Hidden $Z_2 \times Z_2$ symmetry breaking and the Haldane phase in the $S=\frac{1}{2}$ quantum spin chain with bond alternation

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We study the $S=\frac{1}{2}$ spin chain with the Hamiltonian

$$H=\sum_{j=1}^{L-1}\{\sigma_{2j}^x\sigma_{2j+1}^x+\sigma_{2j}^y\sigma_{2j+1}^y+\lambda\sigma_{2j}^z\sigma_{2j+1}\}+\beta\sum_{j=1}^{L}(1-\boldsymbol{\sigma}_{2j-1}\cdot\boldsymbol{\sigma}_{2j}),$$

where $\boldsymbol{\sigma}_i=(\sigma_i^x,\sigma_i^y,\sigma_i^z)$ are the Pauli matrices. We find that a nonlocal unitary transformation reveals the hidden $Z_2\times Z_2$ symmetry of the system. It has been argued that a similar hidden $Z_2\times Z_2$ symmetry of the $S=1$ chain is fully broken when and only when the system exhibits the Haldane gap. We prove that the present system exhibits both an excitation gap and a full breaking of the hidden $Z_2\times Z_2$ symmetry in a range of the parameter space including the line $\beta=0$, $\lambda>-1$. We argue that the range with such properties indeed extends to the limit $\beta\to\infty$ in which the present model reduces to the $S=1$ spin chain. This observation provides support of Hida's conclusion that the Haldane gap in the $S=1$ chain is continuously connected to the gap in the decoupled $S=\frac{1}{2}$ system with $\beta=0$.

I. INTRODUCTION

Haldane[1] argued that, when S is an integer, the spin-S quantum antiferromagnetic chain with the Hamiltonian

$$H=\sum_i S_i^xS_{i+1}^x+S_i^yS_{i+1}^y+\lambda S_i^zS_{i+1}^z+D(S_i^z)^2 \qquad (1.1)$$

has a unique disordered ground state with a gap in a finite region of the parameter space including the SU(2) invariant Heisenberg point $\lambda=1$, $D=0$. This conclusion was somewhat surprising since it had been believed that there should be spin-wave excitations without any energy gap. When S is a half-odd integer in (1.1), it is argued that there is no excitation gap at the SU(2) invariant point. Initial controversy about this fascinating prediction seems to have been resolved by numerous experiments (both in quasi-one-dimensional compounds[2] and in computers[3]) and some theoretical works. There is also an exactly solvable model for $S=1$ with an additional biquadratic interaction which is proved to possess most of the properties Haldane predicted.[4] However, Haldane's conclusion on the standard Heisenberg model with small integer S (say, 1) still remains to be justified theoretically.

The ground state accompanied by the Haldane gap is unique and has exponentially decaying correlation functions. It turned out, however, that the ground state is not simply disordered but has highly nontrivial hidden structures. Den Nijs and Rommelse[5] argued the Haldane-type ground state in an $S=1$ chain has a "hidden antiferromagnetic order" which can be measured by the string order parameter

$$O_{\text{string}}^\alpha=-\lim_{|i-j|\to\infty}\left\langle S_i^\alpha \exp\left[i\pi\sum_{k=i+1}^{j-1}S_k^\alpha\right]S_j^\alpha\right\rangle,$$

where $\alpha=x$, y, or z. (See also Ref. 6.) This string order parameter has been calculated numerically.[7] Kennedy[8] pointed out that, in an $S=1$ Haldane gap system defined on a finite open chain, the four lowest-energy levels are nearly degenerate and are separated from the other eigenstates by a finite (Haldane) gap. This near degeneracy arises from almost free $S=\frac{1}{2}$ degrees of freedom generated at both ends of the chain.[9] In the infinite volume limit, the four nearly degenerate states converge to a single infinite volume ground state since the extra spin $\frac{1}{2}$'s at the boundaries are no longer observable. These two nonstandard properties of the Haldane gap systems can be observed in the solvable model of Ref. 4.

Kennedy and Tasaki[10] argued that these two characteristic features, the hidden antiferromagnetic order and the fourfold near degeneracy, can be understood as consequences of a hidden $Z_2\times Z_2$ symmetry breaking. They introduced a nonlocal unitary transformation for the $S=1$ antiferromagnetic chain and found that the model obtained by applying the transformation to the Hamiltonian (1.1) has a discrete $Z_2\times Z_2$ symmetry. Moreover the $Z_2\times Z_2$ symmetry is fully broken only when the system exhibits the Haldane gap phenomena. The symmetry is partly broken or not broken in other situations.

The existence of a hidden $Z_2\times Z_2$ symmetry breaking is a powerful criterion to distinguish a system exhibiting the Haldane gap from other disordered spin systems. For example, when the uniaxial anisotropy D in the Hamiltonian (1.1) is very large, the ground state is a small perturbation to the state characterized by $S_i^z|0\rangle=0$ for all i. In such a situation, the ground state is unique and there is a finite excitation gap of order D. (This fact can be proved by developing a suitable rigorous perturbation theory.[10]) However, the ground state does not break the hidden $Z_2\times Z_2$ symmetry. The same is true for the disordered ground state observed in an $S=1$ antiferromagnetic chain with strong bond alternation.

Hida[11] recently studied an $S=\frac{1}{2}$ Heisenberg chain with alternating ferromagnetic and antiferromagnetic couplings. [The Hamiltonian (2.1) below with $\lambda=1$.] The model converges to the antiferromagnetic $S=1$ Heisenberg chain as the ferromagnetic coupling β tends to infinity. Hida observed numerically that the model has a unique ground state with a gap for all the values of $\beta>-1$. He also found that the den Nijs–Rommelse string order parameter for the $S=\frac{1}{2}$ chain is nonvanishing in these ground states. This is an interesting observation since it seems to indicate that the Haldane gap in the $S=1$ chain is continuously connected to the gap in the model with $\beta=0$. The latter model decouples into a collection of pairs of interacting spins, and so it is trivial that the ground state is unique and accompanied by a gap.

The purpose of the present paper is to examine whether the disordered ground states observed by Hida exhibits a hidden $Z_2\times Z_2$ symmetry as in the spin-1 models. We find that, in the $S=\frac{1}{2}$ chain with bond alteration, the nonlocal unitary transformation used by Kohmoto, den Nijs, and Kadanoff[12] in 1981 plays the role of the Kennedy-Tasaki unitary transformation for the $S=1$ chain. The unitary transformation maps the $S=\frac{1}{2}$ chain with alternating couplings into an Ashkin-Teller type $S=\frac{1}{2}$ quantum spin system on a pair of chains. [See (3.1) below.] The transformed model has a very natural $Z_2\times Z_2$ symmetry. Moreover, the unitary transformation maps the string order parameters of the original system into ferromagnetic order parameters in the double-chain system. [See (2.2), (3.2), and (3.3) below.] Thus, the breaking of the $Z_2\times Z_2$ symmetry in the transformed system corresponds to the development of the hidden antiferromagnetic order in the original system.

