum spin systems.[3–18] The concept of the string order introduced by den Nijs and Rommelse[4] and later by Tasaki[5] has succeeded in clarifying the physical nature of this peculiar quantum state which possesses a hidden long-range "string" order accompanied by the breakdown of the hidden symmetry.[6,7] The presence of this order is also checked numerically.[8,9] The exactly solvable spin-1 model[12,13] also has this order and the same symmetry breakdown.[6,8] The experimentally observed edge state with spin $\frac{1}{2}$ can be regarded as the evidence of the hidden symmetry breakdown.[10,11]

These observations suggest that further physical insight into this state might be obtained by regarding the spin-1 operator as the strongly coupled two spin-$\frac{1}{2}$ operators. The author thus introduced the spin-$\frac{1}{2}$ ferromagnetic-antiferromagnetic alternating Heisenberg chain which tends to the spin-1 Heisenberg antiferromagnet in the limit of the infinite ferromagnetic coupling. Through the investigation of this model, it is found that the Haldane phase can be regarded as the special case of the dimer phase of the spin-$\frac{1}{2}$ model which also possesses the extended string order.[16] The argument based on the nonlocal unitary transform by Kohmoto and Tasaki[17] and Takada[18] also supports this conclusion.

On the other hand, in the spin-1 Heisenberg antiferromagnetic chain, the on-site easy plane anisotropy is known to destabilize the Haldane phase, leading to the so-called large-D phase, while easy axis anisotropy leads to the transition to the Néel phase.[4,5,14,15] It is the purpose of the present work to investigate the effect of this type of anisotropy in the spin-$\frac{1}{2}$ alternating Heisenberg chain. We consider the Hamiltonian

$$H=2J\sum_{i=1}^{N}\mathbf{S}_{2i}\mathbf{S}_{2i+1}+2J'\sum_{i=1}^{N}\mathbf{S}_{2i-1}\mathbf{S}_{2i}+D\sum_{i=1}^{N}(S^z_{2i-1}+S^z_{2i})^2\ , \tag{1.1}$$

where $\mathbf{S}_i=(S_i^x,S_i^y,S_i^z)$ is the spin operator with spin $\frac{1}{2}$. The suffix i denotes the lattice point and the number of lattice sites in $2N$. The periodic boundary condition $\mathbf{S}_1=\mathbf{S}_{2N+1}$ is assumed. Unless especially mentioned, the coupling J is assumed to be antiferromagnetic (>0) and J' ferromagnetic (<0). For $J'=-\infty$, the spins $\mathbf{S}_{2i-1}$ and $\mathbf{S}_{2i}$ form a local triplet. In this limit, this model reduces to a spin-1 anisotropic antiferromagnetic Heisenberg chain:

$$H^{S=1}=\sum_{i=1}^{N}\tfrac{1}{2}J\hat{\mathbf{S}}_i\hat{\mathbf{S}}_{i+1}+D\sum_{i=1}^{N}\hat{S}_i^{z2}\ , \tag{1.2}$$

where $\hat{\mathbf{S}}_i(=\mathbf{S}_{2i-1}+\mathbf{S}_{2i})$ is the spin operator with spin 1. Thus the last term of Eq. (1.1) is the counterpart of the easy plane anisotropy of the spin-1 model. It should be noted that this term is equivalent to the Ising-type anisotropy $2D\sum_{i=1}^{N}S^z_{2i}S^z_{2i-1}$ except for the c-number terms.

In the next section, we study the several limiting cases where this model is treated exactly and the duality relations hold. Based on the duality relations, we introduce the string order parameter for the large-D phase. The bosonization calculation for $D\sim 2J\sim 2|J'|$ is given in Sec. III. The numerical results are shown in Sec. IV and the ground-state phase diagram is obtained. The case of antiferromagnetic $J'(>0)$ is discussed briefly. The last section is devoted to the summary and discussion.

II. VARIOUS LIMITING CASES

The present model can be treated exactly for several limiting cases, where the duality relations hold. In this section, we study four cases separately.

A. Case $D=2|J'|$

On the line $D=2|J'|$, the Hamiltonian (1.1) becomes

$$H=-2|J'|\sum_{i=1}^{N}(S^x_{2i-1}S^x_{2i}+S^y_{2i-1}S^y_{2i}-S^z_{2i-1}S^z_{2i})+2J\sum_{i=1}^{N}\mathbf{S}_{2i}\mathbf{S}_{2i+1}\ , \tag{2.1}$$

omitting the trivial c-number terms. By the spin rotation around the z axis,

$$\tilde{S}_l^x=-S_l^x,\ \ \tilde{S}_l^y=-S_l^y\ \text{ for } l=4i,4i+1\ ,$$
$$\tilde{S}_l^x=S_l^x,\ \ \tilde{S}_l^y=S_l^y\ \text{ otherwise}\ , \tag{2.2}$$

this Hamiltonian is transformed into the isotropic dimerized Heisenberg Hamiltonian as

$$H=2|J'|\sum_{i=1}^{N}\tilde{\mathbf{S}}_{2i-1}\tilde{\mathbf{S}}_{2i}+2J\sum_{i=1}^{N}\tilde{\mathbf{S}}_{2i}\tilde{\mathbf{S}}_{2i+1}\ . \tag{2.3}$$

