Commun. Math. Phys. 147, 431–484 (1992)

Communications in Mathematical Physics

© Springer-Verlag 1992

Hidden Symmetry Breaking and the Haldane Phase in $S = 1$ Quantum Spin Chains

Tom Kennedy[1] **and Hal Tasaki**[2]

[1] Department of Mathematics, University of Arizona, Tucson, AZ 85721, USA
[2] Department of Physics, Gakushuin University, Mejiro, Toshima-ku, Tokyo 171, Japan

Received September 4, 1991; in revised form November 27, 1991

Abstract. We study the phase diagram of $S = 1$ antiferromagnetic chains with particular emphasis on the Haldane phase. The hidden symmetry breaking measured by the string order parameter of den Nijs and Rommelse can be transformed into an explicit breaking of a $Z_2 \times Z_2$ symmetry by a nonlocal unitary transformation of the chain. For a particular class of Hamiltonians which includes the usual Heisenberg Hamiltonian, we prove that the usual Néel order parameter is always less than or equal to the string order parameter. We give a general treatment of rigorous perturbation theory for the ground state of quantum spin systems which are small perturbations of diagonal Hamiltonians. We then extend this rigorous perturbation theory to a class of "diagonally dominant" Hamiltonians. Using this theory we prove the existence of the Haldane phase in an open subset of the parameter space of a particular class of Hamiltonians by showing that the string order parameter does not vanish and the hidden $Z_2 \times Z_2$ symmetry is completely broken. While this open subset does not include the usual Heisenberg Hamiltonian, it does include models other than VBS models.

1. Introduction

Much of our intuition for quantum spin systems is based on our understanding of the corresponding classical systems. However, occasionally the quantum spin systems surprise us. One of the most interesting surprises is the qualitative dependence of the properties of the one dimensional Heisenberg antiferromagnet on whether the spin is integral or half integral which was discovered by Haldane. He argued that the ground state has an excitation gap and exponentially decaying correlation functions when S is integral, while it has a ground state without a gap and correlation functions with power law decay when S is half integral [22]. Haldane's argument was based on an approximate mapping of the spin chain onto a two dimensional quantum field theory.

The Heisenberg antiferromagnet has a continuous symmetry; we can rotate all the spins by the same amount, and the Hamiltonian will be unchanged. This suggests that it should be possible to construct excitations with arbitrarily low

energy by a gradual twist of the ground state. Haldane's conclusion says that this classical intuition is wrong when the spin is integral. (Note that in the quantum case there is no guarantee that the gradual twist does not simply give you back the ground state.) Even more surprising than this failure of our classical intuition is the way in which the qualitative properties of the chain flip back and forth as the spin varies through half integral and integral values. This is in stark contrast to the universality we have come to expect.

Haldane's theoretical work prompted a great deal of further theoretical work, numerical studies, experiments, and eventually some rigorous work. The numerical work for $S = 1$ now supports Haldane's conclusions rather convincingly [12, 34, 39, 45, 55]. Experimental results in quasi one dimensional systems with an effective spin 1 at each site [6, 15, 21, 24, 43, 51] seem to be consistent with the existence of a gap. For a review, see [2].

The less interesting half of Haldane's conclusions have been proven rigorously. Lieb, Schultz and Mattis [36] proved for $S = 1/2$ that the model must either have no excitation gap or more than one ground state. This proof was extended to all half integral spin by Affleck and Lieb [5] and by Kolb [30]. For any value of the spin the one dimensional Heisenberg antiferromagnet is expected to have a unique infinite volume ground state, in which case the above result implies there is no gap.

There are rigorous results for integral spin for a special class of Hamiltonians. For $S = 1$ the special Hamiltonian is

$$H = \sum_i \mathbf{S}_i \cdot \mathbf{S}_{i+1} + \frac{1}{3}(\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2 \,. \tag{1.1}$$

Affleck, Kennedy, Lieb and Tasaki [4] proved that this model has a unique infinite volume ground state with a gap and exponentially decaying correlation functions. A crucial step in the proof was to realize that the exact ground state of the Hamiltonian (1.1) can be written down compactly using the valence-bond basis. The exact ground state is called the VBS (Valence-Bond-Solid) state. Knabe [29] gave another proof of the existence of a gap in this model. For higher values of the spin the special Hamiltonian is again a polynomial in $\mathbf{S}_i \cdot \mathbf{S}_{i+1}$. The two point function of the ground state of the special model with $S = 1, 2, 3, \ldots$ was computed by Arovas, Auerbach and Haldane [7] and seen to decay exponentially. Fannes, Nachtergaele and Werner [17] studied this class of models in a very general setting. They proved the existence of a gap for all integral spin.

Tasaki [57] proved the existence of the Haldane gap in an $S = 1$ chain in which the usual Heisenberg Hamiltonian is restricted to a subspace of the full Hilbert space. This result is stable in the sense that it established the existence of the Haldane phase in a finite region of the parameter space, and extends even to a quasi-one-dimensional model.

We should emphasize that the most interesting part of Haldane's conclusions, that the integral spin Heisenberg chains are in a massive phase, is still unproven.

Hidden Order and Four-Fold Near Degeneracy. The Haldane phase has no long range order; all the truncated correlation functions are expected to decay exponentially. However, there is a form of hidden order discovered by den Nijs and Rommelse [16]. They introduced the following string order parameter and argued that it should be nonzero in the Haldane phase.

$$O^{\alpha}_{\text{string}} = \lim_{|j-k|\to\infty} \omega\left(-S^{\alpha}_j \exp\left[i\pi \sum_{l=j+1}^{k-1} S^{\alpha}_l \right] S^{\alpha}_k \right). \tag{1.2}$$

Here $\omega(\ )$ denotes the expectation value in the ground state, and α can be x, y or z. (It is not true that if this order parameter is nonzero then the system is in the Haldane phase. We shall return to this point later.) Girvin and Arovas [19] numerically evaluated the above order parameter and concluded it was nonzero for the usual $S = 1$ Heisenberg Hamiltonian. Tasaki [58] reached a picture similar to that of den Nijs and Rommelse by directly treating the path integral representation of the $S = 1$ quantum spin chain and proving some related rigorous results.

The ground state of the VBS model sheds some light on what this string order parameter measures. In the standard basis in which S_i^z at each site is diagonal, the VBS state can be written as follows [4]:

$$\Phi_{\mathrm{VBS}} = \sum_{\sigma} (-1)^{z(\sigma)} 2^{n(\sigma)/2} \Phi_{\sigma} . \tag{1.3}$$

A "classical spin configuration" $\sigma = \{\sigma_1, \sigma_2, \ldots, \sigma_L\}$ is a choice of $\sigma_i = -1, 0$ or $+1$ at each site i, and Φ_σ denotes the eigenstate with $S_i^z \Phi_\sigma = \sigma_i \Phi_\sigma$. Here the summation is over all the configurations σ which satisfy the constraint that nonzero spins must alternate between $+1$ and -1. An example of an allowed configuration is $+00-0+-0+000-0+-+-00+0-$. $z(\sigma)$ is the number of odd sites with $\sigma_i = 0$, and $n(\sigma)$ is the number of nonzero σ_i. Although the allowed configurations have some structure, they do not have long range order. If we fix the spin at the origin to be $+$, then we cannot predict what the spin at a distant site will be since we have no control over the number of 0's that will appear between the origin and our distant site. However, if we keep track of the number of such 0's (or equivalently the number of nonzero's) then we can predict what the spin at the distant site will do. This is precisely what the exponential factor in the string order parameter does. It equals -1 raised to the number of nonzero spins between i and j.

In a Haldane gap system the ground state should be unique in the infinite volume limit. However, it was found in [4] that the Hamiltonian (1.1) on a finite chain with open boundary conditions has exactly four ground states. These ground states all converge to the same infinite volume state as the length of the chain tends to infinity. Such a degeneracy is not observed in a finite chain with periodic boundary conditions. The valence-bond picture of [4] suggests that the four-fold degeneracy is due to the two effective spin 1/2's induced in the boundaries of the chain.

In general in the Haldane phase the ground state of the open chain is not exactly four fold degenerate, but the four lowest eigenvalues are very close. The separation of these eigenvalues converges to zero as $\exp(-L/\xi)$ when the length of the chain L goes to infinity. Here ξ is the correlation length of the ground state. This phenomena was studied by Kennedy [25] and by Affleck and Halperin [3]. The geometric picture in [58] also suggests this phenomena. Experimental consequences of this four-fold near degeneracy of the ground states in a finite open chain (or more precisely the existence of effective spin 1/2's at the boundaries) have been studied by Hagiwara, Katsumata, Affleck, Halperin and Renard [21] and by Glarum, Geschwind, Lee, Kaplan, and Michel [20].

Phase Diagram of Typical Hamiltonians. In this paper we will consider the following two spin 1 Hamiltonians:

$$H_1 = \sum_i [S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \lambda S_i^z S_{i+1}^z + D(S_i^z)^2] , \tag{1.4}$$

$$H_2 = \sum_i J_i [\mathbf{S}_i \cdot \mathbf{S}_{i+1} - \beta(\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2] \tag{1.5}$$

with $J_i = 1$ if i is even and $J_i = \delta \leqq 1$ if i is odd.

One can consider a more general Hamiltonian which includes these two as special cases. Some of our expansion results can be extended to such a Hamiltonian, but we will restrict our attention to (1.4) and (1.5) for the sake of simplicity. The phase diagram of the ground state of H_1 was studied numerically by Botet, Julien and Kolb [12], and further investigated in [16, 47, 48, 57]. Figure 1.1 shows the qualitative phase diagram. We have labelled the Haldane phase with an H. The other phases that appear in these figures are the large D phase (labelled D), the antiferromagnetic Ising phase (labelled I), the XY phase (labelled XY), and the ferromagnetic Ising phase (labelled F). The exact location of the phase boundary between the Haldane and the XY phases is still not clear because of the large numerical ambiguity.

The large D phase of H_1 occurs when D is large and λ is not too large. If D is infinite, then the ground state is simply the configuration with all 0's. The large D phase may be thought of as a perturbation of this state. In this phase H_1 is expected to have a unique infinite volume ground state which has a gap and exponentially decaying correlation functions. Numerical [12, 48] and field theoretic [47] studies indicate that between the Haldane and the large D phases there is

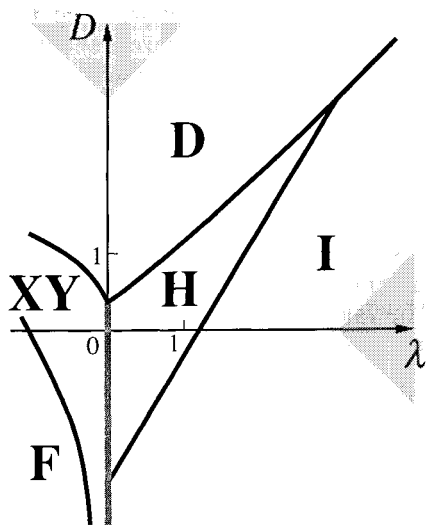

Fig. 1.1. The phase diagram of the ground state of Hamiltonian H_1 obtained by numerical studies. It contains the Haldane phase (labelled H), the antiferromagnetic Ising phase (labelled I), the large-D phase (labelled D), the XY phase (labelled XY), and the ferromagnetic Ising phase (labelled F). The boundary between the Haldane and the XY phases (shaded line) is not yet determined. We have rigorous control of the properties of the ground states in the shaded portions in the phase diagram. These portions just indicate the qualitative shape of the regions, and are not meant to be quantitative

a line of massless models. Initially, the existence of the massless line was the only reason to believe that the large D and Haldane phases are distinct phases, since both of them are characterized by unique massive ground states. But, as we will discuss below, the string order parameter allows one to directly distinguish between these two phases.

The antiferromagnetic Ising phase of H_1 occurs when λ is large and D is not. If λ were infinite then the two Néel states $+ - + - + - \cdots$ and $- + - + - + \cdots$ would be the ground states. In the Ising phase we expect two infinite volume ground states which are perturbations of these two Néel states. Each of these ground states should have Néel order, a gap and exponential decay of the truncated correlation functions.

The ground state phase diagram of H_2 has been studied intensively, especially on the line of translation invariant models with $\delta = 1$. There are four special points on this line where one has exact (or rigorous) results on the ground state. The exact ground states for $\beta = 1$ and $\beta = -1$ were obtained in [9, 32, 56] and [33, 52, 62], respectively. At these points, it appears that the ground state is unique and has no excitation gap. The point $\beta = \infty$ was solved in [10, 28, 42]. It appears to have two ground states and an excitation gap. The Hamiltonian with $\beta = -1/3$ is (1.1), and has a massive unique ground state. It is expected that a similar massive ground state occurs throughout the interval $-1 < \beta < 1$. In the region $\beta > 1$, it is expected that a spontaneous dimerization takes place, and the Hamiltonian has two ground states accompanied by a finite gap. A spontaneous trimerization is expected in the region $\beta < -1$. See [40, 50] for numerical works.

The phase diagram including the nontranslation invariant models with $\delta < 1$ was studied by Singh and Gelfand [49] by Padé analysis of perturbation series. A qualitative phase diagram is shown in Fig. 1.2. The Haldane phase is labelled H and the dimerized phase is labelled D. The VBS state is the exact ground state of H_2 on the line $\beta = -1/3$ and $\delta > 0$.