We show this $Z_2\times Z_2$ symmetry is fully broken in the vicinity of the decoupled model and in the valence-bond-solid (VBS) state which is the exact ground state of a solvable model. This suggests that the symmetry is indeed fully broken in a wide range of the parameter space including the totally decoupled models and the strongly coupled chain, i.e., the $S=1$ model. When there is a long-range Néel order, the $Z_2\times Z_2$ symmetry is partly broken.

The organization of the present paper is as follows. In Sec. II, we define the model and briefly discuss the nature of its ground states. In Sec. III, we describe the nonlocal unitary transformation. In Sec. IV, we discuss properties of typical ground states of the double-chain system with $S=\frac{1}{2}$ obtained in Sec. III. In Sec. V, discussions are given.

II. THE MODEL AND PHASE DIAGRAM

We study the $S=\frac{1}{2}$ spin chain with the Hamiltonian

$$H=\sum_{j=1}^{L-1}\{\sigma_{2j}^x\sigma_{2j+1}^x+\sigma_{2j}^y\sigma_{2j+1}^y+\lambda\sigma_{2j}^z\sigma_{2j+1}^z\}+\beta\sum_{j=1}^{L}(1-\boldsymbol{\sigma}_{2j-1}\cdot\boldsymbol{\sigma}_{2j}), \tag{2.1}$$

where $\boldsymbol{\sigma}_i=(\sigma_i^x,\sigma_i^y,\sigma_i^z)$ are the Pauli matrices which act on the spin at site i, and are related to the spin operators by $\boldsymbol{\sigma}_i=2\mathbf{S}_i$. In the limit $\beta\to\infty$, the ferromagnetic coupling dominates the Hamiltonian and spins on sites $2j-1$ and $2j$ must form an $S=1$ triplet in the ground states. By treating the antiferromagnetic coupling with a degenerate perturbation theory, one exactly recovers the $S=1$ chain with the Hamiltonian (1.1) with $D=0$. To get the Hamiltonian (1.1) with nonvanishing D as the limit, it suffices to add extra interactions $(D/2)\sum_{j=1}^{L}\sigma_{2j-1}^z\sigma_{2j}^z$ to the Hamiltonian (2.1).

Following Hida,[11] we define the den Nijs–Rommelse string operator for the $S=\frac{1}{2}$ chain by

$$\Theta_{\text{string}}^{\alpha}(k,n)=-\sigma_{2k}^{\alpha}\exp\left[\frac{i\pi}{2}\sum_{j=2k+1}^{2n-2}\sigma_j^{\alpha}\right]\sigma_{2n-1}^{\alpha}=(-1)^{n-k}\bigotimes_{j=2k}^{2n-1}\sigma_j^{\alpha}, \tag{2.2}$$

and the corresponding order parameter by

$$O_{\text{string}}^{\alpha}=\lim_{|k-n|\to\infty}\langle\Theta_{\text{string}}^{\alpha}(k,n)\rangle, \tag{2.3}$$

where $\alpha=x$, y, or z. It is straightfoward to check that the string operator and the string order parameter defined in this way converge to the corresponding quantities in the $S=1$ chain as $\beta\to\infty$.

Let us briefly discuss the properties of the ground states of the Hamiltonian (2.1) for various values of β and λ. Figure 1 is the phase diagram that summarizes the expected properties of the ground states.

On the $\beta=\infty$ line, the phase diagram should recover that of the $S=1$ chain with the Hamiltonian (1.1) with $D=0$. It is believed that the ground state of the $S=1$ chain is in the ferromagnetic phase for $\lambda\le-1$, in the massless XY phase for $-1\le\lambda\le\lambda_1$, in the Haldane phase for $\lambda_1\le\lambda\le\lambda_2$, and in the Néel phase for $\lambda_2\le\lambda$. It has been observed numerically that λ_1 lies somewhere around 0, but its precise location is not yet determined. The value of λ_2 is known rather accurately from numerical calculations, and it is slightly larger than 1.

When the ferromagnetic coupling β is vanishing, the model decouples into a collection of independent two-spin systems. We can easily write down its ground states. Let a valence bond (or a singlet pair) v_{ij} be

$$v_{ij}=\frac{1}{\sqrt{2}}(|+\rangle_i|-\rangle_j-|-\rangle_i|+\rangle_j),$$

where $|+\rangle_i$ and $|-\rangle_i$ are the eigenstates of σ_i^z with eigenvalues $+1$ and -1, respectively. For $\beta=0$ and $\lambda>-1$, the ground states of the Hamiltonian (2.1) are

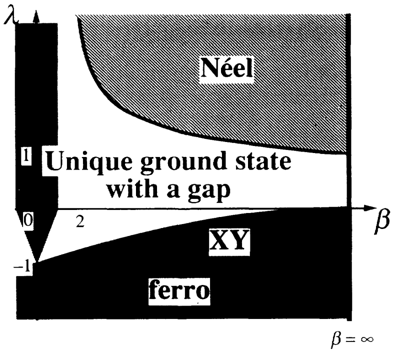

FIG. 1. The expected phase diagram for the ground states of the $S=\frac{1}{2}$ chain with alternating ferromagnetic and antiferromagnetic couplings. The right most line with $\beta=\infty$ corresponds to the $S=1$ antiferromagnetic chain. In the shaded region around the line $\beta=0$, $\lambda>-1$, we have rigorous control of the ground states, and the existence of an excitation gap and a hidden $Z_2\times Z_2$ symmetry breaking is proved. (See Secs. III and IV.) It is expected that the $Z_2\times Z_2$ symmetry breaking takes place in the whole region of the parameter space labeled "unique ground state with a gap" which includes both the decoupled models with $\beta=0$ and the $S=1$ models with $\beta=\infty$. There is also the Néel phase with long-range antiferromagnetic order, the massless XY phase, and the ferromagnetic phase.

the following "dimerized states" which are simple products of the valence bonds:

$$|\Phi_{\rm dimer}\rangle=|a\rangle_1\otimes\left[\bigotimes_{j=1}^{L-1}v_{2j,2j+1}\right]\otimes|b\rangle_{2L}\ . \tag{2.4}$$

Here $a,b=\pm$ are arbitrary. There are two free spin $\frac{1}{2}$'s at the boundaries of the chain. The space of the ground states has dimension four. Figure 2 shows a graphical representation of the ground states. Although one has a fourfold degeneracy in a finite chain, there is a unique ground state in the infinite volume limit. This is because the free spin $\frac{1}{2}$'s are infinitely far away and have no consequences on the physical observations. There is a gap above the ground-state energy which is equal to 4 for $\lambda\geq1$ and $2(\lambda+1)$ for $1\geq\lambda>-1$. The model becomes ferromagnetic for $\beta=0$, $\lambda\leq-1$, and the ground states are highly degenerate. In fact, this line is a critical line. For $\lambda\leq-1$ fixed, the model with β has a phase transition at $\beta=0$.[12]

The calculation of the string order parameter for the dimerized state is trivial[11] and we have

$$\langle\Phi_{\rm dimer}|\Theta^{\alpha}_{\rm string}(k,n)|\Phi_{\rm dimer}\rangle=1$$

for any $n>k$ and $\alpha=x$, y, and z. Thus, we see that

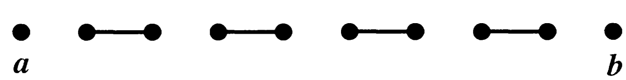

FIG. 2. A graphic representation of the dimerized states. Each bond represents a valence bond (singlet pair).