In this case, the shift of the site index by unity causes the duality transform resulting in the interchange of J and $|J'|$. The region $J>|J'|=D/2$ continues to the point $D=J'=0$ where the ground state is the trivial assembly of the complete local singlets. This state is known to continue to the Haldane phase.[16] Therefore the region $D<2J$ belongs to the Haldane phase. The corresponding string correlation function is defined as

$$O_{\rm str}^{\alpha}(i-j)=-4\langle S_{2i}^{\alpha}\exp\{i\pi(S_{2i+1}^{\alpha}+S_{2i+2}^{\alpha}+\cdots+S_{2j-2}^{\alpha})\}S_{2j-1}^{\alpha}\rangle\ \ (\alpha=x,y,z) \tag{2.4}$$

in terms of the original spin $\mathbf{S}_i$ before the rotation.[16,17] The dual string correlation function $\tilde{O}_{\rm str}^{\alpha}(i-j)$ which characterizes the region $D>2J$ is

$$\tilde{O}_{\rm str}^{z}(i-j)=-4\langle S_{2i-1}^{z}\exp\{i\pi(S_{2i}^{z}+S_{2i+1}^{z}+\cdots+S_{2j-1}^{z})\}S_{2j}^{z}\rangle\ , \tag{2.5}$$

$$\tilde{O}_{\rm str}^{\alpha}(i-j)=4^{j-i+1}\langle S_{2i-1}^{\alpha}S_{2i}^{\alpha}S_{2i+1}^{\alpha}+\cdots S_{2j-1}^{\alpha}S_{2j}^{\alpha}\rangle(\alpha=x,y)\ , \tag{2.6}$$

also in terms of the unrotated spin. The corresponding string order parameter is given by the limit $|i-j|\to\infty$ of Eqs. (2.5) and (2.6). The phase for $D>2J$ belongs to the large-D phase, because this phase persists to the point $D=2|J'|\to\infty$ which belongs to the large-D phase of the spin-1 Heisenberg chain. Therefore we expect the order parameter $\tilde{O}_{\rm str}^{\alpha}$ to characterize the large-D phase. This is verified also in another limiting case in the next subsection and numerical results also support this notion. Thus the transition between the Haldane phase and the large-D phase takes place at $|J'|=J$ on the line $D=2|J'|$.

B. Large-D limit

In the limit $D\to\infty$, the ground states are 2^N-fold degenerate as

$$|G\{\sigma_i{:}i=1.N\}\rangle=\prod_i|\sigma_i\rangle_{2i-1}|-\sigma_i\rangle_{2i}\ , \tag{2.7}$$

where $|\sigma\rangle_i$ denotes the state with spin $\sigma(=\uparrow$ or $\downarrow)$ on the ith site. The degeneracy is removed by the application of J and J' terms within the subspace spanned by the above set of states. In this subspace, we can map the present model onto the one-dimensional N-site Ising model in the transverse magnetic field by the correspondence

$$|\sigma\rangle_{2i-1}|-\sigma\rangle_{2i}\to|\sigma\rangle\rangle_i\ . \tag{2.8}$$

Denoting the newly introduced spin-$\frac{1}{2}$ operator by T_i, the resulting Ising model is

$$H_I=-\sum_{i=1}^{N}(2JT_i^zT_{i+1}^z+2|J'|T_i^x)\ . \tag{2.9}$$

It is well known[19] that this model can be mapped onto the two-dimensional Ising model at finite temperature and satisfies the duality relation with respect to the transform of the spin variable to $\tilde{\mathbf{T}}_i$ defined by

$$T_i^z=\tfrac{1}{2}\prod_{j=1}^{i}(2\tilde{T}_j^x),\ \ T_i^x=2\tilde{T}_i^z\tilde{T}_{i+1}^z\ , \tag{2.10}$$

which transforms the Hamiltonian as

$$\tilde{H}_I=-\sum_{i=1}^{N}(4|J'|\tilde{T}_i^z\tilde{T}_{i+1}^z+J\tilde{T}_i^x)\ . \tag{2.11}$$

Therefore the transition from the ferromagnetic (in terms of T spin) state to the disordered state takes place at $J=2|J'|$. The ferromagnetic state corresponds to the Néel state in terms of the original spin with the spin configuration ↑↓↑↓. We call this type of Néel state the "Néel I" state to distinguish it from the "Néel II" state with spin configuration ↑↑↓↓ which appears for large negative D (see Sec. II D). Here, the Néel I order parameter $O_{\rm NI}^{\alpha}$ defined by

$$O_{\rm NI}^{\alpha}(i-j)=\langle S_i^{\alpha}S_j^{\alpha}\rangle(-1)^{i-j}\ , \tag{2.12}$$

$$O_{\rm NI}^{\alpha}=\lim_{|i-j|\to\infty}O_{\rm NI}^{\alpha}(i-j)\ \ (\alpha=x,y,z) \tag{2.13}$$

remains finite. On the other hand, the disordered state continues to the large-D phase of the spin-1 antiferromagnetic Heisenberg chain for the large- $|J'|$ limit. By the above duality relation, however, this disordered phase can be mapped onto the ferromagnetic phase in terms of the $\tilde{T}$ spin. Therefore we can regard the ferromagnetic order in terms of the $\tilde{T}$ spin as the order parameter which characterizes the large-D phase. This can be written in terms of T spin as

$$\tilde{O}_T=\lim_{|i-j|\to\infty}\tilde{O}_T(i-j)\ , \tag{2.14}$$

where

$$\tilde{O}_T(i-j)=4\langle\tilde{T}_i^z\tilde{T}_j^z\rangle=2^{j-i+1}\langle T_i^xT_{i+1}^x\cdots T_j^x\rangle\ . \tag{2.15}$$

Using the relation

$$2S_{2i-1}^x2S_{2i}^x|\sigma\rangle\rangle_i=2S_{2i-1}^x2S_{2i}^x|\sigma\rangle_{2i-1}|-\sigma\rangle_{2i}$$
$$=|-\sigma\rangle_{2i-1}|\sigma\rangle_{2i}=|-\sigma\rangle\rangle_i\ , \tag{2.16}$$

it is easily verified that $\tilde{O}_{\rm str}^{x}$ defined by Eq. (2.6) coincides with $\tilde{O}_T$ in this limiting case.