The origin of the dimerized phase of H_2, at least for small δ, can be understood as follows. If $\delta = 0$ then the ground state is simply the tensor product of the ground state for each of the bonds with nonzero coupling. If $\beta > -1/3$ the ground state of one of these bonds is the singlet state for two sites. The dimerized phase may be

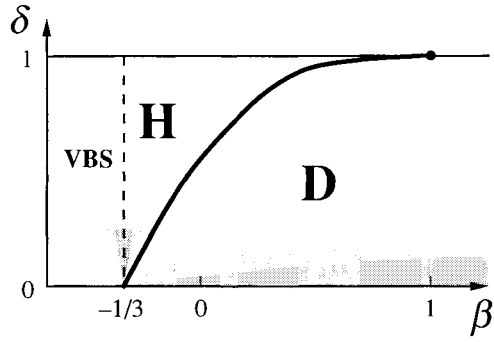

Fig. 1.2. The phase diagram of the ground state of Hamiltonian H_2 obtained by numerical and theoretical studies. It contains the Haldane phase (labelled H) and the dimerized phase (labelled D). On the dashed line (which includes $\delta = 1$ but not $\delta = 0$), the ground state is exactly the VBS state. The shaded regions indicate qualitatively (but not quantitatively) where we have rigorous control of the ground state

thought of as a perturbation of this tensor product of "dimers." Like the large D phase in H_1, the dimerized phase (except the spontaneously dimerized line $\delta = 1, \beta > 1$) is expected to have a unique infinite volume ground state which has a gap and exponentially decaying correlation functions. This phase, like the large D phase, may be distinguished from the Haldane phase by the string order parameter.

As den Nijs and Rommelse [16] pointed out (see also [58]), the string order parameter can be used to distinguish the Haldane phase from other phases with unique massive ground states. The behavior of the string order parameter in the phase diagrams in Figs. 1.1 and 1.2 is believed to be as follows. We will also consider the usual Néel order parameter

$$O^{\alpha}_{\text{Néel}} = \lim_{|j-k|\to\infty} (-1)^{|j-k|}\omega(S^{\alpha}_j S^{\alpha}_k)\,, \tag{1.6}$$

where α is x, y or z. In the Haldane phase (H in Figs. 1.1 and 1.2), all three of $O^{\alpha}_{\text{string}}$ are nonzero while all three of $O^{\alpha}_{\text{Néel}}$ are zero. In the large D phase (D in Fig. 1.1) and the dimerized phase (D in Fig. 1.2) all of the order parameters vanish. Finally, in the Ising phase (I in Fig. 1.1), O^{z}_{string} and $O^{z}_{\text{Néel}}$ are nonzero while the other four order parameters vanish. Hatsugai and Kohmoto [23] numerically evaluated these order parameters for the Hamiltonian H_1 with $\lambda = 1$; their results are consistent with the above picture.

Tasaki [59] recently argued that the sharp singularity experimentally observed in the magnetization process of Haldane gap antiferromagnets [6, 24] can be understood in terms of the behavior of the string order parameter.

Hidden $Z_2 \times Z_2$ Symmetry Breaking. In [26] we introduced a nonlocal unitary transformation U of the spin 1 chain with the following properties. (The definition of the transformation is given again in section two.) If we apply the unitary transformation to the operator that appears in the definition of the string order parameter, we obtain the usual ferromagnetic order parameter $S^{\alpha}_j S^{\alpha}_k$. (See Sect. 2.1.) Thus the nonvanishing of the string order parameter for the system with Hamiltonian H corresponds to the existence of ordinary ferromagnetic order for the system with the transformed Hamiltonian $\tilde{H} = UHU^{-1}$. Since the transformation is nonlocal there is apriori no reason that $\tilde{H}$ should be a sum of local operators. However, for the Hamiltonians above it is. (See Sect. 2.2.)

H_1 has an SO(2) symmetry and H_2 has an $SU(2)$ symmetry. These symmetries are local in the sense that the unitary operators are products of unitary operators that act at a single site. The transformed Hamiltonians $\tilde{H}_1 = UH_1U^{-1}$ and $\tilde{H}_2 = UH_2U^{-1}$ will have the same symmetries as the original Hamiltonian, but there is no reason these symmetries must still be local. It turns out (see Sect. 2.2) that the only local symmetries of $\tilde{H}_1$ and $\tilde{H}_2$ are rotations in spin space by π about one of the three coordinate axes. Thus the local symmetry group is the discrete group $Z_2 \times Z_2$.

In [26] we argued that one can determine which phase the system is in by the extent to which the $Z_2 \times Z_2$ symmetry of the transformed system is broken. In the large D and dimerized phases this symmetry is not broken at all, and the transformed Hamiltonian has a unique ground state. In the antiferromagnetic Ising phase the $Z_2 \times Z_2$ symmetry is partially broken and the transformed Hamiltonian

has two ground states. In the Haldane phase the symmetry is fully broken and the transformed Hamiltonian has four ground states. (Since the transformation is nonlocal the original and transformed Hamiltonians can have different numbers of infinite volume ground states.) We argued [26] that the four infinite volume ground states in the transformed system imply that for a finite chain with open boundary conditions the four lowest eigenvalues of the original system must be very nearly equal. Thus the four fold near degeneracy in the Haldane gap system is a consequence of the hidden $Z_2 \times Z_2$ symmetry breaking.

Results of the Present Paper. In the above we have reviewed some of the properties of the spin 1 chain which are believed to hold. We emphasize that none of the various statements above are theorems except for the few that we have described as "rigorous" or "proven". We turn now to the rigorous results of this paper.

Section 2 is devoted to the nonlocal unitary and the related $Z_2 \times Z_2$ symmetry breaking. We prove the existence of such a symmetry breaking in the Hamiltonian obtained by applying the unitary to the exactly solvable Hamiltonian (1.1). We also present a (highly nonrigorous) variational calculation. The success of this simple approximation indicates the power of the unitary transformation.

We argued above that the string order parameter measures a floating or liquid Néel order in which the nonzero spins alternate between $+$ and $-$, but because of the intervening 0's this alternation does not simply go as $(-1)^{|i-j|}$. It is natural to expect that this floating Néel order appears more easily than the usual Néel order. This observation suggests there should be an inequality

$$O^{\alpha}_{\text{string}} \geqq O^{\alpha}_{\text{Néel}} \,. \tag{1.7}$$

In Sect. 3 of the present paper, we shall prove this inequality for $\alpha = x$, y and z, and other related inequalities for the Hamiltonian H_1 with $\lambda \geqq 0$. The random loop representation used in [58] playes an essential role in the proof.

For certain values of the parameters the Hamiltonians H_1 and H_2 become trivial in the sense that one can find a basis in which they are diagonal. As we saw above, three of the phases (the large D, dimerized and Ising) can be obtained in this trivial way. As $\lambda \to \infty$ with D fixed, H_1 just becomes the spin 1 antiferromagnetic Ising Hamiltonian. As $D \to \infty$ with λ fixed, H_1 also becomes trivial. The Hamiltonian in this limit is just H_1 with $D = 1$ and all the other terms in H_1 deleted. The ground state consists of the state with all spins equal to 0. Hamiltonian H_2 becomes trivial if we set $\delta = 0$. The ground state of $\mathbf{S}_i \cdot \mathbf{S}_{i+1} - \beta(\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2$ is the unique singlet state when $\beta > -1/3$. So for $\delta = 0$ and $\beta > -1/3$ the ground state of H_2 is unique and is just the tensor product of the singlet state on two sites. One can hope to obtain rigorous results in a neighborhood of these trivial Hamiltonians by doing some form of perturbation theory.

In Sect. 4 we prove the convergence of such a perturbation theory for two quite general classes of Hamiltonians. The first class consists of Hamiltonians which are small perturbations of a diagonal Hamiltonian which has a unique ground state. In the second class the Hamiltonian is a small perturbation of a diagonal Hamiltonian which has more than one ground state, and these ground states are related by a symmetry group. In this paper we are primarily interested in the application of this perturbation theory to the one-dimensional systems given by Hamiltonians (1.4) and (1.5). However, we should emphasize that the theory developed in Sects. 4 and 5 is not restricted to one-dimensional systems. By applying these general theorems to Hamiltonians H_1 and H_2 we can prove the following. (The precise

statements of the theorems are given in Sect. 2.2.) In the shaded portion of region D in Fig. 1.1 (the large D phase) and the shaded portion of region D in Fig. 1.2 (the dimerized phase), there is a unique translation invariant ground state. This state has a gap and exponentially decaying correlations. All the string order parameters and the usual Néel order parameters vanish in this state. The transformed Hamiltonian has a unique translation invariant ground state. Thus none of the $Z_2 \times Z_2$ symmetry is broken in these two regions. In the shaded portion of region I in Fig. 1.1 (the Ising phase) there are at least two ground states. The order parameters $O^{\alpha}_{\text{string}}$ and $O^{\alpha}_{\text{Néel}}$ with $\alpha = z$ are nonzero. When $\alpha = x$ or y, both of these order parameters vanish. Thus one of the factors in the $Z_2 \times Z_2$ symmetry is broken, but the other is not. The transformed Hamiltonian also has at least two infinite volume ground states. We stress that these shaded portions in the phase diagrams are not drawn in a quantitative manner (while the phase boundaries are semi-quantitative.) The actual regions where the rigorous perturbation theory works are much smaller or farther away.

The rigorous perturbation theory of Sect. 4 can be thought of as Rayleigh Schrödinger perturbation theory. Rigorous Rayleigh Schrödinger perturbation theory for various quantum spin systems that are perturbations of diagonal Hamiltonians has been done before. The approach we present here is quite general, but the proof of convergence is still relatively simple. Kirkwood and Thomas [27] controlled the perturbation theory for several models by writing the Schrödinger equation in a clever form and developing the expansion directly from this equation. Another approach to controlling the perturbation theory is to use a Feynman–Kac or path space formula to make the quantum spin system look like a classical model in one more dimension. Yin and Thomas took such an approach [61]. See also [46, 57]. Albanese [1] controlled the perturbation theory by constructing a "dressing transformation" which takes the unperturbed ground state into the perturbed ground state.

Our approach in Sect. 4 begins with a path space formula for $\mathrm{Tr}(e^{-\beta H})$. When the Hamiltonian is a small perturbation of a diagonal Hamiltonian the dominant terms in the path space formula consist of large regions of ground state(s) with rare excitations. The usual polymer expansion can be used to control this dilute gas of excitations. To take advantage of the usual polymer expansion we introduce a blocking in the time direction. This blocking of the continuous time direction makes the expansion look more like the usual polymer expansions one encounters in classical lattice systems. Our proof of the convergence of the expansion is greatly facilitated by the introduction of a "comparison Hamiltonian."

Unlike the three phases discussed above there is no diagonal Hamiltonian which is in the Haldane phase. For H_2 with $\beta = -1/3$ the ground state is known exactly, but not all the eigenstates are known. Another way to see that H_2 with $\beta = -1/3$ is quite different from the diagonal Hamiltonians is to consider the correlation length. In the ground states of the trivial Hamiltonians considered above, truncated correlation functions vanish at large enough distances, so the correlation length is 0. By contrast, the correlation function in the ground state of H_2 with $\beta = -1/3$, $\delta > 0$ decays exponentially, but never becomes exactly zero. (The correlation length is $1/\ln 3$.) Attempting to control small perturbations of the $\beta = -1/3$ Hamiltonian is not simply a question of doing rigorous Rayleigh Schrödinger perturbation theory. In Sect. 5 we consider perturbations of Hamiltonians for which the ground state(s) are known and are simple tensor products, but the excited states need not be. Of course we must assume something

about the Hamiltonian we are perturbing. The condition we assume, which we refer to as diagonal dominance, says roughly that each diagonal entry of the unperturbed Hamiltonian is greater than the sum of the absolute values of the off diagonal entries in the same column. We prove a general theorem for these diagonally dominant Hamiltonians which says that we can add a small but essentially arbitrary perturbation to such a Hamiltonian and have a convergent expansion for the ground state(s).

Returning to Hamiltonian H_2, we show in the appendix that for $\beta = -1/3$ and δ sufficiently small but not zero, H_2 satisfies the diagonal dominance condition. The general result of Sect. 5 then gives us a rigorous expansion in the shaded portion of region H in Fig. 1.2. (Again the shaded portion is not quantitative. Also note that the portion does not include the point $\beta = -1/3$, $\delta = 0$.) We use this expansion to prove that this region is indeed in the Haldane phase by showing that the string order parameters are nonzero while the usual Néel order parameters are zero. In this shaded region we also prove that the transformed Hamiltonian H_2 has a least four ground states. It is important to note that when $\beta = -1/3$ and $\delta = 0$ the ground state is highly degenerate. Our results for the shaded portion of Fig. 1.2 cannot be regarded as perturbation theory about this highly singular point.

In previous rigorous examples of the Haldane phase, the proofs that the correlations decay exponentially and there is a gap depended crucially on being able to find the exact ground state and ground state energy explicitly. Aside from the obvious advantage of an explicit solution, there is the disadvantage that this method is not robust, i.e., if one adds a small perturbation to the model then typically one can say nothing about the new model. In this rigorous examples of the Haldane phase that we obtain in this paper, i.e. the shaded portion of region H, we do not find the ground state explicitly, but instead rely on perturbative methods. Thus the results are robust in the sense that they hold in an open region of the parameter space. Unfortunately, the parameter region where our result holds does not include any translation invariant Hamiltonians. As long as β is close to $-1/3$ the ground state of H_2 in the translation invariant case, $\delta = 1$, should be a small perturbation of the VBS state, so one can still hope to do some form of perturbation theory. However, we have not been able to use the methods of Sect. 5 to do so.

2. The Unitary Transformation and $Z_2 \times Z_2$ Symmetry Breaking

2.1. Definition of the Unitary. In the present section we introduce the nonlocal unitary transformation for the $S = 1$ spin chain, and discuss its relevance to the problem of the Haldane gap. Our initial motivation for considering the unitary was to explore the nature of the hidden antiferromagnetic order in the Haldane gap systems. The transformation then lead us to the new $Z_2 \times Z_2$ symmetry breaking picture discussed in the introduction. At the end of Subsect. 2.2 we will argue that this picture gives some insight into the origin of the Haldane gap. Moreover the unitary leads us to a very simple variational calculation which qualitatively recovers the phase diagram (Fig. 1.1) of the Hamiltonian H_1.

