Crossover between the Haldane-gap phase and the dimer phase in the spin-$\frac{1}{2}$ alternating Heisenberg chain

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The ground-state properties of the spin-$\frac{1}{2}$ Heisenberg chain, which has two exchange couplings ($J > J'$) alternatingly, are studied. This model interpolates the spin-1 antiferromagnetic Heisenberg chain (AFHC) ($J' \to -\infty$, $J > 0$), the dimerized spin-$\frac{1}{2}$ AFHC ($J' \simeq J > 0$), and the uniform spin-$\frac{1}{2}$ AFHC ($J' = J > 0$) continuously. The string order introduced by den Nijs–Rommelse and Tasaki changes continuously through the Haldane phase and the dimer phase to vanish at $J = J'$. It is at a maximum for $J' = 0$. This implies that the string order is related to the local singlet correlation in terms of the spin-$\frac{1}{2}$ model. The lowest excitation can be regarded as the renormalized triplet wave. The reversal of the anisotropy effect on the excitation spectrum of the spin-1 AFHC is also explained in a intuitive way based on this picture.

I. INTRODUCTION

Since Haldane's conjecture in 1983,[1,2] the essential difference between the ground-state properties of the antiferromagnetic Heisenberg chain (AFHC) with integer spin and that with half-integer spin has attracted the attention of many physicists. Haldane suggested that the AFHC with integer spin has a finite energy gap (Haldane gap) above the ground state, while that with half-integer spin has no energy gap, as is evident for the case of spin $\frac{1}{2}$.[3] This conjecture was supported by a number of theoretical[4–19] and experimental studies.[20–23]

In this work, we study the spin-$\frac{1}{2}$ alternating Heisenberg chain which has two different exchange couplings J and J' alternatingly. This model has been studied intensively related to the spin-Peirels system for $J' \simeq J$.[24–28] The anisotropic version of this model is equivalent to the highly anisotropic Ashkin-Teller model[29] and has been also studied in this context.[30] Here, we regard the spin-1 AFHC as the alternating spin-$\frac{1}{2}$ Heisenberg chain with antiferromagnetic J and infinitely large ferromagnetic J'. If we change J' from $-\infty$ to J, the ground state of our model changes continuously starting from the Haldane-gap phase to the gapless spin-liquid phase ($J = J'$) passing through the points of the noninteracting singlet state ($J' = 0$) and the dimer phase ($0 < J' \simeq J$). Among these phases, both the Haldane phase and the dimer phase are characterized by the finite energy gap and the exponential decay of the antiferromagnetic correlation. In this work, we clarify that these two phases are two extreme cases of a single phase. This notion also helps us to understand some exotic features of the Haldane-gap phase intuitively.

In order to characterize the Haldane phase, den Nijs and Rommelse[16] and Tasaki[17] introduced the string correlation function $O^z_{\rm str}(i-j)$ and the string order parameter $O^z_{\rm str}$ defined by

$$O^z_{\rm str}(i-j) = -\langle S^z_i \exp[i\pi(S^z_{i+1} + S^z_{i+2} + \cdots + S^z_{j-1})] S^z_j \rangle , \tag{1.1}$$

$$O^z_{\rm str} = \lim_{|i-j| \to \infty} O^z_{\rm str}(i-j) . \tag{1.2}$$

Here S^z_i is the z component of the spin operator $\mathbf{S}_i$ with magnitude 1. In the case of the spin-1 chain, this order parameter remains finite in the Haldane phase and vanishes for the more trivial disordered state which is induced by the anisotropy effect.[16,17] The existence of the string order in the Haldane phase is also checked numerically.[18,19] The order parameters $O^x_{\rm str}$ and $O^y_{\rm str}$ are defined similarly and also remain finite in the Haldane-gap phase. In the present work, we concentrate on the rotationally invariant states. Therefore these three order parameters have the same value and we omit the superscripts x, y, and z.