C. $|J'| \ll J,\ D>0$

In this case, the ground state can be constructed only from the states $|\uparrow\rangle_{2i}|\downarrow\rangle_{2i+1}$ and $|\downarrow\rangle_{2i}|\uparrow\rangle_{2i+1}$ for the 2ith and $(2i+1)$th spin as

$$|G\{\sigma_i : i=1.N\}\rangle = \prod_i |\sigma_i\rangle_{2i}|-\sigma_i\rangle_{2i+1} , \qquad (2.17)$$

due to the following reason.

Even in the absence of the xy component of the J bond, the ground state consists of the above set of states (the Néel I state) for $J'=0$. If the xy component is finite, the $|\uparrow\rangle_{2i}|\downarrow\rangle_{2i+1}$ state is mixed up with the $|\downarrow\rangle_{2i}|\uparrow\rangle_{2i+1}$ state and lowers the energy, while inclusion of $|\uparrow\rangle_{2i}|\uparrow\rangle_{2i+1}$ and $|\downarrow\rangle_{2i}|\downarrow\rangle_{2i+1}$ states provides no way to lower the energy. It should be noted that this does not work unless J' is small enough, because appropriate inclusion of such a configuration can lower the energy by the contribution from the xy component of the J' bond.

Thus we can again map the present model onto the one-dimensional N-site Ising model in the transverse magnetic field by the correspondence

$$|\sigma\rangle_{2i}|-\sigma\rangle_{2i+1} \to \sigma|\sigma\rangle\rangle_i . \qquad (2.18)$$

Denoting the newly introduced spin-$\frac{1}{2}$ operator by $\mathbf{T}'_i$, the resulting Ising model is

$$H_I = -\sum_{i=1}^{N} [2(D+J')T_i'^{z}T_{i+1}'^{z} + 2JT_i'^{x}] . \qquad (2.19)$$

Introducing the dual spin operator $\tilde{\mathbf{T}}'_i$ defined similarly to $\tilde{\mathbf{T}}_i$ as in the preceding subsection, the Hamiltonian is transformed as

$$\tilde{H}_I = -\sum_{i=1}^{N} [4J\tilde{T}_i'^{z}\tilde{T}_{i+1}'^{z} + (D+J')\tilde{T}_i'^{x}] . \qquad (2.20)$$

Therefore the transition from the ferromagnetic (in terms of T' spin) state to the disordered state takes place at $D+J'=2J$. The ferromagnetic state corresponds to the Néel I state in terms of the original spin.

On the other hand, the disordered state continues to the complete local singlet phase at $D=0$ which is known to continue to the Haldane phase of the spin-1 antiferromagnetic Heisenberg chain in the large-J' limit.[16] This phase can be mapped onto the ferromagnetic phase in terms of the $\tilde{T}'$ spin. In a manner similar to that in the preceding subsection, it is easily verified that the x component of the string order parameter (2.4) is mapped into the ferromagnetic order of $\tilde{T}'$ spin.

D. $|J'| \ll J, D<0$

The discussion of this regime proceeds in a way almost parallel to the preceding subsection, except that the ground state is constructed from the states $|\uparrow\rangle_{2i}|\uparrow\rangle_{2i+1}$ and $|\downarrow\rangle_{2i}|\downarrow\rangle_{2i+1}$ for the 2ith and $(2i+1)$th spin as

$$|G\{\sigma_i : i=1.N\}\rangle = \prod_i |\sigma_i\rangle_{2i}|\sigma_i\rangle_{2i+1} . \qquad (2.21)$$

The phase boundary lies at $D=-2J+|J'|$ and the region $D>-2J+|J'|$ continues to the point $J'=D=0$ which belongs to the Haldane phase. On the other hand, the Néel II state with $\uparrow\uparrow\downarrow\downarrow\uparrow\uparrow\downarrow\downarrow$ structure is realized for $D<-2J+|J'|$. This continues to the Néel state of the $S=1$ Heisenberg model for large negative D.[5,14] The Néel II order parameter $O^{\alpha}_{\rm NII}$ is defined by

$$O^{\alpha}_{\rm NII}(i-j) = \langle S_i^{\alpha}S_j^{\alpha}\rangle(-1)^{i'-j'} , \qquad (2.22)$$

with $i'=[(i-1)/2]$, and $j'=[(j-1)/2]$,

$$O^{\alpha}_{\rm NII} = \lim_{|i-j|\to\infty} O^{\alpha}_{\rm NII}(i-j) \quad (\alpha=x,y,z) , \qquad (2.23)$$

where [ ] denotes the Gaussian symbol.