$O^{\alpha}_{\rm string}=1$ for the string order parameter. Since the model with $\beta=0$ is a collection of decoupled two-spin systems, there can be no long-range order in the usual sense. Hida argued that the string order parameter can be understood as a measure of localized singlet (valence bond). We shall see in the next section that the nonvanishing string order parameter corresponds to a spontaneous breakdown of a discrete hidden symmetry.

It is natural to expect that, in a finite region of parameter space surrounding the above line $\beta=0$, $\lambda>-1$, the model has a unique ground state with a gap. Such a statement can be proved rigorously by using the standard rigorous perturbation theory. In Ref. 10, for example, such a rigorous perturbation theory is formulated in a general manner. One finds that the above Hamiltonian falls into class A of Ref. 10, and the following can be proved rigorously. There is a constant $c>0$ such that, for $\lambda>0$, $|\beta|\leq c$ or $0\geq\lambda>-1$, $|\beta|\leq c(1+\lambda)$, the ground state of the Hamiltonian (2.1) in the infinite volume limit is unique, all the truncated correlation functions decay exponentially in this ground state, and there is a finite energy gap. (See Fig. 1 for a schematic view of the region where the rigorous perturbation theory works.) One also expects to have nonvanishing string order parameter in these models. This is proved in Sec. IV by using the nonlocal unitary transformation discussed in Sec. III.

Hida[11] studied the Hamiltonian (2.1) with $\lambda=1$, and observed numerically that the gap and the string order parameter found to be nonvanishing for $\beta=0$ remain finite all the way down to the $S=1$ limit: $\beta\to\infty$. In this limit, the gap is the Haldane gap and the string order parameter measures the hidden antiferromagnetic order. This observation strongly suggests that the line of gapful models for $\beta=0$ belongs to the same phase as the $S=1$ Heisenberg antiferromagnet. (See the phase diagram, Fig. 1).

The spin-1 chain (1.1) with $D=0$ is believed to have two Néel-ordered ground states for $\lambda\gtrsim1$. (The existence of Néel order can be proved rigorously for sufficiently large λ). Since the limit $\beta\to\infty$ of the present model should recover the spin-1 chain, we expect the Hamiltonian (2.1) has two Néel-ordered ground states when β and λ are large. When we have $\lambda\gg\beta\gg1$, the ground states are essentially given by the following classical Néel states:

$$|\Phi_{\rm N\acute{e}el}\rangle=\left[\bigotimes_{j=1}^{[(L+1)/2]}|a\rangle_{4j-3}|a\rangle_{4j-2}\right]\otimes\left[\bigotimes_{j=1}^{[L/2]}|-a\rangle_{4j-1}|-a\rangle_{4j}\right]\ , \tag{2.5}$$

where $a=\pm$. We expect there is a massless XY phase in a part of the phase diagram as is indicated in Fig. 1.

Although we have no results concerning the ground-state properties of H (2.1) for β not small, there is a solvable model which sheds light on the nature of the ground state for large β. The solvable model is the VBS model,[4] reinterpreted as a model of spin-$\frac{1}{2}$ chain with bond alternation. Consider the Hamiltonian

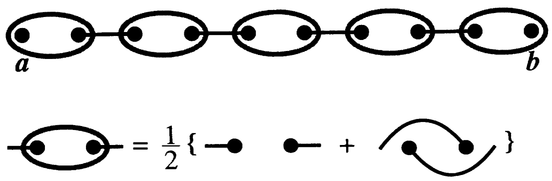

FIG. 3. A graphic representation for the VBS states in the alternating $S=\frac{1}{2}$ spin chain. Two spins surrounded by a gray oval are symmetrized to form a triplet.

$$H_{\rm VBS}=\sum_{j=1}^{L-1} P^{S=2}_{2j-1,2j,2j+1,2j+2}-\beta\sum_{j=1}^{L}\boldsymbol{\sigma}_{2j-1}\cdot\boldsymbol{\sigma}_{2j} \ . \tag{2.6}$$

where $P^{S=2}_{i,j,k,m}$ is the projection operator onto the subspace where the total spin of four sites i,j,k,m is 2. This can be written explicitly by the Pauli matrices as

$$P^{S=2}_{i,j,k,m}=\tfrac{1}{384}(\boldsymbol{\sigma}_i+\boldsymbol{\sigma}_j+\boldsymbol{\sigma}_k+\boldsymbol{\sigma}_m)^4 -\tfrac{1}{48}(\boldsymbol{\sigma}_i+\boldsymbol{\sigma}_j+\boldsymbol{\sigma}_k+\boldsymbol{\sigma}_m)^2 \ .$$

Each term in the first sum of (2.6) favors that there is at least one valence bond within the sites $2j-1$, $2j$, $2j+1$, $2j+2$. On the other hand, each term in the second sum of (2.6) favors the spins at sites $2j-1$ and $2j$ to be in a triplet. Noting that the projection onto a triplet is nothing but the symmetrization operator, we can write down the ground states of (2.6) as

$$|\Phi_{\rm VBS}\rangle=\left\{\bigotimes_{j=1}^{L}\mathcal{S}_{2j-1,2j}\right\}|\Phi_{\rm dimer}\rangle \ , \tag{2.7}$$

where the symmetrization operator is defined by

$$\mathcal{S}_{2j-1,2j}|a\rangle_{2j-1}|b\rangle_{2j}=\tfrac{1}{2}\{|a\rangle_{2j-1}|b\rangle_{2j}+|b\rangle_{2j-1}|a\rangle_{2j}\} \ .$$

for $a,b=\pm$ (Fig. 3). Note that the new states inherit the fourfold degeneracy of the dimerized states. The above VBS states are the exact ground states of (2.6) for all the values of $\beta>0$. (The ground states are highly degenerate at $\beta=0$). Note that these ground states are nothing but the VBS state of Ref. 4 defined for the spin-1 chain if one regards a pair of ferromagnetically coupled spins as a single $S=1$ spin. Unlike the dimerized states, which are the product of noninteracting valence bonds, the VBS states cannot be written as products of decoupled states (unless one performs a nonlocal transformation). In the VBS state, the two-spin correlation function is nonvanishing for any pair of spins. (It decays exponentially.) The string order parameter for the VBS state is nonvanishing and equal to $\frac{4}{9}$.[5] (The easiest way to get this value is to use the nonlocal unitary transformation of Kennedy and Tasaki[10] which maps the VBS state to a simple tensor product of local states.)