In the next section, we explain the model Hamiltonian. We also extend the above definition of the string order parameter to the present model. In Sec. III the bosonization method[24–26] is applied and the string order parameter is calculated analytically within the self-consistent harmonic approximation for $J \simeq J'$. The string order and the energy gap are calculated by the exact diagonalization of small size systems in Sec. IV. The physical picture of the lowest excited state is also given based on the perturbation calculation for $J' \simeq 0$. The last section is devoted to summary and discussion.

II. ALTERNATING HEISENBERG CHAIN

We consider the alternating Heisenberg chain represented by the following Hamiltonian H:

$$H=2J'\sum_{i=1}^{N}\mathbf{S}_{2i-1}\cdot\mathbf{S}_{2i}+2J\sum_{i=1}^{N}\mathbf{S}_{2i}\cdot\mathbf{S}_{2i+1}\ , \tag{2.1}$$

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 is $2N$. The periodic boundary condition $\mathbf{S}_1=\mathbf{S}_{2N+1}$ is assumed. The coupling J is assumed to be antiferromagnetic. For $J'=-\infty$, the spins $\mathbf{S}_{2i-1}$ and $\mathbf{S}_{2i}$ form a local triplet and this model reduces to the spin -1 AFHC:

$$H^{S=1}=\sum_{i=1}^{N}\frac{1}{2}J\hat{\mathbf{S}}_i\cdot\hat{\mathbf{S}}_{i+1}\ , \tag{2.2}$$

where $\hat{\mathbf{S}}_i(=\mathbf{S}_{2i-1}+\mathbf{S}_{2i})$ is the spin operator with spin 1. On the other hand, this model becomes the spin-$\frac{1}{2}$ dimerized antiferromagnetic chain when J' is close to (but not equal to) J.

In the present model, we define the string correlation function $O_{\rm str}(i-j)$ by

$$O_{\rm str}(i-j)=-4\langle S_{2i}^z\exp[i\pi(S_{2i+1}^z+S_{2i+2}^z+\cdots+S_{2j-2}^z)]S_{2j-1}^z\rangle\ . \tag{2.3}$$

The factor 4 is introduced so that this expression reduces to (1.1) in the limit $J'=-\infty$. The string order parameter $O_{\rm str}$ is defined by $O_{\rm str}=\lim_{|i-j|\to\infty}O_{\rm str}(i-j)$.

III. BOSONIZATION FOR $J\simeq J'$

For $J\simeq J'$, we have a weakly dimerized spin-$\frac{1}{2}$ antiferromagnetic chain. In this case, the spin-$\frac{1}{2}$ operators are transformed into the spinless fermions by the Jordan-Wigner transform and further transformed into the boson field ϕ taking the continuum limit.[24–26] The Hamiltonian H is transformed into the form

$$H=\int dx[\,A\phi_x^2+Bp^2-D\cos(\phi)]\ , \tag{3.1}$$

with

$$[p(x),\phi(x')]=-i\delta(x-x')\ . \tag{3.2}$$

The spatial variable is changed from the discrete variable i to the continuous variable x. The parameters are given by

$$A=v_F/8,\quad B=\pi^2v_F/2,\quad D=(J-J')/a,\quad v_F=Ja\ , \tag{3.3}$$

where a is the lattice constant of the original lattice.

Using the identity for the spin-$\frac{1}{2}$ operators, $S_i^z=\exp(i\pi S_i^z)/2i$, the string correlation function $O_{\rm str}(i-j)$ is rewritten as

$$O_{\rm str}(i-j)=\langle\exp[i\pi(S_{2i}^z+S_{2i+1}^z+\cdots+S_{2j-1}^z)]\rangle\ . \tag{3.4}$$