III. BOSONIZATION FOR $J \simeq |J'|$, $D \simeq 2|J'|$

After the spin rotation (2.2), the Hamiltonian (1.1) is rewritten into the form

$$H = 2J' \sum_{i=1}^{N} \tilde{\mathbf{S}}_{2i-1}\tilde{\mathbf{S}}_{2i} + 2J\sum_{i=1}^{N} \tilde{\mathbf{S}}_{2i}\tilde{\mathbf{S}}_{2i+1} + (2D+4J')\sum_{i=1}^{N} \tilde{S}^z_{2i-1}\tilde{S}^z_{2i} , \qquad (3.1)$$

by the transform Eq. (2.2). In the neighborhood of $J=|J'|=D/2$, it is convenient to rearrange the terms as

$$H = 2J_0 \sum_{i=1}^{2N} [(\tilde{S}_i^x\tilde{S}_{i+1}^x + \tilde{S}_i^y\tilde{S}_{i+1}^y + \Delta\tilde{S}_i^z\tilde{S}_{i+1}^z) + \{\delta_{xy}(\tilde{S}_i^x\tilde{S}_{i+1}^x + \tilde{S}_i^y\tilde{S}_{i+1}^y) + \delta_z\tilde{S}_i^z\tilde{S}_{i+1}^z\}(-1)^i] , \qquad (3.2)$$

where

$$J_0 = \frac{J+|J'|}{2} , \quad \delta_{xy} = \frac{J-|J'|}{2J_0} , \quad \delta_z = \frac{J-|J'|-(D-2|J'|)}{2J_0} , \quad \Delta = 1 + \frac{D-2|J'|}{2J_0} . \qquad (3.3)$$

Thus this model can be regarded as the weakly dimerized anisotropic Heisenberg chain.[20–23] The spin-$\frac{1}{2}$ operators are transformed into the spinless fermions by Jordan-Wigner transform and further transformed into the boson field ϕ taking the continuum limit.[20–22]

The bosonized Hamiltonian H is given by[21]

$$H = \int dx \{ A\phi_x^2 + Bp^2 + C_I\cos(2\phi) - C_D\cos(\phi) + E\cos(\phi)\phi_x^2 \} , \qquad (3.4)$$

with

$$[p(x),\phi(x')] = -i\delta(x-x') , \qquad (3.5)$$

where ϕ is the boson field operator. The spatial variable is changed from the discrete variable i to the continuous variable x. For $\Delta>1$, Inagaki and Fukuyama[22] determined the parameters A, B, and C_I from the comparison with the exact solution in the absence of dimerization near the isotropic point ($\Delta \simeq 1$). Other constants are derived directly from the bosonization transform[21,22] as follows:

$$\begin{aligned} A &\simeq \frac{J_0 a}{4}(1+\alpha\sqrt{\Delta-1}) , \\ B &\simeq \pi^2 J_0 a(1-\alpha\sqrt{\Delta-1}) , \\ C_I &\simeq \frac{\pi^2 J_0}{4a}\beta\{1+\alpha'(\sqrt{\Delta-1})\} , \\ C_D &= \frac{2J_0\delta_{xy}}{a} , \quad E=\frac{2J_0\delta_z a}{\pi} , \end{aligned} \tag{3.6}$$

where a is the lattice constant of the original lattice. α, α', and β are numerical constants of the order of unity which cannot be determined by the above method. The values of these numerical constants are unimportant for the following discussion.

Inagaki and Fukuyama[22] used this method to determine the ground state of the model with $\delta_{xy}=\delta_z$. If, as argued by Nakano and Fukuyama,[21] the term with δ_z plays an irrelevant role, our model is equivalent to that of Inagaki and Fukuyama[22] and the Néel state appears around the line $C_D=0$, $\Delta>1$.[22,23] However, this is not true in the present case. If the last term of Eq. (3.4) is decoupled, A and C_D effectively change as

$$A \rightarrow A+E\langle\cos\phi\rangle, \quad C_D \rightarrow C_D - E\langle\phi_x^2\rangle . \tag{3.7}$$

The first effect is only a small correction to A as discussed by Nakano and Fukuyama.[21] The latter, however, is relevant because C_D is also small. We estimate $\langle\phi_x^2\rangle \sim C/a^2$ near the isotropic undimerized point by dimensional consideration where C is a numerical constant of the order of unity. In the case $\delta_{xy}=\delta_z$, which was discussed by Nakano and Fukuyama, this simply changes C_D by a numerical factor and is unimportant qualitatively. However, in the present case, the parameter E contains the anisotropy parameter D while C_D does not. Therefore this term becomes important even for the qualitative argument. The Néel phase appears around the line $C_D - E\langle\phi_x^2\rangle=0$, $\Delta>1$ which leads to

$$J-|J'|=\frac{C(D-2|J'|)}{\pi-C} , \quad D>2|J'| , \tag{3.8}$$

in terms of the parameters for the original spin chain. Unfortunately the appropriate estimation of $\langle\phi_x^2\rangle$ is difficult due to its crucial dependence on the momentum cutoff. We determine this value by comparison with the phase diagram determined by the numerical diagonalization.