III. THE UNITARY TRANSFORMATION

In the present section, we describe the nonlocal unitary transformation which reveals the hidden $Z_2 \times Z_2$ symmetry of the Hamiltonian (2.1). Surprisingly, the transformation is essentially the same as that used by Kohmoto, den Nijs, and Kadanoff[12] to demonstrate the relation between the highly anisotropic version of the $d=2$ Ashkin-Teller model ($d=1$ quantum system) and the staggered XXZ model. It may be worth noting that the present unitary transformation does not converge to the Kennedy-Tasaki transformation in the limit $\beta\to\infty$.

We shall omit a constant in (2.1) and start from the following Hamiltonian:

$$H=\sum_{j=1}^{L-1}\{\sigma^x_{2j}\sigma^x_{2j+1}+\sigma^y_{2j}\sigma^y_{2j+1}+\lambda\sigma^z_{2j}\sigma^z_{2j+1}\} -\beta\sum_{j=1}^{L}\boldsymbol{\sigma}_{2j-1}\cdot\boldsymbol{\sigma}_{2j} \ .$$

First we perform a local gauge transformation by the unitary operator

$$G=\bigotimes_{j=1}^{[L/2]}\exp\left[\frac{i\pi}{2}(\sigma^y_{4j-1}+\sigma^y_{4j})\right] \ ,$$

which generates a rotation of π about the y axis on spins in every other ferromagnetically coupled pairs. This makes the system look as ferromagnetic as possible:

$$GHG^{-1}=-\sum_{j=1}^{L-1}\{\sigma^x_{2j}\sigma^x_{2j+1}-\sigma^y_{2j}\sigma^y_{2j+1}+\lambda\sigma^z_{2j}\sigma^z_{2j+1}\} -\beta\sum_{j=1}^{L}\boldsymbol{\sigma}_{2j-1}\cdot\boldsymbol{\sigma}_{2j} \ .$$

Then we apply the standard duality transformation[13] onto the whole system. In Appendix A, we have defined the duality transformation as the unitary transformation D of the Hilbert space. Using the relations (A2) and (A3), we get

$$(DG)H(DG)^{-1}=-\sum_{j=1}^{L-1}\{\sigma^z_{2j-1/2}\sigma^z_{2j+3/2}+\sigma^z_{2j-1/2}\sigma^x_{2j+1/2}\sigma^z_{2j+3/2}+\lambda\sigma^x_{2j+1/2}\} -\beta\sum_{j=1}^{L}\{\sigma^z_{2j-3/2}\sigma^z_{2j+1/2}-\sigma^z_{2j-3/2}\sigma^x_{2j-1/2}\sigma^z_{2j+1/2}+\sigma^x_{2j-1/2}\} \ ,$$

where we set $\sigma^z_{1/2}=1$. In the next step of the transformation, we merely change the labeling of the lattice sites by the following rule:

$$R: r \to \tfrac{1}{2}(r+\tfrac{1}{2}) .$$

After the relabeling, we shall rewrite the Pauli matrices on the half-odd integer sites as τ. The Hamiltonian then becomes

$$(RDG)H(RDG)^{-1} = -\sum_{j=1}^{L-1}\{\sigma^z_j\sigma^z_{j+1}+\sigma^z_j\tau^x_{j+1/2}\sigma^z_{j+1} + \lambda\tau^x_{j+1/2}\} -\beta\sum_{j=1}^{L}\{\tau^z_{j-1/2}\tau^z_{j+1/2} - \tau^z_{j-1/2}\sigma^x_j\tau^z_{j+1/2}+\sigma^x_j\} .$$

Finally we apply the inverse of the duality transformation only to the τ spins. If we denote by D^τ the dual transformation for the τ spins (which brings a system on the chain $\{1,2,\ldots,L\}$ onto that on the dual chain $\{\frac{3}{2},\frac{5}{2},\ldots,L+\frac{1}{2}\}$), our unitary transformation can be written as

$$U=(D^\tau)^{-1}RDG .$$

Using (A4) and (A5), we find that the final form of the transformed Hamiltonian is

$$\tilde{H}=UHU^{-1} = -\sum_{j=1}^{L-1}\{\sigma^z_j\sigma^z_{j+1}+\lambda\tau^z_j\tau^z_{j+1}+\sigma^z_j\sigma^z_{j+1}\tau^z_j\tau^z_{j+1}\} -\beta\sum_{j=1}^{L}\{\sigma^x_j+\tau^x_j-\sigma^x_j\tau^x_j\} . \quad (3.1)$$

The first part in the Hamiltonian describes two ferromagnetic Ising models coupled by four spin interactions, while the second part is a kind of transverse field. The symmetry of the Hamiltonian $\tilde{H}$ can be easily read off. It is invariant under rotations of π about the x axis applied to σ spins alone or τ spins alone. Thus, it has a $Z_2\times Z_2$ symmetry.

The transformation of the string operators can also be calculated easily. We consider the string operator (2.2) with $a=x$ or z. Then the local gauge transformation G simply gets rid of the extra sign factor in the right-hand side of (2.2) and we have

$$G\Theta^\alpha_{\rm string}(k,n)G^{-1}=\bigotimes_{j=2k}^{2n-1}\sigma^\alpha_j \quad (\alpha=x,z) .$$

Let us consider the case $\alpha=x$ first. Using (A2), we see that the first duality transformation maps the string operator into a product of two local operators as

$$(DG)\Theta^x_{\rm string}(k,n)(DG)^{-1}=\sigma^z_{2k-1/2}\sigma^z_{2n-1/2} .$$

The remaining transformation is the relabeling of the lattice sites, and we get

$$U\Theta^x_{\rm string}(k,n)U^{-1}=\sigma^z_k\sigma^z_n . \quad (3.2)$$

Next we consider the case $\alpha=z$. Using (A3), we find that the result of the first duality transformation is

$$(DG)\Theta^z_{\rm string}(k,n)(DG)^{-1}=\bigotimes_{m=k}^{n-1}\sigma^x_{2m+1/2} .$$

The relabeling transformation maps this operator into the standard string operator of τ spins. The second duality transformation maps this to a simple operator as

$$U\Theta^z_{\rm string}(k,n)U^{-1}=\tau^z_k\tau^z_n . \quad (3.3)$$

The above (3.2) and (3.3) indicate that the nonlocal unitary transformation maps the string correlations in the x and z directions to the standard ferromagnetic correlations of the σ spins and τ spins, respectively. Consequently, the string order parameters (2.3) with $\alpha=x$ and z are mapped to the square of the ferromagnetic order parameters for σ spins and τ spins, respectively, of the double-chain system. These ferromagnetic order parameters measure possible spontaneous breaking of the abovementioned $Z_2\times Z_2$ symmetry.