Because the slowly varying part of the spin density is given by $\partial_x\phi/2\pi$, Eq. (3.4) can be transformed into the boson representation as

$$O_{\rm str}(x-x')=\langle\exp\{i[\phi(x)-\phi(x')]/2\}\rangle\ . \tag{3.5}$$

We apply the self-consistent harmonic approximation (SCHA) to the nonlinear term in the bosonized Hamiltonian.[24–26] The approximate Hamiltonian $H^{\rm SCHA}$ is given by

$$H^{\rm SCHA}=\int dx\left[A\phi_x^2+Bp^2-D_{\rm eff}\left[1-\frac{\phi^2-\langle\phi^2\rangle}{2}\right]\right]\ , \tag{3.6}$$

where the average $\langle\cdots\rangle$ is taken in the ground state of $H^{\rm SCHA}$. The quantity $D_{\rm eff}$ is defined by

$$D_{\rm eff}=D\exp(-\tfrac{1}{2}\langle\phi^2\rangle)\ . \tag{3.7}$$

The expectation value $\langle\phi^2\rangle$ is given by

$$\langle\phi^2\rangle=\frac{B}{2\pi}\int_{-\pi/a}^{\pi/a}dk\frac{1}{\omega(k)}\ , \tag{3.8}$$

where $\omega(k)=(\pi v_F/2)(k^2+m^2)^{1/2}$ and $m^2=D_{\rm eff}/2A$. Then Eq. (3.7) yields

$$m=\left[\frac{aD^2}{8\pi A^2}\right]^{1/3}\ . \tag{3.9}$$

The string order parameter is given by

$$\begin{aligned}O_{\rm str}&=\lim_{|x-x'|\to\infty}O_{\rm str}(x-x')\\&=\lim_{|x-x'|\to\infty}\exp\{-\tfrac{1}{8}\langle[\phi(x)-\phi(x')]^2\rangle\}\\&=(\pi/ma)^{1/4}\sim(1-J'/J)^{1/6}\ .\end{aligned} \tag{3.10}$$

The string long-range order $O_{\rm str}$ disappears for $J'=J$. At this point, the string correlation function $O_{\rm str}(x,x')$ behaves as

$$O_{\rm str}(x-x')\sim|x-x'|^{-1/4}\ . \tag{3.11}$$

Thus the string correlation function decays by this power law in the uniform Heisenberg antiferromagnet with spin $\frac{1}{2}$. This means that the $O_{\rm str}$ in the finite system depends on the system size N as $O_{\rm str}\sim N^{-1/4}$.

IV. NUMERICAL DIAGONALIZATION

We have numerically diagonalized the Hamiltonian (2.1) with $2N=12$, 16, 20, and 24 by the Lanczos method using the program package TITPACK version 2 developed

by Nishimori. The string correlation function $O_{str}(l)$ is shown in Fig. 1(a) ($J'>0$) and Fig. 1(b) ($J'<0$) in the ground state. It is seen from Fig. 1 that $O_{str}(l)$ approaches quickly to the constant value with l except for $J'\simeq J$. This implies the presence of the long-range string order in our model for $J\neq J'$. We estimate the value of O_{str} by extrapolating $O_{str}(N/2)$ to $N\to\infty$. The system size dependence of $O_{str}(N/2)$ for $N=8$, 10, and 12 is negligible in the region $-\infty<J'/J<0.7$. For $0.7<J'/J<0.9$, the extrapolation is made using the Shanks transform.[9,31] For $0.9<J'/J<1.0$, the convergence of the Shanks transform becomes worse. This is due to the divergence of the string correlation length for small $J-J'$.

The J' dependence of O_{str} is shown in Fig. 2(a) ($J'>0$) and Fig. 2 (b) ($J'<0$). According to the bosonization calculation, O_{str} vanishes as $O_{str}\sim(1-J'/J)^{1/6}$ for $J\simeq J'$. Therefore, we plot O_{str} as a function of $(1-J'/J)^{1/6}$ in Fig. 2(a). The plotted data are proportional to $(1-J'/J)^{1/6}$ for $0.9>J'/J>0.7$, in reasonable agreement with the bosonization result. The system size dependence of O_{str} for $J=J'$ is also checked numerically. This is shown in Fig. 3. The data fit approximately with the prediction of bosonization theory $O_{str}\sim N^{-1/4}$. The deviation might be attributed to the smallness of the maximum system size $N=12$. For $J'>0$, the data are plotted against $(1-J'/J)^{-1}$ in Fig. 2(b). It approaches the Haldane value ($\simeq 0.38$),[18] as indicated by the open square.