IV. NUMERICAL DIAGONALIZATION

In this section, we calculate the order parameters defined in Sec. II in the ground state of the present model by the exact numerical diagonalization of finite-size systems. The phase diagram is drawn based on these numerical results. The order parameters are estimated by the

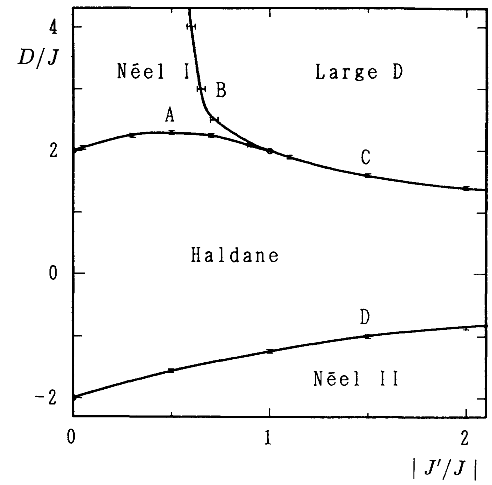

FIG. 1. The ground-state phase diagram on the J'-D plane for $J'=0$.

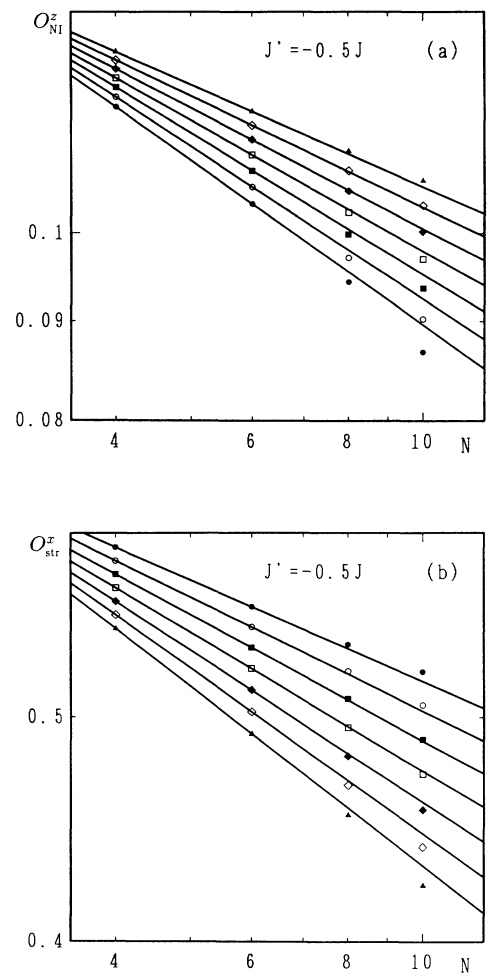

FIG. 2. The log-log plot of the system size dependence of (a) the Néel I order parameter $O^z_{\rm NI}$ and (b) the string order parameter $O^x_{\rm str}$ for $J'=-0.5J$. The values of D/J are 2.23 (●), 2.25 (○), 2.27 (■), 2.29 (□), 2.31 (◆), 2.33 (◇), and 2.35 (▲). The solid lines are linear extrapolation from the data for $N=4$ and 6.

value of the corresponding correlation function at the distance $l=(2N)/2$. They are calculated for $N=4$, 6, 8, and 10. The numerical diagonalization is performed using the program package TITPACK version 2 developed by Nishimori.

The order parameters are plotted versus the system size and the phase boundary is determined by the point at which the log-log plot is best fitted by a straight line. The phase diagram is shown in Fig. 1. The three phases are characterized as follows:

(i) Néel I phase:

$$O^z_{\mathrm{NI}}, O^z_{\mathrm{str}}, \tilde{O}^z_{\mathrm{str}} \neq 0 \ , \tag{4.1}$$

(ii) Néel II phase:

$$O^z_{\mathrm{NII}}, O^z_{\mathrm{str}}, \tilde{O}^z_{\mathrm{str}} \neq 0 \ , \tag{4.2}$$

(iii) Haldane phase:

$$O^\alpha_{\mathrm{str}} \neq 0 \quad (\alpha = x,\ y,\ \text{and}\ z)\ , \tag{4.3}$$

(iv) large-D phase:

$$\tilde{O}^\alpha_{\mathrm{str}} \neq 0 \quad (\alpha = x,\ y,\ \text{and}\ z)\ . \tag{4.4}$$

Other order parameters vanish in each phase. These conditions are the same as the spin-1 case except those which contain $\tilde{O}^\alpha_{\mathrm{str}}$. The error bars show the points at which the numerical calculation is made. The size dependencies of the order parameters near the phase boundary are shown in Fig. 2 (point A), Fig. 3 (point B), Fig. 4 (point C), and Fig. 5 (point D) for the relevant order parameters. Actually, there is a slight discrepancy between the phase boundaries estimated from different order parameters. This is due to the limited system size. This causes the error bars in the phase diagram.

The bosonization argument in the preceding section suggests that the Néel phase persists to the infinitesimal neighborhood of the point $J=|J'|=D/2$. According to the numerically obtained phase diagram, the Néel phase