We consider a finite chain with L sites where L is an even integer, and denote the sites by $i, j, k, \ldots$. We impose open boundary conditions. We associate spin operators S_i^x, S_i^y, S_i^z with $S = 1$ with each site i. We will work in the standard basis

where the S_i^z are diagonal and the matrices of the spin operators are as follows.

$$S_i^x = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad S_i^y = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \quad S_i^z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$

A "configuration" $\sigma = \{\sigma_i\}$ will mean a choice of $\sigma_i = -1, 0$, or $+1$ at each site i, and Φ_σ denotes the eigenstate with $S_i^z \Phi_\sigma = \sigma_i \Phi_\sigma$.

Define $N(\sigma)$ to be the number of odd sites at which there is a 0, and let $\bar{\sigma}$ be the configuration given by

$$\bar{\sigma}_i = \exp\left[i\pi \sum_{l=1}^{i-1} \sigma_l \right] \sigma_i .$$

We define the unitary U by

$$U\Phi_\sigma = (-1)^{N(\sigma)} \Phi_{\bar{\sigma}} . \tag{2.1}$$

If $\sigma_i = 0$ then $\bar{\sigma}_i = 0$. If $\sigma_i \neq 0$, then $\bar{\sigma}_i = \sigma_i$ if the number of nonzero σ_j to the left of i is even and $\bar{\sigma}_i = -\sigma_i$ if this number is odd. We can visualize this transformation in the following way. Beginning at the left end of the chain, we move to the right looking for nonzero spins. The first nonzero spin is left unchanged, the second is flipped, the third is left unchanged, the fourth is flipped, and so on. Here are a few examples of the action of U:

$$(0+0--0++-+0-0) \to (0+0+-0-++++0+0),$$

$$(0+-00+00-+00-) \to -(0++00+00++00+),$$

$$(++0-+00+0-0++) \to (+-0-00+0+0+-).$$

It is immediate from the definition of U that U is unitary and $U^{-1} = U$. Recently, Oshikawa [41] found U can be expressed compactly as

$$U = \prod_{j<k} \exp(i\pi S_j^z S_k^x) .$$

A somewhat more complicated operator representation of U was found in [38, 54].

If O is a local observable, then UOU^{-1} need not be local. The action of U on the Hamiltonian does, however, produce a sum of local operators. This fact can be confirmed easily by an explicit calculation (see Lemma 2.1 below), but let us briefly see why this should be true. Take, for example, the Hamiltonian (1.4) and rewrite it as

$$H_1 = \sum_i S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \lambda S_i^z S_{i+1}^z + D(S_i^z)^2$$

$$= \sum_i \frac{1}{2}(S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+) + \lambda S_i^z S_{i+1}^z + D(S_i^z)^2 ,$$

where $S_j^\pm = S_j^x \pm iS_j^y$.

It is clear that the term $D(S_i^z)^2$ is unchanged by the unitary since this term does not distinguish between $\sigma_i = +1$ and -1. For $S_i^z S_{i+1}^z \Phi_\sigma$ to be nonvanishing, both σ_i and σ_{i+1} must be nonzero. If so, exactly one of the sites i and $i+1$ will be flipped.

Then the unitary changes the sign of $\sigma_i\sigma_{i+1}$. Therefore we find for the diagonal part that $U(\lambda S_i^z S_{i+1}^z + D(S_i^z)^2)U^{-1} = -\lambda S_i^z S_{i+1}^z + D(S_i^z)^2$.

To see how the off-diagonal part transforms, note that the nonvanishing matrix elements of $S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+$ are $(0\,0)\leftrightarrow(+\,-)$, $(0\,0)\leftrightarrow(-\,+)$, $(0\,+)\leftrightarrow(+\,0)$ and $(0\,-)\leftrightarrow(-\,0)$. It is crucial that these actions conserve the number of the nonzero σ_i's or change it by two. Since the unitary only involves the parity of the number of the nonzero spins left of a site, the above matrix elements do not affect the unitary transformation of the spins at sites j with $j > i+1$. Thus the matrix element of $U(S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+)U^{-1}$ are still local and are given by $(0\,0)\leftrightarrow(+\,+)$, $(0\,0)\leftrightarrow(-\,-)$, $(0\,+)\leftrightarrow(+\,0)$ and $(0\,-)\leftrightarrow(-\,0)$.

Now we move on to explicit calculations of the unitary transformation of the spin operators.

Lemma 2.1.

$$
\begin{aligned}
US_j^x U^{-1} &= S_j^x \exp\left(i\pi \sum_{k=j+1}^{L} S_k^x\right), \\
US_j^y U^{-1} &= \exp\left(i\pi \sum_{k=1}^{j-1} S_k^z\right) S_j^y \exp\left(i\pi \sum_{k=j+1}^{L} S_k^x\right), \\
US_j^z U^{-1} &= \exp\left(i\pi \sum_{k=1}^{j-1} S_k^z\right) S_j^z . \qquad (2.2)
\end{aligned}
$$

Proof. It is convenient to explicity write down the matrices of the following operators:

$$
\exp(i\pi S_j^x) = \begin{pmatrix} 0 & 0 & -1 \\ 0 & -1 & 0 \\ -1 & 0 & 0 \end{pmatrix}, \quad \exp(i\pi S_j^y) = \begin{pmatrix} 0 & 0 & 1 \\ 0 & -1 & 0 \\ 1 & 0 & 0 \end{pmatrix},
$$

$$
\exp(i\pi S_j^z) = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}.
$$

We start with S_j^z which is the easiest,

$$
\begin{aligned}
US_j^z U^{-1}\Phi_\sigma &= (-1)^{N(\sigma)} US_j^z \Phi_{\bar\sigma} \\
&= (-1)^{N(\sigma)} \bar\sigma_j U \Phi_{\bar\sigma} \\
&= \bar\sigma_j \Phi_\sigma .
\end{aligned}
$$

The last equality follows from $U\Phi_{\bar\sigma} = (-1)^{N(\bar\sigma)}\Phi_\sigma$ and $N(\bar\sigma) = N(\sigma)$. The definition of $\bar\sigma$ implies that

$$
\begin{aligned}
\bar\sigma_j \Phi_\sigma &= \exp\left(i\pi \sum_{k=1}^{j-1} \sigma_k\right)\sigma_j \Phi_\sigma \\
&= \exp\left[i\pi \sum_{k=1}^{j-1} S_k^z\right] S_j^z \Phi_\sigma .
\end{aligned}
$$

This proves the third identity of (2.2).

Next we consider the transformation of $S_j^{\pm} = S_j^x \pm iS_j^y$,

$$\begin{aligned} US_j^+ U^{-1}\Phi_\sigma &= (-1)^{N(\sigma)} US_j^+ \Phi_{\bar{\sigma}} \\ &= 2^{1/2}(-1)^{N(\sigma)} U\Phi_{\bar{\sigma}+\delta_j}, \end{aligned}$$

where the configuration δ_j is defined so that $(\delta_j)_k$ is the Kronecker delta function δ_{jk}.

When $\bar{\sigma}_j + 1 > 1$, we define $\Phi_{\bar{\sigma}+\delta_j}$ to be zero. Let σ' be the configuration obtained by applying the unitary (2.1) to $\bar{\sigma} + \delta_j$. An explicit calculation shows

$$\begin{aligned} \sigma_k' &= \exp\left[i\pi \sum_{l=1}^{k-1} (\bar{\sigma}_l + \delta_{jl}) \right](\bar{\sigma}_k + \delta_{jk}) \\ &= \exp\left[i\pi \sum_{l=1}^{k-1} (\sigma_l + \delta_{jl}) \right]\left[\exp\left(i\pi \sum_{l=1}^{k-1} \sigma_l \right)\sigma_k + \delta_{jk} \right] \\ &= \exp\left(i\pi \sum_{l=1}^{k-1} \delta_{jk} \right)\sigma_k + \exp\left(i\pi \sum_{l=1}^{k-1} \sigma_l \right)\delta_{jk} \\ &= \begin{cases} \sigma_k & \text{if } k < j \\ \sigma_j + \exp(i\pi \sum_{l=1}^{j-1} \sigma_l) & \text{if } k = j \\ -\sigma_k & \text{if } k > j \end{cases}. \end{aligned}$$

The second equality follows from the fact that $|\bar{\sigma}_l| = |\sigma_l|$. Rewriting the above result in terms of the spin operators, we have

$$\begin{aligned} US_j^+ U^{-1}\Phi_\sigma &= (-1)^j 2^{1/2}\Phi_{\sigma'} \\ &= (-1)^j \left[\frac{1 + \exp(i\pi \sum_{k=1}^{j-1} S_k^z)}{2} S_i^+ + \frac{1 - \exp(i\pi \sum_{k=1}^{j-1} S_k^z)}{2} S_i^- \right] \\ &\quad \prod_{k=j+1}^{L} [-\exp(i\pi S_k^x)]\Phi_\sigma, \end{aligned}$$

where we have used the fact $(-1)^{N(\sigma)+N(\bar{\sigma}+\delta_j)} = (-1)^j$. Note that $-\exp(i\pi S_k^x)$ is the operator that flips the spin at site k. The minus signs cancel out since the number of sites L is even, and we get the transformation of S_j^+.

$$US_j^+ U^{-1} = \left[\frac{1 + \exp(i\pi \sum_{k=1}^{j-1} S_k^z)}{2} S_j^+ + \frac{1 - \exp(i\pi \sum_{k=1}^{j-1} S_k^z)}{2} S_j^- \right] \exp\left(i\pi \sum_{k=j+1}^{L} S_k^x \right).$$

Since $US_j^- U^{-1}$ can be obtained by taking the adjoint of the above, the transformations of S_j^x and S_j^y immediately follow. ∎

The above lemma allows us to calculate the unitary transformation of an arbitrary polynomial of spin operators, i.e., an arbitrary local observable. Of special interest is the following transformation of the products of two spin variables.

Corollary 2.2.

$$US_j^\alpha S_k^\alpha U^{-1} = -S_j^\alpha \exp\left[i\pi \sum_{l=j+1}^{k-1} S_l^\alpha \right] S_k^\alpha, \quad \text{if } \alpha = x, z.$$

We have used the identity $\exp(i\pi S_j^\alpha)S_j^\alpha = -S_j^\alpha$. For $\alpha = y$, the simple transformation above does not hold. It is crucial that the right-hand side of the above equation is nothing but the den Nijs–Rommelse string observable. Therefore we get the following identity between the order parameters:

$$O^\alpha_{\text{string}}(H) = O^\alpha_{\text{Ferro}}(\tilde{H}), \quad \text{for } \alpha = x, z\,, \tag{2.3}$$

where H is a general Hamiltonian and $\tilde{H} = UHU^{-1}$. The ferromagnetic order parameter is defined by

$$O^\alpha_{\text{Ferro}}(\tilde{H}) = \lim_{|j-k|\to\infty} \omega_{\tilde{H}}(S_j^\alpha S_k^\alpha)\,,$$

where $\omega_{\tilde{H}}(\cdot)$ denotes the expectation value in the ground state of $\tilde{H}$.

2.2. Haldane Gap and $Z_2 \times Z_2$ Symmetry Breaking. In the present subsection, we shall apply the nonlocal unitary transformation to the Hamiltonians H_1 and H_2 defined in (1.4) and (1.5), respectively. Let $\tilde{H}_i = UH_iU^{-1}$ $(i = 1, 2)$. Then an explicit calculation using Lemma 2.1 shows that

$$\tilde{H}_1 = \sum_i h_i + (1-\lambda)S_i^z S_{i+1}^z + D(S_i^z)^2\,, \tag{2.4}$$

and

$$\tilde{H}_2 = \sum_i J_i[h_i - \beta(h_i)^2]\,,$$

where

$$h_i = -S_i^x S_{i+1}^x + S_i^y \exp\{i\pi(S_i^z + S_{i+1}^x)\}S_{i+1}^y - S_i^z S_{i+1}^z\,. \tag{2.5}$$

Although the transformed Hamiltonians $\tilde{H}_1, \tilde{H}_2$ are sums of local operators (as we stressed in the previous subsection), it is evident that $\tilde{H}_1, \tilde{H}_2$ have less symmetry than the original Hamiltonians H_1, H_2. We find that $\tilde{H}_1, \tilde{H}_2$ are only invariant under rotations by π about each of the three coordinate axes. They are not invariant under a rotation by π about an arbitrary axis. These three rotations generate the discrete group $Z_2 \times Z_2$. Of course, the transformed Hamiltonians $\tilde{H}_1, \tilde{H}_2$ will have the same symmetries as the original Hamiltonians H_1, H_2 since these operators are related by a unitary, but in general these symmetries for $\tilde{H}_1, \tilde{H}_2$ will be nonlocal. The only local symmetry of the transformed Hamiltonian is the discrete $Z_2 \times Z_2$ symmetry. We shall think of this group as being generated by the rotations by π around the x and the z axes, i.e., $\Phi \to \exp(i\pi\sum_j S_j^x)\Phi$ and $\Phi \to \exp(i\pi\sum_j S_j^z)\Phi$. As we shall discuss in the following, these symmetries may be spontaneously broken. Spontaneous breaking of these symmetries can be measured by the order parameters $O^z_{\text{Ferro}}(\tilde{H})$ and $O^x_{\text{Ferro}}(\tilde{H})$, respectively.

Let us investigate what happens to this $Z_2 \times Z_2$ symmetry in various regions of the phase diagrams. First we look at the ground state of H_1 in the region where the anisotropy parameter D is large. Then we have the following theorem which is proved in Sect. 4 as a special case of a general theorem.