It should be remarked that O_{str} takes the maximum at $J'=0$. At this point, the string order parameter is exactly equal to unity as follows:

The ground state $|G\rangle$ for $J'=0$ is given by

$$|G\rangle=\prod_{i=1}^{N}|s\rangle_i\ , \tag{4.1}$$

with

$$|s\rangle_i=\frac{1}{\sqrt{2}}(|\uparrow\rangle_{2i}|\downarrow\rangle_{2i+1}-|\downarrow\rangle_{2i}|\uparrow\rangle_{2i+1})\ , \tag{4.2}$$

where $|\sigma\rangle_i$ denotes the state with spin $\sigma(=\uparrow$ or $\downarrow)$ on

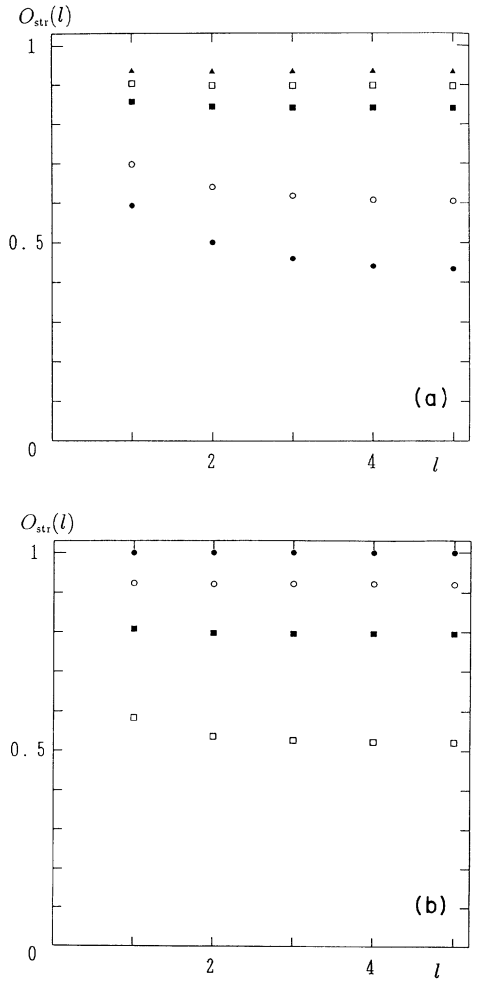

FIG. 1. l dependence of the string correlation function $O_{str}(l)$ for $N=10$. The parameters are: (a) $J'/J=1$ (●), 0.9 (○), 0.8 (■), 0.7 (□), 0.6 (▲), and (b) $J'/J=-0.1$(●), -1.0 (○), -2.0 (■), -5.0 (□).