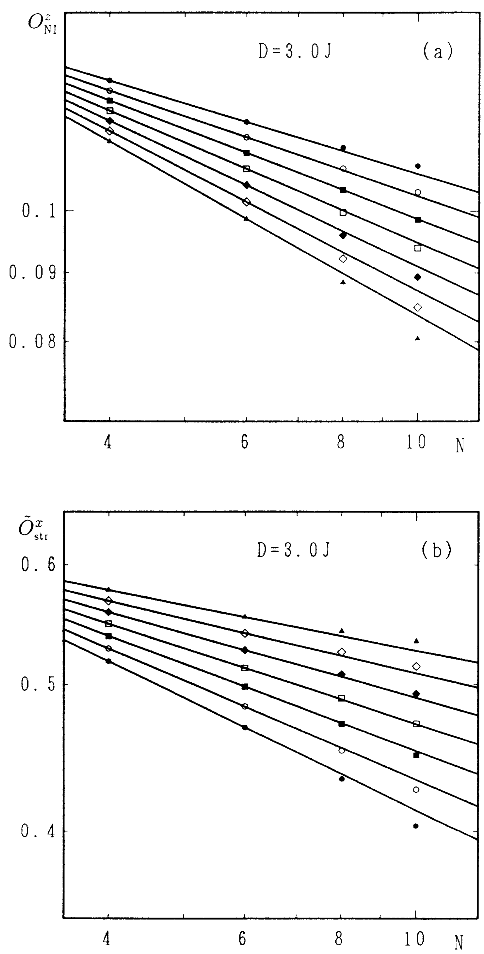

FIG. 3. The log-log plot of the system size dependence of (a) the Néel I order parameter O^z_{NI} and (b) the large-D string order parameter $\tilde{O}^x_{\mathrm{str}}$ for $D/J=3$. The values of $|J'|/J$ are 0.62 (●), 0.63 (○), 0.64 (■), 0.65 (□), 0.66 (♦), 0.67 (◇), and 0.68 (▲). The solid lines are linear extrapolation from the data for $N=4$ and 6.

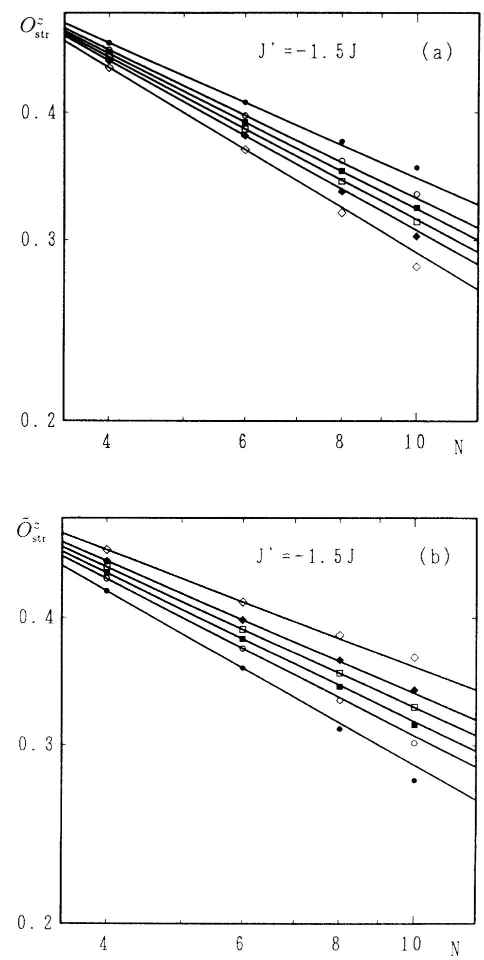

FIG. 4. The log-log plot of the system size dependence of (a) the string order parameter O^z_{str} of the Haldane phase and (b) the string order parameter $\tilde{O}^z_{\mathrm{str}}$ of the large-D phase for $J'/J=-1.5$. The values of D/J are 1.58 (●), 1.60 (○), 1.61 (■), 1.62 (□), 1.63 (♦), and 1.65 (◇). The solid lines are linear extrapolation from the data for $N=4$ and 6.

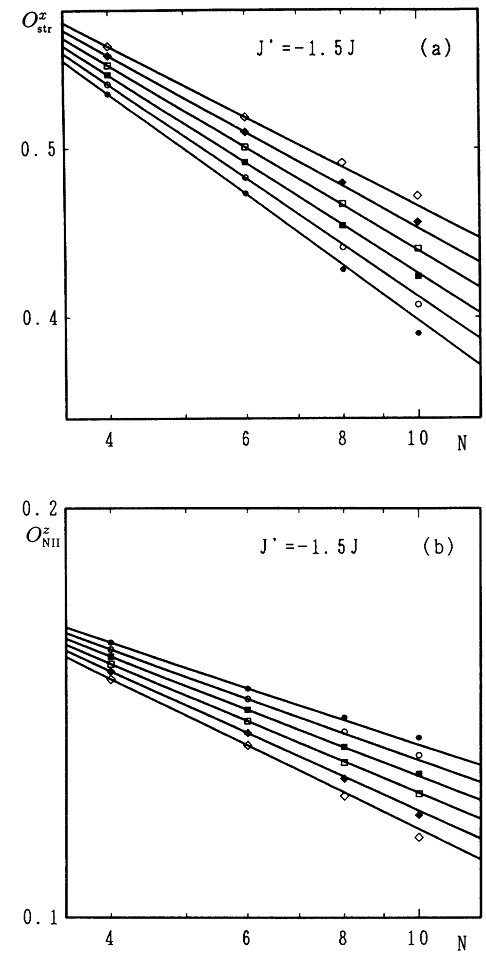

FIG. 5. The log-log plot of the system size dependence of (a) the string order parameter $O^x_{\rm str}$ and (b) the Néel II order parameter $O^x_{\rm NII}$ for $J'/J=-1.5$. The values of D/J are -1.06 (●), -1.04 (○), -1.02 (■), -1.00 (□), -0.98 (♦), and -0.96 (◇). The solid lines are linear extrapolation from the data for $N=4$ and 6.

appears around the line $J-|J'|\simeq D-2|J'|$, $D>2|J'|$. This suggests that the constant C introduced in the preceding section is close to $\pi/2$.