Theorem 2.3. *If D is sufficiently large, then the Hamiltonian H_1 has a unique translation invariant ground state. In this ground state $O^\alpha_{\text{Néel}}(H_1) = 0$ and $O^\alpha_{\text{string}}(H_1) = 0$ for $\alpha = x, y, z$. This ground state has a gap, and truncated correlation functions decay exponentially. Under the same condition on the parameters the*

Hamiltonian $\tilde{H}_1$ has a unique translation invariant ground state and in this ground state $O^{\alpha}_{\text{Ferro}}(\tilde{H}_1) = 0$ for $\alpha = x, y, z$. (How large D should be depends on the value of λ. There are constants c, c' such that the theorem holds if $D \geqq c + c'|\lambda|$.)

The above theorem states that the $Z_2 \times Z_2$ symmetry of the transformed Hamiltonian $\tilde{H}_1$ is completely unbroken for sufficiently large D. (In [60], a convergent cluster expansion for the random loop representation described in Sect. 3 was developed. The above theorem was proved for $D - 2|\lambda| \geqq 28$.) Although our proof requires that D be large, we expect that the conclusions of the theorem are valid throughout the large-D phase in Fig. 1.1.

Similarly we have the following theorem for the ground state of the Hamiltonian H_2 in the region with strong bond alternation.

Theorem 2.4. *If $\beta > -1/3$ and δ is sufficiently small, then the Hamiltonian H_2 has a unique translation invariant ground state. In this ground state $O^{\alpha}_{\text{Néel}}(H_2) = 0$ and $O^{\alpha}_{\text{string}}(H_2) = 0$ for $\alpha = x, y, z$. This ground state has a gap, and truncated correlation functions decay exponentially. Under the same conditions on the parameters the Hamiltonian $\tilde{H}_2$ has a unique translation invariant ground state and in this ground state $O^{\alpha}_{\text{Ferro}}(\tilde{H}_2) = 0$ for $\alpha = x, y, z$. (How small δ should be depends on the value of β. See the shaded portion of the region labelled* D *in Fig. 1.2. In particular, there is a constant c such that when β is near $-1/3$ the theorem holds in the wedge $0 < \delta < c|\beta + 1/3|$.)*

Again, we expect that the conclusions of the theorem, in particular the absence of any breaking of the $Z_2 \times Z_2$ symmetry, are true throughout the dimerized phase in Fig. 1.2 although our proof only works in a subset of this region.

Next we consider H_1 in the region with strong Ising-like anisotropy. We prove the following theorem in Sect. 4.

Theorem 2.5. *If λ is sufficiently large, then H_1 has at least two translation invariant infinite volume ground states. In each of these ground states we have $O^{\alpha}_{\text{Néel}}(H_1) = 0$ and $O^{\alpha}_{\text{string}}(H_1) = 0$ for $\alpha = x, y$, while $O^{z}_{\text{Néel}}(H_1) > 0$ and $O^{z}_{\text{string}}(H_1) > 0$. Under the same condition on the parameters $\tilde{H}_1$ has at least two translation invariant infinite volume ground states. In each of them $O^{\alpha}_{\text{Ferro}}(\tilde{H}_1) = 0$ for $\alpha = x, y$ and $O^{z}_{\text{Ferro}}(\tilde{H}_1) > 0$. (How large λ should be depends on the value of D. There are constants c, c' such that the theorem holds if $\lambda \geqq c + c'|D|$.)*

Thus the ground states for large enough λ spontaneously break the symmetry of rotation by π about the x axis. Note that they break only half of the $Z_2 \times Z_2$ symmetry, since the ground states are still invariant under the rotation by π about the z axis. We expect that the same is true in the entire Ising phase in the phase diagram of Fig. 1.1.

As we discussed in the introduction, the above theorems are proved by an expansion that can be regarded as rigorous Rayleigh Schrödinger perturbation theory. Several authors have put this perturbation theory on a rigorous footing for various quantum spin systems, and we expect that their approaches can also be used to prove Theorems 2.3, 2.4, and 2.5. Our next theorem concerns the Haldane phase, and its proof is much more subtle. For the Hamiltonian H_2 we can rigorously establish the existence of the Haldane phase in an open region in the phase diagram in Fig. 1.2. Unfortunately we have not been able to do this for the Hamiltonian H_1.

Theorem 2.6. *There are positive constants ε, δ_0 and γ such that if $|\beta + 1/3| < \varepsilon$ and $\gamma|\beta + 1/3| < \delta < \delta_0$ then the transformed Hamiltonian $\tilde{H}_2$ has at least four translation invariant infinite volume ground states. In each of them $O^{\alpha}_{\text{Ferro}}(\tilde{H}_2) > 0$ for $\alpha = x, z$.* Let H_2^L *denote Hamiltonian H_2 on sites $-L$ to L with open boundary conditions, and let*

$$\langle \cdot \rangle_{\beta, L} = \frac{\mathrm{Tr}(\cdot \exp(-\beta H_2^L))}{\mathrm{Tr}(\exp(-\beta H_2^L))} .$$

Then under the above conditions on the parameters we have

$$\liminf_{|j-k|\to\infty} \liminf_{L\to\infty} \liminf_{\beta\to\infty} \left\langle -S_j^{\alpha} \exp\left[i\pi \sum_{l=j+1}^{k-1} S_l^{\alpha} \right] S_k^{\alpha} \right\rangle_{\beta, L} > 0 ,$$

and there exist constants $c, \mu > 0$ *such that*

$$\limsup_{L\to\infty} \limsup_{\beta\to\infty} |\langle S_j^{\alpha} S_k^{\alpha} \rangle_{\beta, L}| \leqq c e^{-\mu|j-k|}$$

for any j and k.

In Theorems 2.3, 2.4, and 2.5 we have convergent expansions for both the original and transformed Hamiltonians. In Theorem 2.6 we only have a convergent expansion for the transformed Hamiltonian. This expansion proves most but not all of the properties that should hold in the Haldane phase. For example, although we prove that all the Néel order parameters vanish, we do not prove that the original Hamiltonian has a unique ground state. This is why the statements in the theorem about the string order parameter and the decay of the two point correlation function are somewhat cumbersome. We cannot simply refer to "the ground state," but must instead use $\langle \ \rangle_{\beta, L}$.

The theorem says that $\tilde{H}_2$ has at least four infinite volume ground states in at least part of the Haldane phase. We expect that this is true in the entire Haldane phase for both $\tilde{H}_1$ and $\tilde{H}_2$. This may seem somewhat puzzling since the original Hamiltonian H should have a unique infinite volume ground state. Of course our unitary is nonlocal, so the number of infinite volume ground states of the original Hamiltonian does not have to equal the number of infinite volume ground states for the transformed Hamiltonian. Recall that the number of infinite volume ground states is unchanged by the unitary when we are in the Ising, the large-D, and the dimerized phases. The nonlocal unitary changes the physics drastically, but only does so when we are in the Haldane phase!

The four infinite volume ground states of the transformed Hamiltonian in the Haldane phase have an important consequence for the original Hamiltonian. For a long finite open chain the four lowest eigenvalues of the transformed Hamiltonian should be almost degenerate. For a finite open chain the original and transformed Hamiltonians have the same eigenvalues, so the four lowest eigenvalues of the original Hamiltonian must also be almost degenerate. We conclude that the near degeneracy in the Haldane phase discussed in Sect. 1 is an inevitable consequence of the $Z_2 \times Z_2$ symmetry breaking.

Moreover, one may argue that the spontaneous breaking of the $Z_2 \times Z_2$ symmetry is the origin of the Haldane gap itself. The spontaneous breaking of a continuous symmetry is usually accompanied by massless excitations (Goldstone bosons), while the breaking of a discrete symmetry is usually accompanied by the

appearance of a gap. Since the ground states of the transformed Hamiltonian spontaneously break the $Z_2 \times Z_2$ symmetry in the Haldane phase, it is natural that each of the four ground states will be accompanied by a finite excitation gap. Then the most natural scenario (but not the only possible one) for a finite open chain is that the four lowest eigenvalues of the transformed Hamiltonian are separated from the other eigenvalues by a finite gap which is uniform in the size of the system. Since the spectrum of the original and transformed Hamiltonians are identical, this suggests that the original Hamiltonian should have a gap above the ground state energy.

2.3. The Solvable Model. In this subsection we prove that the full $Z_2 \times Z_2$ symmetry is broken in the solvable model of Affleck, Kennedy, Lieb and Tasaki [4]. The Hamiltonian is

$$H_{\mathrm{VBS}} = \sum_i \left[\mathbf{S}_i \cdot \mathbf{S}_{i+1} + \frac{1}{3} (\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2 \right].$$

This Hamiltonian is special because $\mathbf{S}_i \cdot \mathbf{S}_{i+1} + 1/3(\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2 = 2P_{i,i+1}^{S=2} - 2/3$, where $P_{i,i+1}^{S=2}$ is the projection onto the states with spin 2 on sites i and $i+1$. Using this fact the following statements have been proven for the Hamiltonian H_{VBS} [4]. There is a unique infinite volume ground state. In this ground state the truncated correlation functions decay exponentially. There is a gap in the energy spectrum. For a finite open chain the ground state subspace of H_{VBS} is four dimensional. In the infinite volume limit these ground states all yield the same infinite volume state. The Hamiltonian $\tilde{H}_{\mathrm{VBS}}$ for a finite chain with open boundary conditions must also have a four dimensional ground state subspace. However, we will prove below that these finite chain ground states yield four distinct ground states in the infinite volume limit.

There are explicit formulae for the ground states of H_{VBS} [4], e.g., Eq. (1.3). We will not need these formulae here, but we should emphasize that these ground states cannot be written as a single tensor product of states at each site. We denote the transformed Hamiltonian $UH_{\mathrm{VBS}}U^{-1}$ by $\tilde{H}_{\mathrm{VBS}}$. As we will now show the ground states of $\tilde{H}_{\mathrm{VBS}}$ can be written as a simple tensor product. Using our calculations above, $\tilde{H}_{\mathrm{VBS}} = \sum_i [h_i + \frac{1}{3} h_i^2]$, with h_i defined in (2.5). The two site Hamiltonian $h_i + \frac{1}{3} h_i^2$ is easily diagonalized, and we find that the ground state subspace is four dimensional and is spanned by the states $\phi_k \otimes \phi_k$, $k = 1, 2, 3, 4$, where

$$\phi_1 = [|0\rangle + \sqrt{2}|+\rangle]/\sqrt{3},$$

$$\phi_2 = [|0\rangle - \sqrt{2}|+\rangle]/\sqrt{3},$$

$$\phi_3 = [|0\rangle + \sqrt{2}|-\rangle]/\sqrt{3},$$

$$\phi_4 = [|0\rangle - \sqrt{2}|-\rangle]/\sqrt{3}.$$

For convenience we work with a finite chain running from $-L$ to L. The modifications needed for other finite chains should be clear. Let ψ_k^L be the state on this finite chain formed by tensoring together $2L+1$ copies of ϕ_k. It follows immediately from the two site calculation that these four states are ground states for the $-L$ to L chain.

Lemma 2.7. *For a finite chain with open boundary conditions the ground state subspace for $\tilde{H}_{\mathrm{VBS}}$ is four dimensional and is spanned by the states ψ_k^L, $k = 1, 2, 3, 4$, defined above.*

Proof. The ground state subspaces of H_{VBS} and $\tilde{H}_{\mathrm{VBS}}$ have the same dimension. In [4] it was proven that the former has dimension four. As noted above the states ψ_k^L are ground states, so we need only show that these four states are linearly independent. This is an easy exercise that we omit. ∎

We can define four infinite volume states $\omega_1, \omega_2, \omega_3$, and ω_4 as follows. For any local observable O let

$$\omega_k(O) = \lim_{L\to\infty} (\psi_k^L, O\psi_k^L) .$$

For sufficiently large L, $(\psi_k^L, O\psi_k^L)$ is independent of L, so the existence of the limit is trivial.

In general the ground state energy per bond is defined to be

$$e_0 = \inf_{\rho} \lim_{L\to\infty} \frac{1}{2L} \rho(H_{-L,L}) ,$$

where $H_{-L,L}$ is the Hamiltonian for a chain running from $-L$ to L, and the infimum over ρ is over all states on the infinite chain. The Hamiltonian H_{VBS} is unusual in that the ground state energy for a finite chain is just equal to the number of bonds times the lowest eigenvalue of the two site Hamiltonian. Thus $e_0 = -2/3$, where $-2/3$ is the lowest eigenvalue of $h_i + \frac{1}{3}h_i^2$. We will say that an infinite volume state ω is a ground state if for every i, $\omega(h_i + \frac{1}{3}h_i^2) = e_0$. Clearly each ω_k is an infinite volume ground state.

Theorem 2.8. *$\tilde{H}_{\mathrm{VBS}}$ has exactly 4 infinite volume ground states.*

Proof. We first show that one can find local observables O_k, $k = 1, 2, 3, 4$, such that $w_k(O_j) = \delta_{kj}$. An immediate consequence of this is that the ω_k are linearly independent. Let P_j be the orthogonal projection onto the subspace spanned by states of the form $\chi \otimes \phi_j \otimes \phi_j \otimes \xi$, where χ is any state on sites $-L$ to -1 and ξ is any state on sites 2 to L. So the factor $\phi_j \otimes \phi_j$ lives at sites 0 and 1. Some calculation shows that $\omega_k(P_j) = M_{kj}$, where

$$M_{kj} = \begin{cases} 1 & \text{if } j = k \\ 1/81 & \text{if } j \neq k \end{cases} .$$

One can check that the matrix M_{kj} is invertible. We define

$$O_j = \sum_{k=1}^{4} (M^{-1})_{jk} P_k .$$

Then $\omega_k(O_j) = \delta_{kj}$.