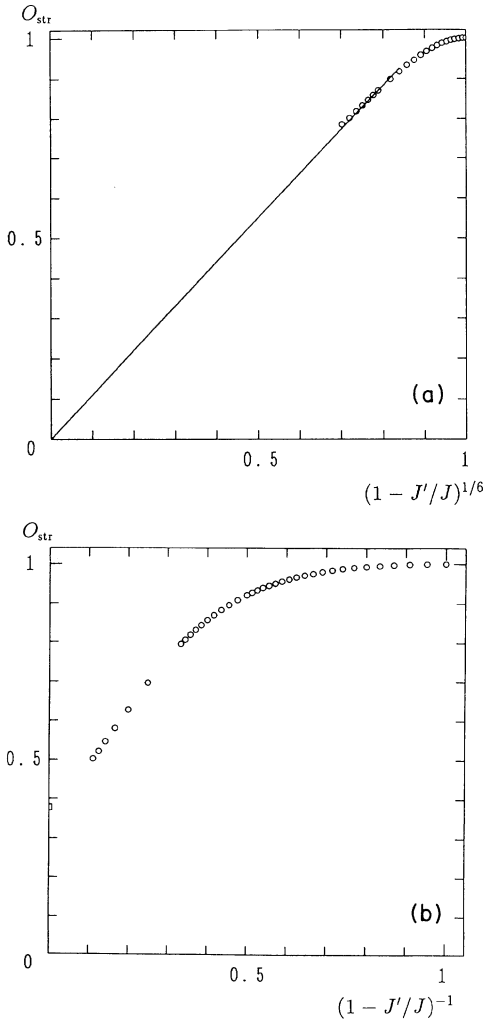

FIG. 2. String order parameter O_{str}. (a) $1>J'>0$: plotted against $(1-J'/J)^{1/6}$. The solid line is a guide for the eye. (b) $0>J'/J>-\infty$: plotted against $(1-J'/J)^{-1}$. The open square is the value for the spin-1 AFHC.

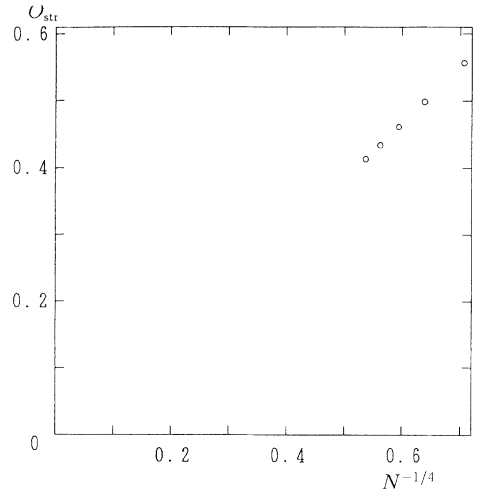

FIG. 3. System size dependence of the string order parameter O_{str} for $J=J'$ plotted against $1/N^{1/4}$.

the ith site. Using the identity

$$\exp[i\pi(S^z_{2i}+S^z_{2i+1})]|s\rangle_i=-4S^z_{2i}S^z_{2i+1}|s\rangle_i =|s\rangle_i \ , \tag{4.3}$$

on expression (3.4), it is easily verified that O_{str} is equal to unity.

In this context, we may interpret the string order parameter as the measure of the strength of the localized singlet correlation. In the presence of finite J', the perfectly localized singlets are perturbed by the interaction with other spins. Both the Haldane phase and the dimer phase are characterized as the phase in which the localized singlets survive such perturbation, while the string order decays by the power law in the spin-liquid phase ($J'=J$). It should be noted that the antiferromagnetic J' is more effective than the ferromagnetic J' to reduce the string order.

The energy gap ΔE between the ground state and the first excited state also characterizes both the dimer phase and the Haldane phase. The J' dependence of the gap is shown in Fig. 4. The system size dependence is very weak except the regions $J\simeq J'$ and $-J'\gg J$. The Shanks transform is again used for the extrapolation to $N\to\infty$. The gap tends to the Haldane value ($\simeq 0.41J/2$) as $J'\to-\infty$, which is indicated by the open square in Fig. 4. The factor $\frac{1}{2}$ comes from the overall factor $\frac{1}{2}$ in (2.2). It is remarkable that the energy gap has a cusp at $J'=0$. This can be understood by the first-order perturbation in J' as follows.