IV. TYPICAL GROUND STATES OF THE TRANSFORMED SYSTEM

We discuss the properties of typical ground states of the double-chain $S=\frac{1}{2}$ system (3.1) obtained by the nonlocal unitary transformation. We will see that the $Z_2\times Z_2$ symmetry is fully broken in the following cases A and C. In case B, the symmetry is partly broken or fully broken depending on the values of the parameters.

(A) $\beta=0$ case. We have the simplest situation in this case. The transformed Hamiltonian

$$\tilde{H}=-\sum_{j=1}^{L-1}\{\sigma^z_j\sigma^z_{j+1}+\lambda\tau^z_j\tau^z_{j+1}+\sigma^z_j\sigma^z_{j+1}\tau^z_j\tau^z_{j+1}\}$$

is diagonal in the standard basis, so its ground states are classical spin configurations which minimize the energy. One finds that, for $\lambda>-1$, there are four ground states given by

$$\bigotimes_{j=1}^{L}|+\rangle^\sigma_j|+\rangle^\tau_j ,$$

$$\bigotimes_{j=1}^{L}|+\rangle^\sigma_j|-\rangle^\tau_j ,$$

$$\bigotimes_{j=1}^{L}|-\rangle^\sigma_j|+\rangle^\tau_j ,$$

$$\bigotimes_{j=1}^{L}|-\rangle^\sigma_j|-\rangle^\tau_j ,$$

where $|\pm\rangle^\sigma_j$, $|\pm\rangle^\tau_j$ are the states for the σ spin and τ spin, respectively, at site j characterized by $\sigma^z_i|\pm\rangle^\sigma_j=\pm|\pm\rangle^\sigma_j$, $\tau^z_i|\pm\rangle^\tau_j=\pm|\pm\rangle^\tau_j$. The above ground states fully break the $Z_2\times Z_2$ symmetry. As is expected, we recover these states by applying the unitary transformation U to the dimerized state (2.4). See Appendix B for details.

The existence of similar $Z_2\times Z_2$ symmetry breaking can be proved rigorously in a neighborhood of the above trivially solvable model. These models fall into class B of Ref. 10, and one can prove rigorously that they have four infinite volume ground states with nonvanishing ferromagnetic order. Therefore, the unique ground state of the original Hamiltonian (2.1) has nonvanishing string order. The region in which such a rigorous perturbation theory works is the same as that described in Sec. II.

Based on Hida's numerical calculation,[11] we expect this $Z_2\times Z_2$ symmetry breaking to continue to the region of the parameter space with large β. But we have no way of controlling this symmetry breaking theoretically. The only case we can control the effect of large (or even infinite) β is the generalized VBS model discussed in Sec. II C below.

(B) $\lambda \gg \beta$, 1 case. Since the ground state for the part of the Hamiltonian including λ is easily obtained in this case, we shall treat the other parts by a degenerate perturbation theory within the states spanned by

$$|\Phi^\sigma\rangle\otimes\left[\bigotimes_{j=1}^{L}|+\rangle_j^\tau\right]$$

and

$$|\Psi^\sigma\rangle\otimes\left[\bigotimes_{j=1}^{L}|-\rangle_j^\tau\right],$$

where $|\Phi^\sigma\rangle$ and $|\Psi^\sigma\rangle$ are arbitrary states for the σ spins. Since the operators τ^x have no nonvanishing matrix elements between the above two types of states, we only have to treat the Hamiltonian

$$\tilde{H}^\sigma=-2\sum_{j=1}^{L-1}\sigma_j^z\sigma_{j+1}^z-\beta\sum_{j=1}^{L}\sigma_j^x$$

for the σ spins. This is nothing but the solvable Ising chain under transverse magnetic field. When $\beta<2$, the σ spins break the Ising symmetry, thus leading to the full $Z_2\times Z_2$ symmetry breaking. When $\beta>2$, the Ising symmetry for the σ spins is restored, and the whole ground state breaks half of the $Z_2\times Z_2$ symmetry. Such partial symmetry breaking is exhibited in the ground state for $\lambda\gg\beta>2$:

$$\bigotimes_{j=1}^{L}\frac{1}{\sqrt{2}}\{(|+\rangle_j^\sigma+|-\rangle_j^\sigma)|+\rangle_j^\tau\}$$

or

$$\bigotimes_{j=1}^{L}\frac{1}{\sqrt{2}}\{(|+\rangle_j^\sigma+|-\rangle_j^\sigma)|-\rangle_j^\tau\},$$

which is also obtained by applying the unitary transformation U to the Néel state (2.5). (See Appendix B.)

(C) Valence-bond-solid case. Let us discuss the VBS model with the Hamiltonian (2.6) introduced in Sec. II. As has been stressed, this is the only model in which we can control the effect of large or infinite β. In the exact ground state of this model, the ground state is much more complicated than the trivial model with $\beta=0$, since the interaction between two ferromagnetically coupled spins are taken into account.

A tedious but straightforward calculation described in Appendix B shows that the VBS states (2.7) transform as follows:

$$U|\Phi_{\rm VBS}\rangle=\begin{cases}\bigotimes_{j=1}^{L}\frac{1}{\sqrt{12}}(3|+\rangle_j^\sigma|+\rangle_j^\tau+|+\rangle_j^\sigma|-\rangle_j^\tau+|-\rangle_j^\sigma|+\rangle_j^\tau-|-\rangle_j^\sigma|-\rangle_j^\tau)\\ \bigotimes_{j=1}^{L}\frac{1}{\sqrt{12}}(3|-\rangle_j^\sigma|-\rangle_j^\tau+|-\rangle_j^\sigma|+\rangle_j^\tau+|+\rangle_j^\sigma|-\rangle_j^\tau-|+\rangle_j^\sigma|+\rangle_j^\tau)\\ \bigotimes_{j=1}^{L}\frac{1}{\sqrt{12}}(3|+\rangle_j^\sigma|-\rangle_j^\tau+|+\rangle_j^\sigma|+\rangle_j^\tau+|-\rangle_j^\sigma|-\rangle_j^\tau-|-\rangle_j^\sigma|+\rangle_j^\tau)\\ \bigotimes_{j=1}^{L}\frac{1}{\sqrt{12}}(3|-\rangle_j^\sigma|+\rangle_j^\tau+|-\rangle_j^\sigma|-\rangle_j^\tau+|+\rangle_j^\sigma|+\rangle_j^\tau-|+\rangle_j^\sigma|-\rangle_j^\tau)\,.\end{cases}$$