The system size dependence of the energy gap ΔE is also calculated. Near the boundary between the Néel phase and the large-D phase, the lowest excited state has $S_z^{\rm tot}=0$ where $S_z^{\rm tot}$ is the z component of the total spin.

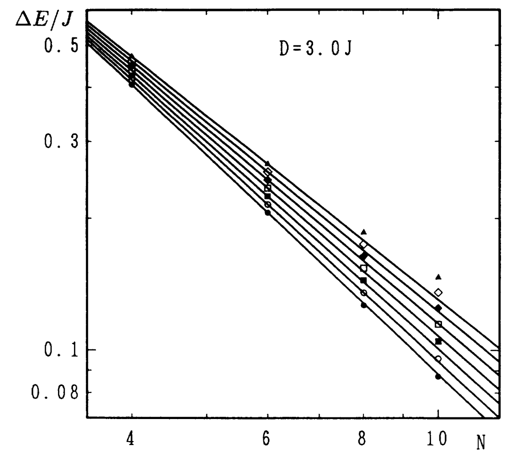

FIG. 6. The log-log plot of the system size dependence of the energy gap ΔE for $D/J=3$. The values of $|J'|/J$ are 0.62 (●), 0.63 (○), 0.64 (■), 0.65 (□), 0.66 (♦), 0.67 (◇), and 0.68 (▲). The solid lines are linear extrapolation from the data for $N=4$ and 6.

In the Néel states, the gap tends to zero as the system size becomes large reflecting the degeneracy of the ground state, while it remains finite in the large-D phase. This is shown in Fig. 6 for point A. Similar behavior is observed in the neighborhood of the phase boundary between the Haldane phase and the Néel I and Néel II phases.

The behavior of the energy gap across the boundary between the Haldane phase and the large-D phase is shown in Fig. 7. In this case, the lowest excited state has $S_z^{\rm tot}=1$. The gap of the finite-size system takes the minimum around the phase boundary and the gap seems to vanish in the thermodynamic limit reflecting the change in the symmetry of the phase.

So far we have only been concerned with the case $J'<0$, because we are mainly interested in the relation of the present model to the $S=1$ spin chain. Before closing this section, however, let us briefly discuss the case $J'>0$ (antiferromagnetic-antiferromagnetic alternating chain), because the phase diagram for this case can easily be obtained by the spin rotation (2.2) from that for $J'<0$. The parameters change as $J'\to -J'$ and $D\to D+2J'$ as seen by comparing Eqs. (1.1) and (3.1). For large enough J', there appears a new disordered phase where the following order parameter $\tilde{O}^\alpha_{\rm str}$ remains finite:

$$\hat{O}^\alpha_{\rm str}=\lim_{|i-j|\to\infty} -4\langle S^\alpha_{2i-1}\exp\{i\pi(S^\alpha_{2i}+S^\alpha_{2i+1}+\cdots+S^\alpha_{2j-1})\}S^\alpha_{2j}\rangle(\alpha=x,y,z)\ . \tag{4.5}$$

We may call this phase the large-J' phase. In the limit of infinitely large D, the boundary between this phase and the Néel phase tends to $J'=0.5J$. For small J', the boundary between the Haldane phase and the Néel phase tends to $D=2J$ continuing to the region $J'<0$. The overall phase diagram is shown in Fig. 8.

V. SUMMARY AND DISCUSSION

We have studied the ground-state properties of the anisotropic alternating Heisenberg chain with spin-$\frac{1}{2}$ which has exchange couplings $J(>0)$ between $(2i-1)$th and $2i$th spin and $J'(<0)$ between $2i$th and $(2i+1)$th spin.

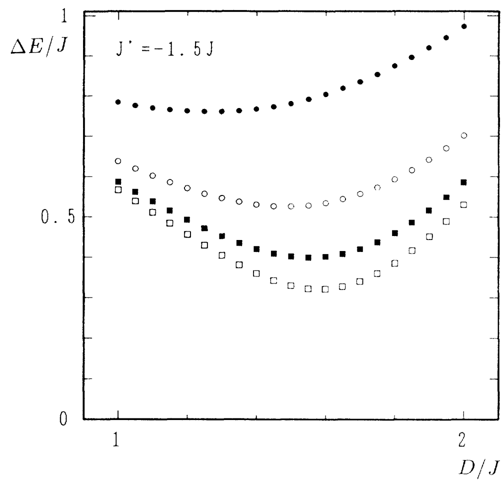

FIG. 7. The smallest energy gap ΔE for $J'/J=-1.5$ and $1.0<D/J<2.0$ for finite systems with $N=4$ (●), 6 (○), 8 (■), and 10 (□).

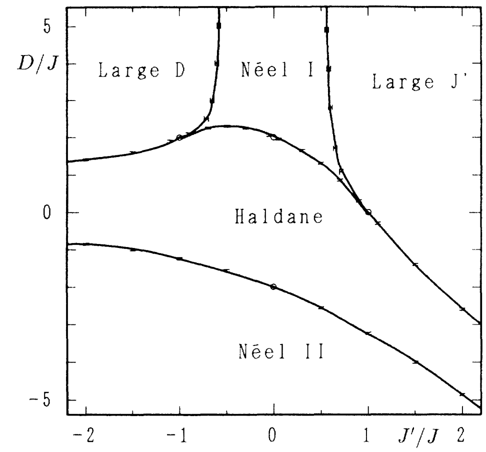

FIG. 8. The ground-state phase diagram on the whole J'-D plane.