Now let ω be an infinite volume ground state. Using the observables O_k defined above we let $c_k = \rho(O_k)$. We will show that

$$\omega = \sum_{k=1}^{4} c_k \omega_k .$$

It suffices to show that $\omega(O) = \sum_{k=1}^{4} c_k \omega_k(O)$ for any local observable O. We can also assume that the observable O has $\|O\| \leqq 1$. Choose l large enough that the

support of O is contained in sites $-l$ to l. Consider the restrictions of the states ω and $\sum_{k=1}^{4} c_k \omega_k$ to the finite chain which contains sites $-L$ to L. These restrictions can be written as density matrices for the $-L$ to L chain. Furthermore, since the expectations in ω and $\sum_k c_k \omega_k$ of the Hamiltonian for this finite chain are equal to the ground state energy of the finite chain, these density matrices can only involve the ground state vectors for the finite chain. Using the lemma above this implies that there are four by four matrices a_{ij} and $\tilde{a}_{ij}$ such that

$$\omega(O) = \sum_{i,j} a_{ij}(\psi_i^L, O\psi_j^L) ,$$

$$\sum_k c_k \omega_k(O) = \sum_{i,j} \tilde{a}_{ij}(\psi_i^L, O\psi_j^L) .$$

In these sums i, j and k all run from 1 to 4. The states ψ_k^L are not orthonormal, so the matrices a_{ij} and $\tilde{a}_{ij}$ do not have all the properties they would have if we used an orthonormal basis, but this does not affect our proof.

For $i \neq j$, $|(\phi_i, \phi_j)| = 1/3$. Thus $i \neq j$ implies

$$|(\psi_i^L, O\psi_j^L)| \leqq 3^{-2(L-l)}$$

which implies

$$\left| \omega(O) - \sum_i a_{ii}(\psi_i^L, O\psi_i^L) \right| \leqq 12 \cdot 3^{-2(L-l)} .$$

Similarly,

$$\left| \sum_k c_k \omega_k(O) - \sum_i \tilde{a}_{ii}(\psi_i^L, O\psi_i^L) \right| \leqq 12 \cdot 3^{-2(L-l)} .$$

The definition of the c_k and the properties of the observables O_k imply that $\omega(O_l) = \sum_k c_k \omega(O_l)$. Thus if we take $O = O_l$ in the above bounds we find that $|a_{ll} - \tilde{a}_{ll}|$ is of order $3^{-2(L-l)}$. Thus $|\omega(O) - \sum_k c_k \omega_k(O)|$ is of order $3^{-2(L-l)}$. We can take L as large as we like, so this proves the theorem. ∎

2.4. A Variational Calculation. There is a simple variational calculation which qualitatively recovers the phase diagram (Fig. 1.1) of the Hamiltonian H_1 and the $Z_2 \times Z_2$ symmetry breaking picture discussed in Sect. 2.2. The success of our simple calculation indicates that the nonlocal unitary transformation provides a natural viewpoint for studying the Haldane gap phenomena. We believe that the unitary also provides a good starting point for developing approximate theories for the Haldane gap.

Let $\phi = a(0) + b(+) + c(-)$ be a state on a single site, and $\Phi = \bigotimes_i \phi$ be the state on the whole lattice obtained by tensoring together copies of the state ϕ at each site. We shall take Φ as our variational state, and minimize the energy expectation value of $\tilde{H}_1$. It is crucial that we use the transformed Hamiltonian rather than the original one here.

By an explicit calculation using (2.4), (2.5), we find

$$\begin{aligned} E(a, b, c) &= \frac{1}{L}(\Phi, \tilde{H}_1 \Phi) \\ &= (|a|^2 + |b|^2 + |c|^2)^{-2} \{ -2\mathrm{Re}(a^2(\bar{b}^2 + \bar{c}^2)) - 2|a|^2(|b|^2 + |c|^2) \\ &\quad - \lambda(|b|^2 - |c|^2)^2 + D(|a|^2 + |b|^2 + |c|^2)(|b|^2 + |c|^2) \} . \end{aligned}$$

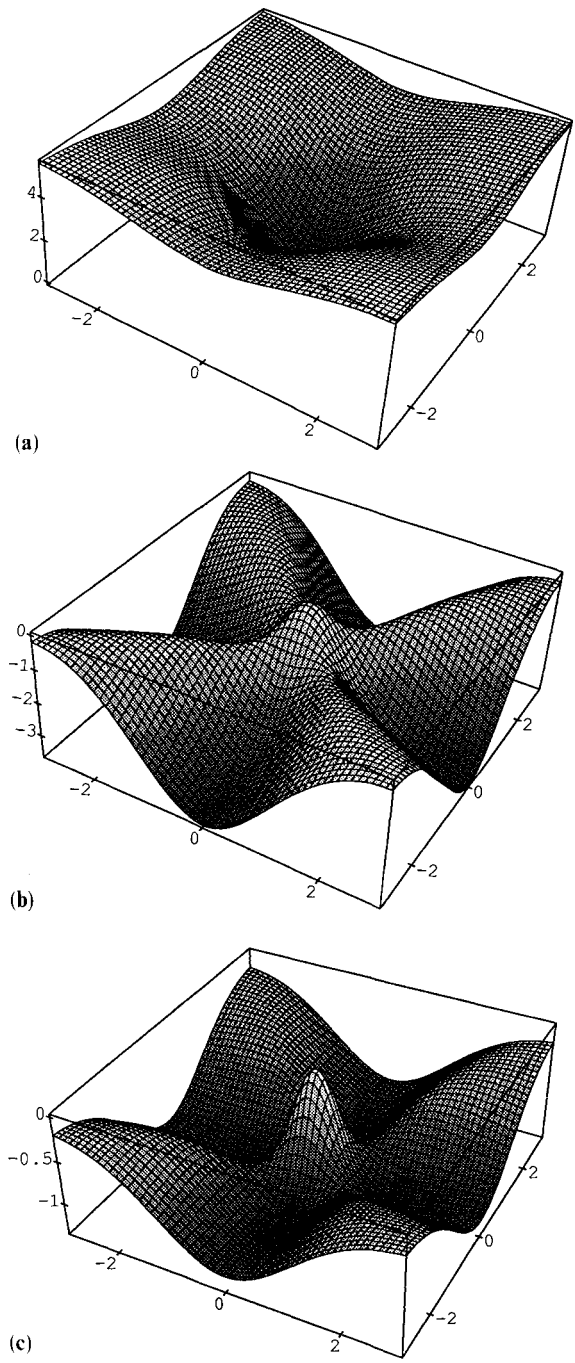

Fig. 2.1. Typical energy landscape encountered in the variational calculation of the ground state of H_1. The expectation value of the energy is plotted against the variational parameters b/a and c/a. a. The large D phase; $\lambda = 0$, $D = 4$. There is a unique minimum at the origin, which preserves the symmetry. b. The Ising phase; $\lambda = 4$, $D = 0$. There are two minima at b/a, $c/a = \pm\infty$, corresponding to the breaking of half of the $Z_2 \times Z_2$ symmetry. c. The Haldane phase; $\lambda = 1$, $D = 0$. There are four minima, indicating the full $Z_2 \times Z_2$ symmetry breaking

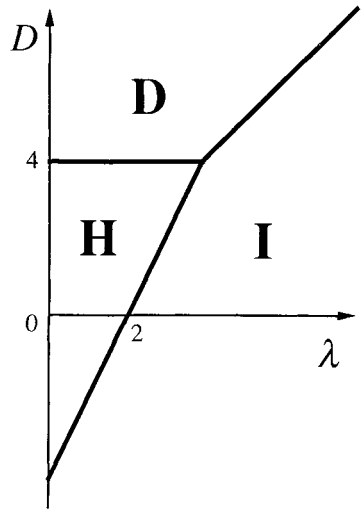

Fig. 2.2. The phase diagram for H_1 obtained by the variational calculation. It contains the Haldane phase (labelled H), the antiferromagnetic Ising phase (labelled I), and the large-D phase (labelled D). This qualitatively recovers the phase diagram of Fig. 1.1

It is clear that a minimum of $E(a, b, c)$ is attained when a, b, c are all real. When we minimize $E(a, b, c)$, we find that the number of states at which the minimum occurs, i.e., the number of variational ground states, can be one, two or four depending on the values of the parameters in the Hamiltonian. Figure 2.1 shows typical energy landscapes in each of the three cases. In this figure we have plotted $E(a, b, c)$ as a function of b/a and c/a.

i) *The large-D Phase*: In the region $D > 4$, $D > \lambda > 0$, we find that $\phi = (0)$ is the unique variational ground state (i.e., minimizer of the energy expectation value). This state does not break the $Z_2 \times Z_2$ symmetry at all.
ii) *The Ising Phase*: In the region $2\lambda - D > 4$, $\lambda > D$, $\lambda > 0$, we find two distinct variational ground states, $\phi = |+\rangle$ and $\phi = |-\rangle$. These states breaks half of the $Z_2 \times Z_2$ symmetry, i.e., the rotation by π about the x axis.
iii) *The Haldane Phase*: In the region $D < 4$, $2\lambda - D < 4$, $\lambda > 0$, we find there are four different variational ground states, $\phi = \alpha|0\rangle \pm \beta|+\rangle$, $\phi = \alpha|0\rangle \pm \beta|-\rangle$, where $\alpha = \sqrt{(4 + D - 2\lambda)/(8 - 2\lambda)}$, $\beta = \sqrt{(4 - D)/(8 - 2\lambda)}$. They clearly break the full $Z_2 \times Z_2$ symmetry. These variational ground states at the Heisenberg point $\lambda = 1, D = 0$ are the exact VBS ground states of the solvable model discussed in the previous subsection. Given the fact that the unitary U transforms the VBS states into simple tensor product states, this coincidence is not surprising since the SU(2) invariance requires $\langle (S_i^z)^2 \rangle = 2/3$ and thus uniquely determines the coefficients α and β.

Figure 2.2 shows the phase diagram that results from this variational calculation. It shows a striking similarity with the expected diagram in Fig. 1.1.

3. String Order Parameters and Random Loop Representation

3.1. Main Results. In the present section, we study the den Nijs–Rommelse string correlation functions for $S = 1$ quantum spin chains. The main goal here is to

establish the bound between the string order parameters and the Néel order parameters. To prove the bound, we develop a stochastic geometric representation of the spin chain. Relations between the string order parameters and percolation phenomena in the representation are also discussed.

We consider a finite chain of length L with open boundary conditions, where L is a finite integer. As in the previous sections, a "configuration" $\sigma = \{\sigma_i\}$ will mean a choice of $\sigma_i = -1, 0$, or $+1$ at each site i, and Φ_σ denotes the eigenstate with $S_i^z \Phi_\sigma = \sigma_i \Phi_\sigma$.

We consider the antiferromagnetic Hamiltonian with uniaxial anisotropy

$$H = \sum_i S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \lambda S_i^z S_{i+1}^z + D(S_i^z)^2 , \tag{3.1}$$

where $\lambda \geqq 0$. This is precisely the Hamiltonian H_1 in the introduction. We denote by $\omega_L(\cdot)$ the ground state expectation value in the finite chain. We shall prove the following inequalities between the string correlation function and the standard antiferromagnetic correlation function.

Theorem 3.1. *In the ground state of the Hamiltonian* (3.1) *with* $\lambda \geqq 0$, *we have*

$$\omega_L\left(-S_i^\alpha \exp\left(i\pi \sum_{k=i+1}^{j-1} S_k^\alpha \right) S_j^\alpha \right) \geqq |\omega_L((-1)^{|i-j|} S_i^\alpha S_j^\alpha)| \tag{3.2}$$

for any i, j *and* $\alpha = x, y, z$. *For the antiferromagnetic correlation function, we have*

$$\omega_L((-1)^{|i-j|} S_i^\alpha S_j^\alpha) \geqq 0 \tag{3.3}$$

for $\alpha = x, y$.

By letting $L \to \infty$ and $|i-j| \to \infty$ in the above inequalities, we get the following bounds which were claimed in the introduction.

Corollary 3.2. *The string order parmeters and the Néel order parameters satisfy*

$$O^\alpha_{\text{string}}(H) \geqq |O^\alpha_{\text{Néel}}(H)|$$

where $\alpha = x, y$ or z.

Remarks.

1. For the antiferromagnetic correlation function in the z direction, we do not prove the bound (3.3). This bound may be violated when D is very large.
2. Our proof of the theorem requires open boundary conditions for some technical (but essential) reasons. We could prove the theorem for a periodic chain with an even number of sites if we knew that the (finite volume) ground state had $\sum_i S_i^z = 0$. This can be proved if i) $\lambda \geqq 1$, $D \leqq 0$, ii) $-1 < \lambda \leqq 1, D \geqq 0$, or iii) $D - 2\lambda \geqq 4$. The proof of cases i) and ii) is a straightforward extension of the method used in [5, 35], while case iii) is proved using the random loop representation [60].
3. It is straightforward to extend our theorem to the Hamiltonian

$$H = \sum_i J_i(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \lambda_i S_i^z S_{i+1}^z) + D_i(S_i^z)^2$$

with site dependent couplings $J_i > 0$, $\lambda_i \geqq 0$, and D_i. But the proof fails if the Hamiltonian contains a nonnearest neighbor interaction or a biquadratic term $(\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2$.