These states clearly break the full $Z_2\times Z_2$ symmetry. Unlike the case for $\beta=0$, there is a correlation between the σ spins and the τ spins. It is notable that, as in the case of the Kennedy-Tasaki transformation in the $S=1$ chain,[10] the VBS states have been transformed into a simple tensor product of single-spin states. This is a highly nontrivial fact since the VBS states cannot be written as products of local states in the standard basis.[4]

V. DISCUSSIONS

We have presented some results which indicate that the $S=\frac{1}{2}$ chain (2.1) with alternating ferromagnetic and antiferromagnetic couplings fully breaks the hidden $Z_2\times Z_2$ symmetry in a wide region of the parameter space. The region includes both the decoupled models and the strongly coupled chain, i.e., the $S=1$ model. Since the full breaking of the $Z_2\times Z_2$ symmetry is believed to be a fundamental property of a Haldane gap system,[10] this observation provides further support of Hida's conclusion[11] that the Haldane gap is continuously connected to the gap in the model with $\beta=0$.

The ground state of the $S=\frac{1}{2}$, chain (2.1) with $\beta=0,\lambda>-1$ is a product of local valence bands. Note that the physical idea behind the construction of the solvable VBS model of Affleck, Kennedy, Lieb, and Tasaki[4] was that the ground state of the $S=1$ chain in the Haldane phase may be understood as a modification of such valence-bond states.

Hida's and the present observation suggest that the $S=1$ chain exhibiting the Haldane gap belongs to the same phase as the decoupled $S=\frac{1}{2}$ chain with $\beta=0$. Even though the latter model has a gap generated by a trivial reason, one should not regard that the mechanism that generates the Haldane gap has been resolved. These observations simply lift the problem to a different stage. Now the really hard problem is to find out why the gapful phase continues all the way to $\beta\to\infty$ when λ is close to 1. As far as we know, such a problem is understood only in the solvable VBS models.

To see that this is really a nontrivial problem, consider the model with $\lambda=0$. For β not too large, the behavior of the model is more or less the same as that with $\lambda=1$. However, the two models behave quite differently as β becomes large. The model with $\lambda=0$ is expected to undergo a phase transition and is massless at $\beta=\infty$, while the model with $\lambda=1$ is believed to be massive even at $\beta=\infty$.

Den Nijs and Rommelse[5] pointed out that the phase diagram of the $S=1$ Hamiltonian (2.1) is similar to that of the Ashkin-Teller model in the strong anisotropy limit.[12] Then den Nijs[14] argued that the two models have the same Coulomb gas representation in the continuum limit and should be in the same universality class.

One might imagine that the transformation of Sec. III provides further support to this mapping since the double-chain model (3.1) obtained by the unitary transformation is of the Ashkin-Teller type. However, the Hamiltonian (3.1) lacks the positivity property which would allow one to rewrite a quantum system as a classical system in one higher dimension. Our transformation maps the spin chain to the "outside" of the standard phase diagram of the Ashkin-Teller model. It is interesting that the quantum antiferromagnetic chain is related to the Ashkin-Teller-type model in two different ways.

The Kennedy-Tasaki unitary transformation[10] for the $S=1$ chain not only reveals the hidden symmetry, but also provides a useful basis to study the Haldane gap and the related phenomena. Kennedy and Tasaki developed a simple but powerful variational calculation for the ground state of the $S=1$ chain (1.1). Kennedy[15] constructed a one-parameter family of SU(2) noninvariant $S=1$ chains which includes the VBS model. We believe the unitary transformation studied in the present paper can be used to extend these ideas to the $S=\frac{1}{2}$ chain with bond alternation.

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APPENDIX A: THE DUALITY TRANSFORMATION

Here we define the duality transformation[13] used in Sec. III. The transformation, which is quite standard, is usually defined by writing down the transformation rule of the spin operators. [See (A2)–(A5) below.] Here we shall define the transformation explicitly as a unitary transformation of the Hilbert space on which the spin operators act. Such a formulation is necessary for us when we calculate the transformation of various states explicitly as in Sec. IV and in Appendix B.

Consider a chain $\{1,2,\ldots,M\}$ of $S=\frac{1}{2}$ spins. $\boldsymbol{\sigma}_j$ $(j=1,2,\ldots,M)$ denote the Pauli matrices. The duality transformation D is an unitary transformation which maps a state of this system onto a state of the "dual chain" $\{\frac{3}{2},\frac{5}{2},\ldots,M+\frac{1}{2}\}$ of $S=\frac{1}{2}$ spins. $\boldsymbol{\sigma}_{j+1/2}$ $(j=1,2,\ldots,M)$ denote the Pauli matrices for the dual chain.

In the original system, we take the x axis as the quantization axis and define basis vectors by

$$|+\rangle_j^x=\frac{1}{\sqrt{2}}(|+\rangle_j^z+|-\rangle_j^z)\ ,$$

$$|-\rangle_j^x=\frac{1}{\sqrt{2}i}(|+\rangle_j^z-|-\rangle_j^z)\ ,$$

where $|\pm\rangle_j^z$ are the standard basis vectors. Let the classical configuration $c=\{c_j\}$ be a collection of variables $c_j=\pm 1$ for $j=1,2,\ldots,M$. We denote by $|c\rangle^x$ a basis state defined by

$$|c\rangle^x=\bigotimes_{j=1}^{M}|c_j\rangle_j^x\ .$$

We define a classical configuration c^* on the dual lattice by

$$c^*_{j+1/2}=\prod_{k=1}^{j}c_k\ . \tag{A1}$$

In the dual system, we take (as usual) the z axis as the quantization axis, and denote by $|c^*\rangle^z$ a basis state defined by

$$|c^*\rangle^z=\bigotimes_{j=1}^{M}|c^*_{j+1/2}\rangle_{j+1/2}^z\ .$$

We define the duality transformation as

$$D=\tilde{D}\exp\left[\frac{i\pi}{4}\sum_{i=1}^{M}\sigma_i^x\right]\ .$$

The main body of the transformation is defined by

$$\tilde{D}\sum_c\varphi_c|c\rangle^x=\sum_c\varphi_c|c^*\rangle^z\ ,$$

where φ_c are arbitrary complex coefficients. It is clear from the definition that D is unitary. Note that we do not have a relation like $D^2=1$.