The unperturbed ground state is given by (4.1). The ground-state energy has no first-order correction in J' and is equal to $-3JN/2$ up to this order. The unperturbed excited state is obtained by replacing one of the singlet pairs in the ground state by a triplet pair as

$$|l;S^z\rangle=\prod_{i\neq l}|s\rangle_i|t;S^z\rangle_l \ , \tag{4.4}$$

where

$$|t;0\rangle_i=\frac{1}{\sqrt{2}}(|\uparrow\rangle_{2i}|\downarrow\rangle_{2i+1}+|\downarrow\rangle_{2i}|\uparrow\rangle_{2i+1}) \ , \tag{4.5}$$

$$|t;+1\rangle_i=|\uparrow\rangle_{2i}|\uparrow\rangle_{2i+1} \ , \tag{4.6}$$

$$|t;-1\rangle_i=|\downarrow\rangle_{2i}|\downarrow\rangle_{2i+1} \ . \tag{4.7}$$

Because the position l of the triplet pair is arbitrary, the first excited states are N-fold degenerate. The first-order correction in J' removes the degeneracy within the subspace $\Sigma(S^z)=\{|l;S^z\rangle:l=1,N\}$ ($S^z=0,\pm1$). The perturbation Hamiltonian H_p is the first term of (2.1). The application of H_p on the state $|l;S^z\rangle$ results in the expression

$$H_p|l;S^z\rangle=-\frac{J'}{2}|l+1;S^z\rangle-\frac{J'}{2}|l-1;S^z\rangle \ . \tag{4.8}$$

Diagonalizing H_p within this subspace, the excited states are given by the following extended states:

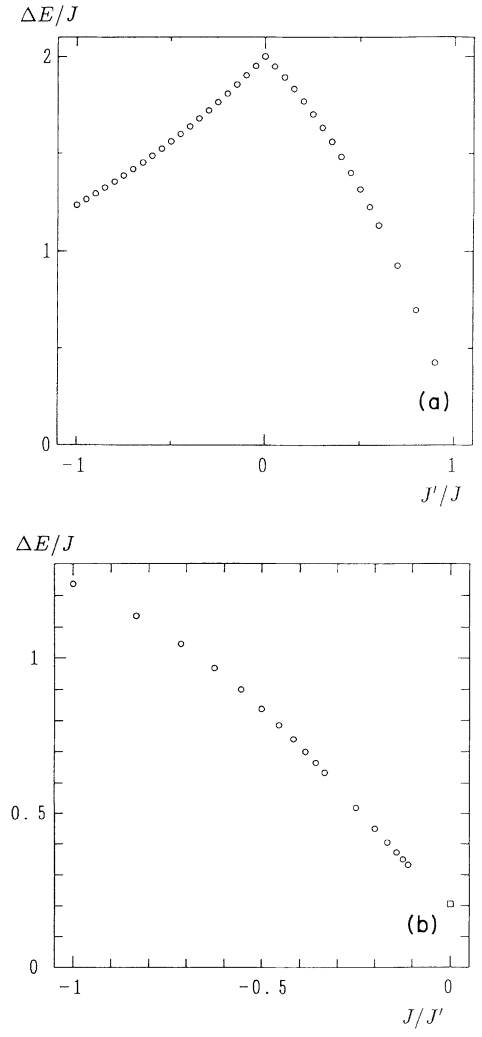

FIG. 4. J' dependence of the energy gap ΔE for (a) $1>J'/J>-1$ and (b) $-1>J'/J>-\infty$ ($\circ$). The open square is the value for the spin-1 AFHC.

$$|k;S^z\rangle = \left[\frac{1}{N}\right]^{1/2} \sum_{l=1}^{N} \exp(2ikla)|l;S^z\rangle \ , \tag{4.9}$$

where $k = n\pi/Na$ ($-N/2 < n \leq N/2$; n = integer). The energy eigenvalue $E(k)$ of the state $|k;S^z\rangle$ is given by

$$E(k) = -\tfrac{3}{2}JN + 2J - J'\cos(2ka) \ . \tag{4.10}$$

We may call these excited states the "triplet wave" states, because a triplet pair is wandering around in the background of singlet pairs. The energy spectrum of the triplet wave forms a band with width $2J'$ and the first excited state is the bottom of the band at $2J - |J'|$ measured from the ground state. For $J' > 0$, the bottom of the triplet wave band is located at $k = 0$. As J' approaches J, this gap continues to the dimer gap at $k = 0$. For $J' < 0$, the bottom of the triplet wave band is located at $k = \pi/(2a)$. Taking into account that $2a$ corresponds to the size of the unit cell for $J' \neq 0$, this point is the zone boundary. Thus the gap at $J' < 0$ continues to the Haldane gap, which also lies at the zone boundary. Because the numerical data shows no discontinuity between $J' = 0$ and $J' \to \infty$, it would be reasonable to expect that the excited state above the Haldane gap also keeps the character of the renormalized triplet wave state. Although this picture is not rigorous, it helps to understand some exotic features of the Haldane phase in a simple way.