3.2. Random Loop Representation. In order to prepare for the proof of the theorem, we develop a random loop representation for the ground state. The representation follows the standard philosophy of path integrals. In a finite system, the ground state expectation value can be realized as the zero temperature limit of the Gibbs state,

$$\omega_L(A) = \lim_{\beta \to \infty} \frac{\mathrm{Tr}(Ae^{-\beta H})}{\mathrm{Tr}(e^{-\beta H})} .$$

We use the standard path space formula [8, 18, 53, 44] to represent the above expectation value as that of a classical system. From the Lie product formula, we have

$$e^{-\beta H} = \lim_{N \to \infty} (T_{xy} T_z)^{N\beta} ,$$

where the "time evolution operators" T_{xy}, T_z are defined by

$$T_{xy} = \prod_i \left[1 - \frac{1}{2N} (S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+) \right] ,$$

$$T_z = \exp\left[- \sum_i \left\{ \frac{\lambda}{N} S_i^z S_{i+1}^z + \frac{D}{N} (S_i^z)^2 \right\} \right] .$$

We let $N\beta$ be a finite even integer, and study the expectation value

$$\omega_{L,\beta,N}(A) = \frac{1}{Z_{L,\beta,N}} \mathrm{Tr}(A(T_{xy} T_z)^{N\beta}) , \tag{3.4}$$

where

$$Z_{L,\beta,N} = \mathrm{Tr}((T_{xy} T_z)^{N\beta}) . \tag{3.5}$$

Note that we have

$$\omega_L(A) = \lim_{\beta \to \infty} \lim_{N \to \infty} \omega_{L,\beta,N}(A)$$

for any local observable A. We shall prove (3.2), (3.3) for the expectation value $\omega_{L,\beta,N}(A)$. The resulting bounds are uniform in N, $N\beta$ and L, and thus are also valid in the limits $N, \beta, L \to \infty$.

By inserting the complete basis Φ_σ, we can rewrite $Z_{L,\beta,N}$ as

$$Z_{L,\beta,N} = \sum_{\{\sigma_\tau\}_{\tau=0,1/N,\ldots,\beta-1/N}} \prod_{\tau=0}^{\beta-(1/N)} (\Phi_{\sigma_{\tau+1/N}}, (T_{xy} T_z) \Phi_{\sigma_\tau}) , \tag{3.6}$$

where σ_τ is a classical spin configuration indexed by $\tau = 0, 1/N, 2/N, \ldots, \beta - 1/N, \beta$. We impose periodic boundary conditions (in the temporal direction), $\sigma_0 = \sigma_\beta$, and sum σ_τ over all the classical spin configurations for each τ. As usual, it is convenient to interpret i and τ as spatial and temporal coordinates, respectively, of an $L \times \beta$ space-time lattice. The lattice spacing in the spatial direction is 1 while that in the temporal direction is $1/N$. Then the summation in (3.6) can be regarded as being over all the classical spin configuration $\{\sigma_{i,\tau}\}$ in the space-time lattice where $\sigma_{i,\tau} = 0, \pm 1$.

Now we develop a geometric representation of (3.6). For each space-time point (i, τ) with $\sigma_{i,\tau} \neq 0$, we draw a vertical line of length $1/N$ which has the point as its

midpoint, i.e., $(i, \tau + 1/2N) - (i, \tau - 1/2N)$. We put an up-going arrow on the bond if $\sigma_{i,\tau} = +1$ and a down-going arrow if $\sigma_{i,\tau} = -1$.

Next we expand the operator T_{xy}. When a term in T_{xy} acts on a basis state, each bond may be hit by an operator $S_i^- S_{i+1}^+$, by an operator $S_i^+ S_{i+1}^-$, or by 1. A graphical rule to represent these contributions to the matrix element $(\Phi_{\sigma_{\tau+1/N}}, T_{xy}\Phi_{\sigma_\tau})$ in (3.6) is as follows. Each horizontal bond $(i, \tau + 1/2N) - (i + 1, \tau + 1/2N)$ can be occupied by a right-going or a left-going arrow, or left vacant. Given a graph G of such horizontal arrows, we define operators $O_i(G)$ as follows. We set $O_i(G) = S_i^- S_{i+1}^+$ if the element in G on the bond $(i, \tau + 1/2N) - (i + 1, \tau + 1/2N)$ is a right-going arrow, $O_i(G) = S_i^+ S_{i+1}^-$ if it is a left-going arrow, and $O_i(G) = 1$ if it is empty. Then we can write

$$(\Phi_{\sigma_{\tau+1/N}}, T_{xy}\Phi_{\sigma_\tau}) = \sum_G \left(\Phi_{\sigma_{\tau+1/N}}, \prod_i O_i(G)\Phi_{\sigma_\tau} \right),$$

where G is summed over all the possible graphs of horizontal arrows.

We have constructed a graph Γ which is a collection of vertical and horizontal arrows. See Fig. 3.1 for an example of a classical spin configuration on the space-time lattice, and the corresponding graph Γ. (We have omitted the arrows in the figure.) Now (3.6) can be rewritten as

$$Z_{L,\beta,N} = \sum_\Gamma W(\Gamma),$$

where Γ is summed over all the possible graphs. Note that Γ satisfies a self-avoiding condition in the sense that each bond in the lattice can be occupied by at most one arrow in a graph Γ. It also turns out that the only graphs Γ we should take into account are those satisfying a kind of "current conservation."

Lemma 3.3. *The weight $W(\Gamma)$ is nonvanishing if and only if, at each space-time point $(i, \tau + 1/2N)$, the numbers of incoming arrows and outgoing arrows are identical.*

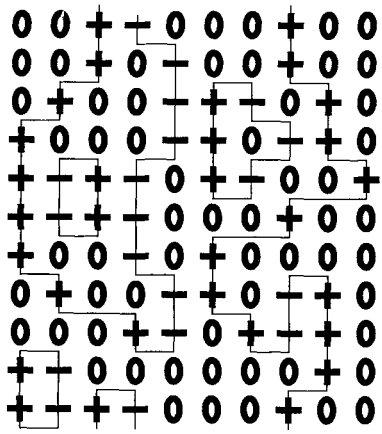

Fig. 3.1. A typical space-time configuration of classical spins, where we regard the horizontal and vertical axes as spatial and temporal axes, respectively. We draw closed loops which show the time-evolution of the nonzero spins to construct the random loop representation

Proof. The statement follows easily from the construction of the graphic expansion and the fact that $((s)_i, S_i^+(s')_i) = ((s')_i, S_i^-(s)_i) = \sqrt{2}\delta_{s,s'+1}$ for $s, s' = -1, 0, 1$. ∎

A graph Γ which satisfies the above "current conservation" can be uniquely decomposed into a union of loops as $\Gamma = \gamma_1 \cup \ldots \cup \gamma_N$, where we do not allow a loop γ_α to have self-intersections. (An 8-shaped graph, for example, is regarded as two loops.) We denote by each γ_α an unoriented loop, and represent its orientation by an accompanying parity variable $p_\alpha = \pm 1$. For a reason which will become clear later, we use the following procedure to determine p_α. Suppose that we are given a graph Γ of oriented loops. Take a loop γ_α, and pick an arbitrary point (i, τ) on it. The classical spin $\sigma_{i,\tau}$ at the point must be either $+1$ or -1. Let $N_{i,\tau}(\{\gamma_\alpha\})$ be the number of vertical bonds in $\{\gamma_\alpha\}$ that cross the line $(1/2, \tau) - (i - 1/2, \tau)$. (We assume that $i = 1, L$ are the boundary sites.)

Lemma 3.4.

$$p_\alpha = (-1)^{N_{i,\tau}(\{\gamma_\alpha\})}\sigma_{i,\tau} . \tag{3.7}$$

is independent of the specific choice of the point (i, τ) *on* γ_α.

Proof. Given $(i, \tau) \in \gamma_\alpha$, let (j, τ) be the left-most point on γ_α with the same τ. The loop γ_α crosses the line $(j + 1/2, \tau) - (i - 1/2, \tau)$ an even number of times if $\sigma_{i,\tau} = \sigma_{j,\tau}$, and an odd number of times if $\sigma_{i,\tau} = -\sigma_{j,\tau}$. This is because the up-going and down-going arrows alternate in a constant τ slice of the oriented loop γ_α. All the other loops cross the line $(j + 1/2, \tau) - (i - 1/2, \tau)$ an even number of times. Thus we see that

$$(-1)^{N_{i,\tau}(\{\gamma_\alpha\})}\sigma_{i,\tau} = (-1)^{N_{j,\tau}(\{\gamma_\alpha\})}\sigma_{j,\tau} .$$

Next we shall see that (3.7) gives the same value for an arbitrary point (k, τ') which is the left-most point in γ_α for a fixed τ'. Note that our space-time lattice has a cylindrical topology, so a self-avoiding loop on it must have the winding number 0 or ± 1. Any loop γ_β $(\alpha \neq \beta)$ with the winding number 0 crosses the line $(1/2, \tau') - (k - 1/2, \tau')$ an even number of times. A loop γ_β with the winding number ± 1 crosses the same line an even number of times if it is right of γ_α, and an odd number of times if it is left of γ_α. Thus the definition of p_α is independent of (k, τ'). ∎

Now we can rewrite the representation (3.6) as

$$Z_{L,\beta,N} = \sum_{\{\gamma_\alpha\}} U(\{\gamma_\alpha\}) \sum_{\{p_\alpha\}} V_{\{\gamma_\alpha\}}(\{p_\alpha\}) , \tag{3.8}$$

where $\{\gamma_\alpha\}$ is summed over all the configurations of unoriented loops, and $\{p_\alpha\}$ over all the ways of assigning orientations to the loops. We have factorized the whole weight as $W(\Gamma) = U(\{\gamma_\alpha\})V_{\{\gamma_\alpha\}}(\{p_\alpha\})$. The weight $U(\{\gamma_\alpha\})$ comes from the operator T_{xy} and the D-dependent part of T_z, while $V_{\{\gamma_\alpha\}}(\{p_\alpha\})$ from the λ-dependent part of T_z. It immediately follows from the construction of the geometric representation that

$$U(\{\gamma_\alpha\}) = \prod_i \left(-\frac{1}{N}\right)^{N_{\text{hor}}} \exp\left(-\frac{D}{N} N_{\text{vert}}\right) , \tag{3.9}$$

where N_{hor} is the number of horizontal bonds and N_{vert} the number of vertical bonds in $\{\gamma_\alpha\}$. Note that the weight $U(\{\gamma_\alpha\})$ is nonnegative because any loop

contains an even number of horizontal bonds. As for the other weight, we have the following.

Lemma 3.5. *The weight* $V_{\{\gamma_\alpha\}}(\{p_\alpha\})$ *can be written as*

$$V_{\{\gamma_\alpha\}}(\{p_\alpha\}) = \exp\Big(\sum_{\alpha,\alpha'} J_{\alpha,\alpha'} p_\alpha p_{\alpha'}\Big), \tag{3.10}$$

where the sum is over all pairs of loop indices α, α' *including the case* $\alpha = \alpha'$. *Here*

$$J_{\alpha,\alpha'} = \frac{\lambda}{N} \times (\#\text{ of horizontal bonds that connect } \gamma_\alpha \text{ and } \gamma'_\alpha)$$

for $\alpha = \alpha'$ *and*

$$J_{\alpha,\alpha} = \frac{\lambda}{N} \times (\#\text{ of horizontal bonds that connect two points on } \gamma_\alpha)\,.$$

In particular, we have $J_{\alpha,\alpha'} \geqq 0$ *for any* α, α'.

Proof. Note that, in terms of the classical spin configuration $\{\sigma_{i,\tau}\}$, the weight can be written as

$$V_{\{\gamma_\alpha\}}(\{p_\alpha\}) = \exp\Big(-\frac{\lambda}{N}\sum_{i,\tau}\sigma_{i,\tau}\sigma_{i+1,\tau}\Big)\,.$$

Suppose $(i,\tau) \in \gamma_\alpha$ and $(i+1,\tau) \in \gamma_{\alpha'}$. Then we have $N_{i+1,\tau}(\{\gamma_\alpha\}) = N_{i,\tau}(\{\gamma_\alpha\}) + 1$, and hence $p_\alpha p_{\alpha'} = -\sigma_{i,\tau}\sigma_{i+1,\tau}$ by (3.7). Summing up the contributions from all the bonds connecting γ_α and γ'_α, we get the desired expression for $J_{\alpha\alpha'}$. ∎

It should be noted that the expression (3.10) can be regarded as the Boltzman factor of a *ferromagnetic* Ising model where the parity variable of each loop plays the role of an Ising spin. We used a somewhat involved definition of p_α to implicitly perform a local gauge transformation to make the model ferromagnetic. Note that this gauge transformation is closely related to the nonlocal unitary transformation discussed in the previous section. This ferromagnetic property is essential for our proof of the desired bounds.

Since the statistical weights $U(\{\gamma_\alpha\})$, $V_{\{\gamma_\alpha\}}(\{p_\alpha\})$ are nonnegative, we can make use of probabilistic concepts. The quantity

$$\mathrm{Prob}_{L,\beta,N}(\{\gamma_\alpha\}) = \frac{1}{Z_{L,\beta,N}} U(\{\gamma_\alpha\}) \sum_{\{p_\alpha\}} V_{\{\gamma_\alpha\}}(\{p_\alpha\}) \tag{3.11}$$

can be interpreted as the probability that a loop configuration $\{\gamma_\alpha\}$ appears.

3.3. Proof of the Bounds. We shall construct representations for the expectation values of various operators, and complete the proof of Theorem 3.1. First we investigate the order parameters in the z direction.

Consider an observable which can be written as $F(\{S_i^z\})$, where F is an arbitrary real polynomial. Inserting the complete basis into the expectation value

(3.4), and noting that $F(\{S_i^z\})\Phi_{\sigma_0} = F(\{\sigma_{i,0}\})\Phi_{\sigma_0}$, we get

$$\omega_{L,\beta,N}(F(\{S_i^z\})) = Z_{L,\beta,N}^{-1} \sum_{\{\sigma_\tau\}} \prod_{\tau=1/N}^{\beta-1/N} (\Phi_{\sigma_{\tau+1/N}}, (T_{xy}T_z)\Phi_{\sigma_\tau})(\Phi_{\sigma_{1/N}}, (T_{xy}T_z)F(\{S_i^z\})\Phi_{\sigma_0})$$

$$= Z_{L,\beta,N}^{-1} \sum_{\{\gamma_\alpha\}} U(\{\gamma_\alpha\}) \sum_{\{p_\alpha\}} F(\{\sigma_{i,0}\}) V_{\{\gamma_\alpha\}}(\{p_\alpha\}) . \tag{3.12}$$

The classical spin variables $\{\sigma_{i,0}\}$ can be expressed in terms of p_α as

$$\sigma_{i,0} = (-1)^{N_{i,0}(\{\gamma_\alpha\})} p_{\alpha(i,0)} , \tag{3.13}$$

where $\alpha(i,0)$ denotes the index of the loop to which the space-time point $(i,0)$ belongs. We set $p_{\alpha(i,0)} = 0$ if $(i,0)$ does not belong to any loop.