The transformation of the operators by D are given by the following:

$$D\sigma_j^xD^{-1}=\sigma_{j-1/2}^z\sigma_{j+1/2}^z\ , \tag{A2}$$

$$D\sigma_j^zD^{-1}=\bigotimes_{k=j}^{M}\sigma_{k+1/2}^x\ , \tag{A3}$$

$$D^{-1}\sigma_{j+1/2}^xD=\sigma_j^z\sigma_{j+1}^z\ , \tag{A4}$$

$$D^{-1}\sigma^z_{j+1/2}D=\bigotimes_{k=1}^{j}\sigma^x_k\ . \tag{A5}$$

The relation (A2) should be read $D\sigma^x_1D^{-1}=\sigma^z_{3/2}$ for $j=1$, and (A4) should be read $D^{-1}\sigma^x_{M+1/2}D=\sigma^z_M$ for $j=M$. The transformation rules for σ^y follow from the identity $\sigma^y_j=i\sigma^x_j\sigma^z_j$ for the Pauli matrices.

We show the relations (A2)–(A5) in the rest of the Appendix. Let us start from (A5), which is the easiest. By applying the operator on the left-hand side onto an arbitrary basis state (quantized in the x direction) of the original system, we get

$$\begin{aligned}D^{-1}\sigma^z_{j+1/2}D|c\rangle^x&=\exp\left[\frac{i\pi}{4}\sum c_i\right]D^{-1}\sigma^z_{j+1/2}|c^*\rangle^z\\&=\exp\left[\frac{i\pi}{4}\sum c_i\right]D^{-1}c^*_{j+1/2}|c^*\rangle^z\\&=\exp\left[\frac{i\pi}{4}\sum c_i\right]\prod_{k=1}^{j}c_k\exp\left[-\frac{i\pi}{4}\sum c_i\right]|c\rangle^x\\&=\bigotimes_{k=1}^{j}\sigma^x_k|c\rangle^x\ ,\end{aligned}$$

which is the desired (A5). Similarly we apply the left-hand side of (A3) to a basis state to get

$$\begin{aligned}D\sigma^z_jD^{-1}|c^*\rangle^z&=\exp\left[-\frac{i\pi}{4}\sum c_i\right]D\sigma^z_j|c\rangle^x\\&=\exp\left[-\frac{i\pi}{4}\sum c_i\right]Dic_j|\bar{c}\rangle^x\ ,\end{aligned}$$

where $\bar{c}$ is defined by

$$\bar{c}_k=\begin{cases}c_k & \text{for } k\neq j\\ -c_j & \text{for } k=j\ .\end{cases}$$

From the definition of D we get

$$\begin{aligned}&D\sigma^z_jD^{-1}|c^*\rangle^z\\&=\exp\left[-\frac{i\pi}{4}\sum c_i\right]ic_j\exp\left[\frac{i\pi}{4}\sum \bar{c}_i\right]|(\bar{c})^*\rangle^z\\&=|(\bar{c})^*\rangle^z=\bigotimes_{k=j}^{M}\sigma^x_{k+1/2}|c^*\rangle^z\ ,\end{aligned}$$

where

$$(\bar{c})^*_{k+1/2}=\begin{cases}c^*_{k+1/2} & \text{for } k<j\\ -c^*_{k+1/2} & \text{for } k\geq j\ ,\end{cases}$$

by the definitions. Thus, (A3) follows. The other two relations [(A2) and (A4)] follow from (A3) and (A5) by noting that $(\sigma^\alpha_i)^2=1$.

APPENDIX B: UNITARY TRANSFORMATION OF TYPICAL STATES

Here we outline how to calculate the unitary transformation of typical states discussed in Sec. IV. In the following calculations, we consider only one typical state from each class. The other states can be obtained in a similar manner. We also omit the constants multiplying the states since they do not have any physical information.

Néel state. Consider a Néel state (2.5) with $a=+$. By applying the local gauge transformation G, it becomes the ferromagnetic state as

$$G|\Phi_{\text{Néel}}\rangle=\bigotimes_{j=1}^{2L}|+\rangle^z_j=\bigotimes_{j=1}^{2L}\frac{1}{\sqrt{2}}(|+\rangle^x_j+i|-\rangle^x_j)\ .$$

We then apply the dual transformation D. The first part of the transformation is the multiplication by a phase factor, and we get

$$\begin{aligned}\exp\left[\frac{i\pi}{4}\sum_{i=1}^{2L}\sigma^x_i\right]G|\Phi_{\text{Néel}}\rangle&=e^{i\pi L/2}\bigotimes_{j=1}^{2L}\frac{1}{\sqrt{2}}(|+\rangle^x_j+|-\rangle^x_j)\\&=\text{const}\times\sum_{\substack{c_j=\pm1\\(j=1,2,\ldots,2L)}}\bigotimes_{j=1}^{2L}|c_j\rangle^x_j\ .\end{aligned}$$

It is clear from (A1) that, when we sum over all the possible $\{c_j\}$, the dual configuration $\{c^*_{j+1/2}\}$ is also summed over all the possible combinations with $c^*_{j+1/2}=\pm1$. Thus, we get

$$\begin{aligned}DG|\Phi_{\text{Néel}}\rangle&=\text{const}\times\sum_{\substack{c^*_{j+1/2}=\pm1\\(j=1,2,\ldots,2L)}}\bigotimes_{j=1}^{2L}|c^*_{j+1/2}\rangle^z_{j+1/2}\\&=\text{const}\bigotimes_{j=1}^{2L}(|+\rangle^z_{j+1/2}+|-\rangle^z_{j+1/2})\ .\end{aligned}$$

After the trivial relabeling and renaming of the spin operators, we have to apply the inverse duality transformation to the following state for τ spins:

$$\bigotimes_{j=1}^{L}(|+\rangle^z_{j+1/2}+|-\rangle^z_{j+1/2})\ .$$

But the result of the transformation is obvious from the above calculations. Our final result is

$$U|\Phi_{\text{Néel}}\rangle=\text{const}\bigotimes_{j=1}^{L}(|+\rangle_j^{z,\sigma}+|-\rangle_j^{z,\sigma})|+\rangle_j^{z,\tau}\ .$$

Dimerized state. We consider a dimerized state

$$|\Phi_{\text{dimer}}\rangle=|+\rangle_1^x\otimes\left[\bigotimes_{j=1}^{L-1}v_{2j,2j+1}\right]\otimes(|+\rangle_{2L}^x+i|-\rangle_{2L}^x)\ .$$

The valence bond is written in the present basis as

$$v_{ij}=\frac{1}{\sqrt{2}i}(|+\rangle_i^x|-\rangle_j^x-|-\rangle_i^x|+\rangle_j^x)\ .$$