For example, one remarkable characteristic of the excited states of the Haldane phase is the anisotropy effect. In the presence of the single-site anistoropy, the triplet states with total spin $S_{\rm tot} = 1$ are decomposed into the doublet with $S^z_{\rm tot} = \pm 1$ and the singlet with $S^z_{\rm tot} = 0$. In contrast to simple minded intuition, the doublet has lower energy than the singlet for easy-plane anistropy.[5,22] this can be easily understood by the triplet wave picture above as follows.

The single-site easy-plane anistropy in the spin-1 model corresponds to the additional term

$$H_{\rm an} = D \sum_{i=1}^{N} (S^z_{2i-1} + S^z_{2i})^2 \ , \tag{4.11}$$

with $D > 0$ in the present model Hamiltonian (2.1). Omitting the trivial c-number terms, $H_{\rm an}$ has no matrix elements in the subspace $\Sigma(\pm 1)$, while in $\Sigma(0)$ the application of $H_{\rm an}$ gives

$$H_{\rm an}|l;0\rangle = -\frac{D}{2}|l+1;0\rangle - \frac{D}{2}|l-1;0\rangle \ . \tag{4.12}$$

Thus the bottom of the triplet wave band at the zone boundary becomes $2J - |J' + D|$ for $S^z = 0$, while it does not change for $S^z = \pm 1$. For negative J' and positive D ($< |J'|$) this implies that the doublet ($S^z = \pm 1$) has lower energy than the singlet ($S^z = 0$).

V. SUMMARY AND DISCUSSION

We have studied the ground-state properties of the alternating Heisenberg chain with spin $\frac{1}{2}$, which has two exchange couplings $J(>0)$ and $J'(J \geq J' > -\infty)$ alternatingly. The string order parameter $O_{\rm str}$ is defined and calculated. It is found that $O_{\rm str}$ remains finite not only in the Haldane-gap phase ($J' < 0$, $|J'| \gg J$) but also in the dimer phase ($J' \simeq J$). It takes the maximum value for $J' = 0$ where the ground state is simply the assembly of perfectly localized singlet pairs. This observation suggests that the string order is the measure of the localized singlet correlation. Therefore this order parameter must be useful to distinguish the static valence-bond-type disordered states from other disordered states. It should be remarked that the relevance of this type of disordered state to high-T_c superconductivity was recently pointed out.[32]

From the present viewpoint, the Haldane-gap state is characterized as a special case of the static valence-bond state of the spin-$\frac{1}{2}$ model. The valence-bond solid state proposed by Affleck *et al.*[12,13] also possesses this character. On the other hand, in the field-theoretical approach, the Haldane state is characterized by the absence of the topological term in the corresponding nonlinear σ model.[1,2,10] The relation between these two characterizations of the Haldane phase is not quite clear.

The lowest excitation is the extended triplet wave for $J' \simeq 0$, which has a gap $2J - |J'|$ above the ground state. This gap continues to the dimer gap for small $J - J'$ and to the Haldane gap for $J' \ll -J$. It is speculated that the excited state in the Haldane phase has also the character of the renormalized triplet wave. This picture gives an intuitive explanation of the reversal of the anisotropy effect on the excitation spectrum of the Haldane-gap system. Although not rigorous, such a physical picture must be useful in the phenomenological interpretation of the experimental results. Further investigation of the anisotropy effect in this model also must be interesting. This is left for future study.

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