Since the weight $V_{\{\gamma_\alpha\}}(\{p_\alpha\})$ can be regarded as the Boltzman factor of an Ising model, it is natural to define the corresponding expectation value by

$$\langle F(\{p_\alpha\})\rangle_{\{\gamma_\alpha\}} = \frac{\sum_{\{p_\alpha\}} F(\{p_\alpha\}) V_{\{\gamma_\alpha\}}(\{p_\alpha\})}{\sum_{\{p_\alpha\}} V_{\{\gamma_\alpha\}}(\{p_\alpha\})} , \tag{3.14}$$

where F is an arbitrary function of $\{p_\alpha\}$.

By putting together (3.4), (3.8), (3.11), (3.12), and (3.14), we finally get the desired random loop representation

$$\omega_{L,\beta,N}(F(\{S_i^z\})) = \sum_{\{\gamma_\alpha\}} \mathrm{Prob}_{L,\beta,N}(\{\gamma_\alpha\}) \langle F(\{\sigma_{i,0}\})\rangle_{\{\gamma_\alpha\}} , \tag{3.15}$$

where we use (3.13) to interpret F as a function of $\{p_\alpha\}$. It is interesting that the right-hand-side of the above representation can be regarded as the expectation value in a random Ising ferromagnet, in which the parity variables $\{p_\alpha\}$ play the role of the Ising spins, and the random loop configuration $\{\gamma_\alpha\}$ determines the random lattice.

We now apply the representation to investigate the properties of the string correlation function. We note that

$$-S_i^z \exp\left(i\pi \sum_{k=i+1}^{j-1} S_k^z\right) S_j^z \Phi_{\sigma_0} = -\sigma_{i,0} \exp\left(i\pi \sum_{k=i+1}^{j-1} \sigma_{k,0}\right) \sigma_{j,0} \Phi_{\sigma_0}$$

$$= -\sigma_{i,0}(-1)^{N_{j,\tau}(\{\gamma_\alpha\}) - N_{i+1,\tau}(\{\gamma_\alpha\})} \sigma_{j,0} \Phi_0$$

$$= p_{\alpha(i,0)} p_{\alpha(j,0)} \Phi_{\sigma_0} .$$

Therefore the representation (3.15) for the string correlation function becomes extremely simple,

$$\omega_{L,\beta,N}\left(-S_i^z \exp\left(i\pi \sum_{k=i+1}^{j-1} S_k^z\right) S_j^z\right)$$

$$= \sum_{\{\gamma_\alpha\}} \mathrm{Prob}_{L,\beta,N}(\{\gamma_\alpha\}) \langle p_{\alpha(i,0)} p_{\alpha(j,0)}\rangle_{\{\gamma_\alpha\}} . \tag{3.16}$$

Moreover, since $\langle \cdots \rangle_{\{\gamma_\alpha\}}$ is the expectation value of *a ferromagnetic* Ising model, Griffiths' first inequality implies

$$\langle p_{\alpha(i,0)} p_{\alpha(j,0)}\rangle_{\{\gamma_\alpha\}} \geqq 0 .$$

We see that (3.16) represents the string correlation function as a sum of nonnegative terms. Thus we have proved that the string correlation function, and hence the string order parameter in the z direction are nonnegative.

To compare the string correlation function with the antiferromagnetic correlation function, we write down the representation (3.15) for the standard S^z correlation function,

$$\omega_{L,\beta,N}(S_i^z S_j^z) = \sum_{\{\gamma_\alpha\}} (-1)^{N_{j,0}(\{\gamma_\alpha\})+N_{i,0}(\{\gamma_\alpha\})} \mathrm{Prob}_{L,\beta,N}(\{\gamma_\alpha\}) \langle p_{\alpha(i,0)} p_{\alpha(j,0)} \rangle_{\{\gamma_\alpha\}} .$$

By taking the absolute value, we see that

$$\begin{aligned} |\omega_{L,\beta,N}(S_i^z S_j^z)| &\leqq \sum_{\{\gamma_\alpha\}} \mathrm{Prob}_{L,\beta,N}(\{\gamma_\alpha\}) \langle p_{\alpha(i,0)} p_{\alpha(j,0)} \rangle_{\{\gamma_\alpha\}} \\ &= \omega_{L,\beta,N}\left(-S_i^z \exp\left(i\pi \sum_{k=i+1}^{j-1} S_k^z \right) S_j^z \right) \end{aligned}$$

which, in the limits $\beta, N \to \infty$, becomes the desired bound (3.2) for $\alpha = z$.

Next we consider the order parameters in the x and y directions. By symmetry, it suffices to consider only the x direction.

The string operator in the x direction can be conveniently rewritten as

$$-S_i^x \exp\left(i\pi \sum_{k=i+1}^{j-1} S_k^x \right) S_j^x = \frac{(-1)^{|j-i|}}{4} (S_i^+ + S_i^-) \left(\prod_{k=i+1}^{j-1} P_k \right) (S_j^+ + S_j^-) ,$$

where $P_k = -\exp(i\pi S_k^x)$ is the spin-flip operator which flips the spin at site k.

We will develop a geometric representation of the following quantity:

$$\begin{aligned} X_{L,\beta,N}(i,j) &= Z_{L,\beta,N} \omega_{L,\beta,N}\left(-S_i^x \exp\left(i\pi \sum_{k=i+1}^{j-1} S_k^x \right) S_j^x \right) \\ &= \frac{(-1)^{|j-i|}}{4} \sum_{\{\sigma_\tau\}} \sum_{\tau=1/N}^{\beta-1/N} (\Phi_{\sigma_{\tau+1/N}}, (T_{xy} T_z) \Phi_{\sigma_\tau}) \\ &\quad \times \left(\Phi_{\sigma_{1/N}}, (T_{xy} T_z)(S_i^+ + S_i^-) \left(\sum_{k=i+1}^{j-1} P_k \right) (S_j^+ + S_j^-) \Phi_{\sigma_0} \right) . \end{aligned}$$

We follow every step in the previous subsection to get graphs of vertical and horizontal arrows, and represent the above quantity as

$$X_{L,\beta,N}(i,j) = \sum_{\Gamma} W'(\Gamma) . \tag{3.17}$$

The "current conservation rule" stated in the Lemma 3.3 is still valid except for those space-time points on which the string operator directly acts. At the points $(i, 1/2)$ and $(j, 1/2)$, there can be an extra in-coming or out-going current because the creation-annihilation operators $S^\pm$ act here. When a current crosses (vertically) through the horizontal line $(i + 1/2, 1/2) - (j - 1/2, 1/2)$, the direction of the current is reversed because the spin-flip operators act here. Besides these exceptions, any graph Γ with nonvanishing weight $W'(\Gamma)$ must conserve the current.

An allowed graph Γ can again be decomposed as $\Gamma = w \cup \gamma_1 \cup \ldots \gamma_N$, where each $\{\gamma_\alpha\}$ is a loop, and w is a walk connecting the space-time points $(i, 1/2)$ and $(j, 1/2)$. We assume $\{\gamma_\alpha\}$ and w are unoriented and non-self-intersecting (Fig. 3.2).

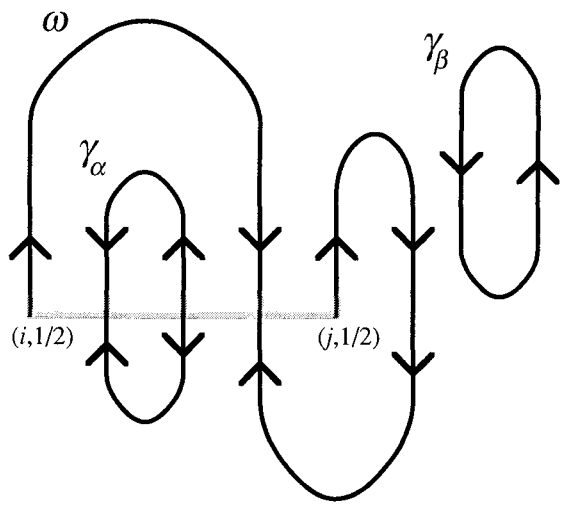

Fig. 3.2. A graph that contributes to the calculation of the string correlation function in the x direction. Note that the direction of the current is reversed when it crosses the spin flip line indicated by the shaded line

Note that the weight $W'(\Gamma)$ is again nonnegative. This is most easily seen by noting that the sign from T_{xy} associated with the walk w exactly cancels out the factor $(-1)^{|i-j|}$.

We further follow the previous subsection to associate a parity variable p_α ($\alpha = 1, \ldots, N$) with each loop, and a parity variable P_0 with the walk w. Even though the topology of the graphs are different from the previous subsection, the construction (3.7) works consistently in this case also. This is because the anomaly caused by the current sources at $(i, 1/2)$ and $(j, 1/2)$ is precisely canceled by the spin-flip on the line between the sources.

Therefore we arrive at the representation

$$X_{L,\beta,N}(i,j) = \sum_{\{w,\gamma_\alpha\}} |U(\{w,\gamma_\alpha\})| \sum_{\{p_\alpha\}} V_{\{w,\gamma_\alpha\}}(\{p_\alpha\}) , \tag{3.18}$$

where U, V are again defined by (3.9), (3.10), and Lemma 3.5 is still valid. Thus V can be regarded as the Boltzman factor of a ferromagnetic Ising model.

In order to compare the string correlation function with the standard antiferromagnetic correlation function, we now repeat the same construction for the quantity

$$\begin{aligned} Y_{L,\beta,N}(i,j) &= Z_{L,\beta,N}\omega_{L,\beta,N}((-1)^{|i-j|}S_i^x S_j^x) \\ &= \frac{(-1)^{|j-i|}}{4} \sum_{\{\sigma_\tau\}} \prod_{\tau=1/N}^{\beta-1/N} (\Phi_{\sigma_{\tau+1/N}}, (T_{xy}T_z)\Phi_{\sigma_\tau}) \\ &\quad \times (\Phi_{\sigma_{1/N}}, (T_{xy}T_z)(S_i^+ + S_i^-)(S_j^+ + S_j^-)\Phi_{\sigma_0}) . \end{aligned}$$

It is now straightforward to get a representation

$$Y_{L,\beta,N}(i,j) = \sum_{\Gamma} W''(\Gamma) ,$$

where the weight $W''(\Gamma)$ is nonnegative. This proves the nonnegativity of the antiferromagnetic correlation function (3.3) claimed in Theorem 3.1. We also note that the graphs Γ summed over here are in one-to-one correspondence with those summed over in (3.17).

Although an allowed Γ can again be decomposed as $\Gamma = w \cup \gamma_1 \cup \ldots \gamma_N$, the construction of the parity variables $\{p_\alpha\}$ does not extend to this situation. Our definition (3.7) gives inconsistent values of p_α for a loop that crosses the line $(i + 1/2, 1/2) - (j - 1/2, 1/2)$. For such a loop, we chose an arbitrary point on it and apply (3.7) to define p_α.

Because of this arbitrariness in the definition of p_α, Lemma 3.5 need not hold. As a consequence, the final representation for $Y_{L,\beta,N}(i,j)$ becomes

$$Y_{L,\beta,N}(i,j) = \sum_{\{w,\gamma_\alpha\}} |U(\{w,\gamma_\alpha\})| \sum_{\{p_\alpha\}} \tilde{V}_{\{w,\gamma_\alpha\}}(\{p_\alpha\}) , \tag{3.19}$$

where

$$\tilde{V}_{\{w,\gamma_\alpha\}}(\{p_\alpha\}) = \exp\left(\sum_{\alpha,\alpha'} \tilde{J}_{\alpha,\alpha'} p_\alpha p_{\alpha'} \right) .$$

The interaction $\tilde{J}_{\alpha,\alpha'}$ satisfies $|\tilde{J}_{\alpha,\alpha'}| \leqq J_{\alpha,\alpha'}$ with $J_{\alpha,\alpha'}$ defined as in (3.10). The effective Ising model of the parity variables $\{p_\alpha\}$ may not be ferromagnetic in this situation.

Lemma 3.6.

$$\sum_{\{p_\alpha\}} V_{\{w,\gamma_\alpha\}}(\{p_\alpha\}) \geqq \sum_{\{p_\alpha\}} \tilde{V}_{\{w,\gamma_\alpha\}}(\{p_\alpha\}) .$$

Proof. Note that the quantities in the inequality are partition functions of Ising models. By using the identity $\exp(J\sigma) = \cosh(J) + \sigma \sinh(J)$ for $\sigma = \pm 1$, we expand the partition functions in standard high temperature series. Comparing the terms corresponding to the same graph using $|\tilde{J}_{\alpha,\alpha'}| \leqq J_{\alpha,\alpha'}$, we get the desired bound. ∎

By inserting the above bound into the representations (3.18) and (3.19), and noting that there is a one-to-one correspondence between the walk-loop configurations, we get the desired inequality in Theorem 3.1.

3.4. Geometric Interpretation of the String Order. In [58, 60] a stochastic geometric picture of the Haldane gap was developed. The point of this work was that the three phases (the Ising phase, the large-D phase, and the Haldane phase) of the Hamiltonian (3.1) can be fully characterized by using the notion of percolation. In the present subsection, we briefly see how the string order parameters are related to percolation phenomena.