After the gauge transformation and the multiplication by a phase factor, we get

$$\exp\left[\frac{i\pi}{4}\sum_{i=1}^{2L}\sigma_i^x\right]G|\Phi_{\text{dimer}}\rangle=\text{const}|+\rangle_1^x\otimes\left[\bigotimes_{j=1}^{L-1}g_{2j,2j+1}\right]\otimes(|+\rangle_{2L}^x+|-\rangle_{2L}^x)\ ,$$

where

$$g_{ij}=\frac{1}{\sqrt{2}}(|+\rangle_i^x|+\rangle_j^x+|-\rangle_i^x|-\rangle_j^x)\ .$$

The above can be rewritten as

$$\exp\left[\frac{i\pi}{4}\sum_{i=1}^{2L}\sigma_i^x\right]G|\Phi_{\text{dimer}}\rangle=\text{const}\times\sum_{\substack{u_j=\pm1\\(j=1,2,\ldots,L)}}|+\rangle_1^x\otimes\left[\bigotimes_{j=1}^{L-1}|u_j\rangle_{2j}^x|u_j\rangle_{2j+1}^x\right]\otimes|u_L\rangle_{2L}^x\ .$$

For a fixed $\{u_j\}$, the corresponding dual spin configuration can be easily obtained by using (A1) as

$$c_{2j-1/2}^*=1,\quad c_{2j+1/2}^*=u_j\ .$$

Thus, we get

$$\begin{aligned}DG|\Phi_{\text{dimer}}\rangle&=\text{const}\times\sum_{\substack{u_j=\pm1\\(j=1,2,\ldots,L)}}\bigotimes_{j=1}^{L}|+\rangle_{2j-1/2}^z|u_j\rangle_{2j+1/2}^z\\&=\text{const}\bigotimes_{j=1}^{L}|+\rangle_{2j-1/2}^z(|+\rangle_{2j+1/2}^z+|-\rangle_{2j+1/2}^z)\ .\end{aligned}$$

Fortunately, we find that the inverse dual transformation (after the relabeling) is exactly the same as the previous Néel state. So we get

$$U|\Phi_{\text{dimer}}\rangle=\text{const}\bigotimes_{j=1}^{L}|+\rangle_j^{z,\sigma}|+\rangle_j^{z,\tau}\ .$$

VBS state. We consider the VBS state obtained by applying the symmetrization operator onto the dimerized state considered above. Then the calculation similar to the above shows that

$$\exp\left[\frac{i\pi}{4}\sum_{i=1}^{2L}\sigma_i^x\right]G|\Phi_{\text{VBS}}\rangle=\text{const}\times\sum_{\substack{u_j=\pm1\\(j=1,2,\ldots,L)}}\left\{\bigotimes_{j=1}^{L}\mathcal{S}_{2j-1,2j}\right\}\left[|+\rangle_1^x\otimes\left[\bigotimes_{j=1}^{L-1}|u_j\rangle_{2j}^x|u_j\rangle_{2j+1}^x\right]\otimes|u_L\rangle_{2L}^x\right]\ .$$

For a fixed $\{u_j\}$, the corresponding dual spin configuration can be obtained by using (A1) as

$$c_{2j-1/2}^*=\begin{cases}u_{j-1}u_j & \text{exchanged}\\ 1 & \text{unexchanged,}\end{cases}\quad c_{2j+1/2}^*=u_j\ ,$$

where the condition in the first equality refers to whether the spins at $2j-1$ and $2j$ are exchanged by the symmetrization operator or left unexchanged. Thus, we get

$$DG|\Phi_{\text{VBS}}\rangle=\text{const}\times\sum_{\substack{u_j=\pm1\\(j=1,2,\ldots,L)}}\bigotimes_{j=1}^{L}\{(|+\rangle_{2j-1/2}^z+|u_{j-1}u_j\rangle_{2j-1/2}^z)\otimes|u_j\rangle_{2j+1/2}^z\}\ .$$

After the relabeling transformation, we should apply the inverse dual transformation to the state for τ spins. By letting $c_{j+1/2}^*=u_j$ and solving (A1) for $\{c_j\}$, we get

$$(D^{\tau})^{-1}\bigotimes_{j=1}^{L}|u_j\rangle_{j+1/2}^{z,\tau}=\bigotimes_{j=1}^{L}\exp\left[-\frac{i\pi}{4}u_{j-1}u_j\right]|u_{j-1}u_j\rangle_j^{x,\tau}\ .$$

Noting that

$$\exp\left[-\frac{i\pi}{4}v_j\right]|v_j\rangle_j^{x,\tau}=\frac{e^{-i\pi/4}}{\sqrt{2}}(|+\rangle_j^{z,\tau}+v_j|-\rangle_j^{z,\tau}) ,$$

and writing $u_{j-1}u_j=v_j$, we can express the final result as

$$U|\Phi_{\text{VBS}}\rangle=\text{const}\times\sum_{\substack{v_j=\pm1\\(j=1,2,\ldots,L)}}\bigotimes_{j=1}^{L}(|+\rangle_j^{z,\sigma}+|v_j\rangle_j^{z,\sigma})\otimes(|+\rangle_j^{z,\tau}+v_j|-\rangle_j^{z,\tau})\}$$

$$=\text{const}\bigotimes_{j=1}^{L}(3|+\rangle_j^{z,\sigma}|+\rangle_j^{z,\tau}+|+\rangle_j^{z,\sigma}|-\rangle_j^{z,\tau}+|-\rangle_j^{z,\sigma}|+\rangle_j^{z,\tau}-|-\rangle_j^{z,\sigma}|-\rangle_j^{z,\tau}) .$$

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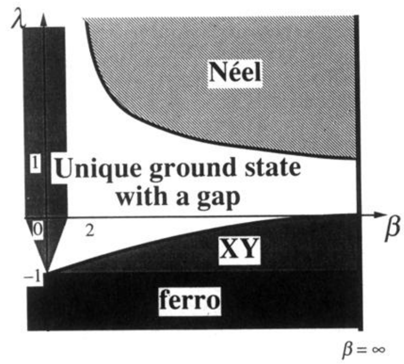

FIG. 1. The expected phase diagram for the ground states of the $S=\frac{1}{2}$ chain with alternating ferromagnetic and antiferromagnetic couplings. The right most line with $\beta=\infty$ corresponds to the $S=1$ antiferromagnetic chain. In the shaded region around the line $\beta=0$, $\lambda>-1$, we have rigorous control of the ground states, and the existence of an excitation gap and a hidden $Z_2\times Z_2$ symmetry breaking is proved. (See Secs. III and IV.) It is expected that the $Z_2\times Z_2$ symmetry breaking takes place in the whole region of the parameter space labeled "unique ground state with a gap" which includes both the decoupled models with $\beta=0$ and the $S=1$ models with $\beta=\infty$. There is also the Néel phase with long-range antiferromagnetic order, the massless XY phase, and the ferromagnetic phase.