The Ising-type anisotropy D is assumed between $2i$th and $(2i+1)$th spin. This model tends to the spin-1 Heisenberg chain with on-site anisotropy D in the limit $J'\rightarrow-\infty$.

The string order parameter $\tilde{O}^{\alpha}_{\rm str}$ which characterizes the large-D phase is introduced based on the analysis of the various limiting cases and calculated by the diagonalization of the finite-size systems for more general parameter range. The ground-state phase diagram is obtained. It is also shown that the energy gap tends to zero at the phase boundary, justifying the relevance of the order parameters. The presence of the order parameter in the large-D phase implies that this phase is not a simply disordered phase but is accompanied by the breakdown of the hidden symmetry like the Haldane phase. The case of the antiferromagnetic-antiferromagnetic alternating chain $(J,J'>0)$ is briefly discussed. It is shown that another type of disordered phase with string order $\hat{O}^{\alpha}_{\rm str}$ appears for large positive J'.

The detailed study of the critical behavior at the phase boundary is left for future study. The larger system size is required for the accurate determination of the critical exponents.

The effect of the anisotropy on the J bond is discussed by Kohmoto and Tasaki[17] using the nonlocal unitary transform introduced by Kohmoto, den Nijs, and Kadanoff.[24] This type of anisotropy corresponds to the Ising-type anisotropy in the spin-1 model. They predict the presence of the Néel phase, XY phase, and ferromagnetic phase for $J'<0$. It should be noted the regime $J'>0$ of this model corresponds to the region $J'>0$ of the present model. The region $J'<0$ of this model, which is discussed by Kohmoto and Tasaki,[17] has no correspondence with the present model. The numerical study of this model will be reported elsewhere.

The relation of the present model to the mechanism of superconductivity should also be noted. Imada suggested that the superconductivity may arise by the doping of holes into the dimer-type ground state.[25] In this context, it might be interesting to study the effect of the hole doping in various phases of this model.

ACKNOWLEDGMENTS

The author is indebted to H. Nishimori for providing him TITPACK version 2. He thanks M. Imada, M. Kohmoto, H. Tasaki, and S. Takada for sending him their works prior to publication and for useful comments. This work is supported by the Grant-in-Aid for Scientific Research from the Ministry of Education, Science and Culture. The numerical calculation is performed on the HITAC S820/80 at the Computer Center of the University of Tokyo and Hokkaido University, and HITAC S820/15 at the Information Processing Center of Saitama University.

[1] F. D. M. Haldane, Phys. Lett. **93A**, 464 (1983).
[2] F. D. M. Haldane, Phys. Rev. Lett. **50**, 1153 (1983).
[3] I. Affleck, J. Phys. Condens. Matter. **1**, 3047 (1989), and references therein.
[4] M. den Nijs and K. Rommelse, Phys. Rev. B **40**, 4709 (1989).
[5] H. Tasaki, Phys. Rev. Lett. **66**, 798 (1991).
[6] T. Kennedy and H. Tasaki, Phys. Rev. B **45**, 304 (1992).
[7] S. Takada and K. Kubo, J. Phys. Soc. Jpn. **60**, 4026 (1991).
[8] S. M. Girvin and D. P. Arovas, Phys. Scr. T **27**, 156 (1989).
[9] Y. Hatsugai and M. Kohmoto, Phys. Rev. B **44**, 11 789 (1991).
[10] M. Hagiwara, K. Katsumata, I. Affleck, B. I. Halperin, and J. P. Renard, Phys. Rev. Lett. **65**, 3181 (1990).
[11] S. H. Glarum, S. Geschwind, K. M. Lee, M. L. Kaplan, and J. Michel, Phys. Rev. Lett. **67**, 1614 (1991).
[12] I. Affleck, T. Kennedy, E. Lieb, and H. Tasaki, Phys. Rev. Lett. **59**, 799 (1987).
[13] I. Affleck, T. Kennedy, E. Lieb, and H. Tasaki, Commun. Math. Phys. **115**, 477 (1988).

[14]R. Botet, R. Julien, and M. Kolb, Phys. Rev. B **28**, 3914 (1983).
[15]H. J. Schulz, Phys. Rev. B **34**, 6372 (1986).
[16]K. Hida, Phys. Rev. B **45**, 2207 (1992).
[17]M. Kohmoto and H. Tasaki (unpublished).
[18]S. Takada, J. Phys. Soc. Jpn. **61**, 428 (1992).
[19]D. C. Mattis, *The Theory of Magnetism II* (Springer-Verlag Berlin, 1985), Chap. 3.
[20]H. Fukuyama and H. Takayama, in *Electronic Properties of Inorganic Quasi-One-Dimensional Compounds,* edited by Pierre Monceau (Reidel, Dordrecht, 1985), Part I, and references therein.
[21]T. Nakano and H. Fukuyama, J. Phys. Soc. Jpn. **50**, 2489 (1981).
[22]S. Inagaki and H. Fukuyama, J. Phys. Soc. Jpn. **52**, 2504 (1983).
[23]H. Nishimori, K. Okamoto, and M. Yokozawa, J. Phys. Soc. Jpn. **56**, 4126 (1987).
[24]M. Kohmoto, M. den Nijs, and L. P. Kadanoff, Phys. Rev. B **24**, 5229 (1981).
[25]M. Imada, J. Phys. Soc. Jpn. **60**, 1877 (1991).