Theorem 3.7. *The string correlation function in the z direction satisfies the lower bound*

$$\omega\left(-S_i^z \exp\left(i\pi \sum_{k=i+1}^{j-1} S_k^z \right) S_j^z \right) \geqq \mathrm{Prob}(i \leftrightarrow j) , \tag{3.20}$$

where

$$\mathrm{Prob}(i \leftrightarrow j) = \lim_{L,\beta,N\to\infty} \sum_{\{\gamma_\alpha\}} \mathrm{Prob}(\{\gamma_\alpha\}) \chi((i,0),(j,0) \in \gamma_\alpha \text{ for some } \alpha)$$

denotes the probability (in the $L, \beta, N \to \infty$ limits) that the two space-time points are connected with each other by a single loop. Here χ(event) is one if the event is true and zero if it is false. The probability of the basic event $\{\gamma_\alpha\}$ is defined in (3.11).

Proof. The inequality follows by taking only those loop configurations $\{\gamma_\alpha\}$ where the two sites are connected, and noting that (in such a configuration) one has $p_{\alpha(i,0)} p_{\alpha(j,0)} = 1$. ∎

An interesting lower bound for the string order parameter O^z_{string} follows from (3.20). If we define the percolation probability P_∞ of our random loop system by

$$P_\infty^2 = \lim_{|i-j| \to \infty} \text{Prob}(i \leftrightarrow j)$$

we have

$$O^z_{\text{string}} \geqq P_\infty^2 \,.$$

The inequality is reminiscent of the picture developed in [58] that the percolation in the random loop system (formed by + and − states) generates the alternating order of + and − in the $S = 1$ quantum antiferromagnet. It is expected that the percolation takes place in the Ising phase and the Haldane phase, but not in the large-D phase.

The string correlation function in the x (or y) direction cannot be bounded by the probability of a simple event. However the geometric representation developed in the previous subsection suggest an interesting connection between the percolation phenomena and the behavior of the string order parameter in the x (or y) directions.

In a graph contributing to the quantity $X_{L,\beta,N}(i,j)$, the space-time points $(i, 1/2)$ and $(j, 1/2)$ become sources of flux carried by the bonds. Since flux is conserved (or changes by two at the spin-flip line) in all the other points, these two points must be connected by a random walk w consisting of the + and − states. It is likely that the percolation of the loops formed by + and − is necessary for the string order parameter in the x direction to become nonvanishing.

However this is not the only geometric condition required. To see this, we consider different geometric objects. Given a classical configuration on the space-time lattice, we draw a vertical line of the unit time length through each point with 0 on it. When drawing the horizontal lines, we use the same rule as before but omit its arrow. Figure 3.3 shows the same configuration as in Fig. 3.1, and the corresponding graph constructed in the new way. There is again a current conservation rule which says that each space-time point is attached to an even number of lines. A graph contributing to $Z_{L,\beta,N}$ consists of unoriented closed loops formed by the 0 states.

If we apply the new geometric construction to the quantity $X_{L,\beta,N}$, we find that the points $(i, 1/2)$ and $(j, 1/2)$ again become sources of 0-lines. Thus we must have a random walk of 0 states connecting these points. This suggests that the percolation in the new geometric system of 0 states is also necessary to get a nonvanishing string order in the x direction. It is expected [58] that the percolation of the 0-loop system takes place in the large-D and the Haldane phase, but not in the Ising phase.

In the previous section, we have characterized the Haldane phase by nonvanishing string order parameters in both the z and x directions. The above observation reveals that this characterization is perfectly consistent with the

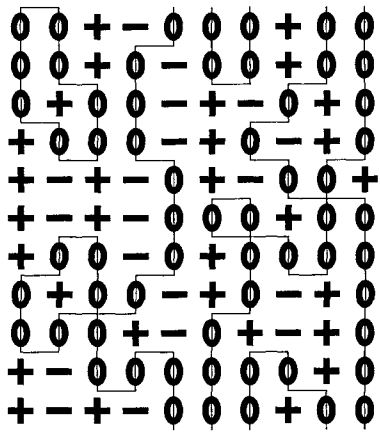

Fig. 3.3. The same classical spin configuration as in Fig. 3.1 is shown, but now the random loops formed by 0 spins are drawn. In the Haldane phase the $\pm$ loops (drawn in Fig. 3.1) and the 0 loops (drawn here) both percolate

percolation picture in [58], where the Haldane phase was characterized by the coexistence of percolation of $\pm$ loops and percolation of 0 loops.

4. Rigorous Perturbation Theory for Quantum Spin Systems

4.1. Statement of Results. In the present section we study Hamiltonians that are small perturbations of Hamiltonians which are trivially diagonalizable. When the unperturbed Hamiltonian is a sum of independent terms and the unperturbed ground state is unique and has a gap, we can allow an essentially arbitrary finite range perturbation if it is sufficiently small. In this case we prove there is a unique translation invariant ground state, a finite correlation length and a nonzero excitation gap. For unperturbed Hamiltonians which have multiple ground states related by a symmetry group, we can allow perturbations which preserve this symmetry. We prove that each of the unperturbed ground states gives rise to a ground state for the perturbed model. These ground states have a finite correlation length and a nonzero excitation gap.

Theorems 2.3, 2.4 and 2.5 follow from the results of this section. While these applications are all one-dimensional, the perturbation theory of this section and the following section is valid in any number of dimensions. Some examples of applications of the general theorems to models other than the spin 1 chains are briefly discussed below. As we emphasized in the introduction, other authors have done similar rigorous perturbation theory for a variety of quantum spin systems. See the introduction for references.

We consider an arbitrary translation invariant infinite lattice whose sites are denoted by $i, j, \ldots$. On each site we have a finite dimensional state space. A "site" in the present section need not be an atomic site of a quantum spin system. For example, a pair of strongly coupled (atomic) sites in the dimerized Hamiltonian H_2 in the introduction is treated here as a single "site."

We consider the following two classes of systems.

A: *Unique Ground State.* The models in this class have translation invariant Hamiltonians of the form

$$H = V + \varepsilon P\,,$$
$$V = \sum_i V_i, \quad P = \sum_i P_i\,, \tag{4.1}$$

where V_i acts only on the spin at site i. We assume that V_i restricted to site i has a unique ground state. We normalize V_i so that the ground state energy is 0, and denote by g the first nonzero eigenvalue (i.e., the gap) of V_i. The only conditions on the perturbation P are as follows. P_0 is an arbitrary hermitian operator whose support is a finite set including the origin 0. P_i is obtained by translating P_0 so that the origin is mapped onto the site i.

B: *Multiple Ground States.* The models in this class have translation invariant Hamiltonians of the form

$$H = V + \varepsilon P\,,$$
$$V = \sum_{i,j} V_{ij}, \quad P = \sum_i P_i\,, \tag{4.2}$$

where i, j is summed over all the nearest neighbor pairs of sites. As in class A, the perturbation P_0 must have finite support, and P_i is the translation of P_0. We assume that there is an orthonormal basis $\{e_\mu^{(i)}\}_{\mu=1}^{d}$ for the single site i and an integer $m \leqq d$, such that V_{ij} is diagonal in the basis $\{e_\mu^{(i)} \otimes e_{\mu'}^{(j)}\}$ and the ground state subspace of V_{ij} is spanned by $\{e_\mu^{(i)} \otimes e_\mu^{(j)}\}_{\mu=1,\ldots,m}$. If we normalize the ground state energy to zero, we have

$$(e_\mu^{(i)} \otimes e_{\mu'}^{(j)},\, V_{ij} e_\mu^{(i)} \otimes e_{\mu'}^{(j)}) \begin{cases} = 0 & \text{if } \mu = \mu' \leqq m \\ \geqq g & \text{otherwise} \end{cases} \tag{4.3}$$

for some positive constant g. The unperturbed model with $\varepsilon = 0$ has m ground states $|\mu\rangle = \bigotimes_i e_\mu^{(i)}$ with $\mu = 1, \ldots, m$. Finally, we require that V and P are invariant under a symmetry group that acts transitively on the m unperturbed ground states of the model.

In the following theorems and throughout the present section, an infinite volume ground state $\omega(\ )$ will mean a state for the infinite system which satisfies

$$\omega(A^*[H, A]) \geqq 0$$

for an arbitrary local operator A. This is a fairly standard definition in the mathematical literature. Note that we used a slightly different definition when we discussed the ground states of $\tilde{H}_{\mathrm{VBS}}$ in Sect. 2. See the remark in [4, page 493] for the relation between these two definitions.

Theorem 4.1. *Consider a model in class* A. *There is a positive constant* ε_0 *such that for any* ε *with* $|\varepsilon| \leqq \varepsilon_0$ *the model has a unique translation invariant infinite volume ground state.*

Theorem 4.2. *Consider a model in class* B. *There is a positive constant* ε_0 *such that for any* ε *with* $|\varepsilon| \leqq \varepsilon_0$ *the model has (at least)* m *distinct translation invariant infinite volume ground states. When* $\varepsilon = 0$ *these ground states equal the states* $|\mu\rangle = \bigotimes_i e_\mu^{(i)}$. *If the Hamiltonian* H *has additional symmetry under which the unperturbed ground*

states $|\mu\rangle^{\wedge}$ *are invariant, then the m ground states are also invariant under this additional symmetry.*

We denote by $\omega(A)$ the expectation value in the above ground state of a local observable A. We also define the ground state energy per spin by

$$E_0 = -\lim_{\Lambda\to\infty}\lim_{\beta\to\infty}\frac{1}{\beta|\Lambda|}\operatorname{Tr} e^{-\beta H}, \tag{4.4}$$

where H denotes the Hamiltonian of the corresponding finite system with Λ sites.

Theorem 4.3. *Consider a model in class* A *or* B. *There is a positive constant* ε_0 *such that for any* ε *with* $|\varepsilon| \leqq \varepsilon_0$ *we have the following.*

i) *The ground state energy per spin* E_0 *is an analytic function of the parameters in* P_i.

ii) *Let A be an arbitrary local observable. The expectation value* $\omega(A)$ *is an analytic function of the parameters in* P_i.

iii) *Let A and B be arbitrary local observables which contain the origin of the lattice in their supports, and let* B_i *be the operator obtained by translating B so that the origin is translated to the site i. Then we have*

$$|\omega(AB_i) - \omega(A)\omega(B)| \leqq C_A C_B \exp(-|i|/\xi_0)$$

(*in one of the m ground states in the case of class* B) *where* $|i|$ *is the graph theoretic distance between the origin and the site i.* C_A *and* C_B *are positive constants that depend on A and B, and* ξ_0 *is a finite constant that does not. Thus the ground state has a finite correlation length.*

iv) *There is a positive constant* γ *such that if A is any local observable with* $\omega(A) = 0$ *then*

$$\omega(A^*[H, A]) \geqq \gamma\omega(A^*A).$$

(*In the case of class* B, ω *is any one of the ground states of Theorem* 4.2.) *Thus the ground state has a nonzero excitation gap.*

Remarks.

1. One can extend class B so that the interaction V includes general n-spin interactions which allow the standard Peierls argument.

2. We have restricted ourselves to translation invariant models. But our expansion and the convergence proof work in models without translation invariance as well.

4.2. Applications. The theorems above are quite general. Before proving them, we list some examples to which they apply.

i) *Large-D Hamiltonian.* Consider the Hamiltonian H_1 in the introduction and its unitary transformation $\tilde{H}_1$. These Hamiltonians fall into class A if we regard $\sum_i D(S_i^z)^2$ as an unperturbed Hamiltonian V and the rest of the Hamiltonians as perturbations. Thus we can show the convergence of the rigorous perturbation theory when the uniaxial anisotropy D is sufficiently large (compared to 1 and λ). This proves Theorem 2.3.

ii) *Large-*λ *Hamiltonian.* We again consider H_1 and $\tilde{H}_1$, but we now regard $\pm\sum_i \lambda S_i^z S_{i+1}^z$ as unperturbed Hamiltonians. Then H_1 and $\tilde{H}_1$ fall into class B. The perturbation theory works when λ is positive and sufficiently large (compared to 1 and D). This proves Theorem 2.5.

One might ask whether we are able to prove the existence of a Néel order in the ground state of H_1 when $\lambda > 0$ is not large, but D is negative and its absolute value is large. In this region, we should regard $\sum \lambda S_i^z S_{i+1}^z + D(S_i^z)^2$ as the unperturbed Hamiltonian. The perturbation $\sum S_i^x S_{i+1}^x + S_i^y S_{i+1}^y$ is not small in norm, but is effectively small since there are no matrix elements between the ground states. One must always go through an excited state (which costs an energy roughly equal to $|D|$) to get from one ground state to the other, and this fact should assume the convergence of the cluster expansion. This model does not belong to class B, but it is not difficult to modify the methods of this section to handle this model.

iii) *Dimerized Hamiltonian.* First we describe a general class of models which can be handled by our theorem. Consider an arbitrary translation invariant lattice, and let $\tilde{B} = \{(i_n, j_n)\}$ be a set of bonds (indexed by n) with the property that each site in the lattice belongs to exactly one of the bonds in $\tilde{B}$. Let V_n be an arbitrary Hamiltonian which acts only on the spins at sites i_n, j_n and has a unique ground state. Consider an arbitrary Hamiltonian of the form

$$H = \sum_n V_n + \varepsilon P$$

which is of finite range and invariant under any translation that leaves $\tilde{B}$ invariant. Such a model falls into class A if we regard each bond in $\tilde{B}$ as a "site." Thus it has a unique ground state, a finite correlation length and a gap, provided that ε is sufficiently small.

In a chain, we let $\tilde{B} = \{(2n, 2n+1)\}_{n \in Z}$. Consider the Hamiltonians H_2 and $\tilde{H}_2$, and let V_n be the parts of the Hamiltonians corresponding to the interactions between sites $2n$ and $2n+1$. Then H_2 and $\tilde{H}_2$ fall into the general class described above. This proves Theorem 2.4.

Note that there is no reason to limit ourselves only to dimerized models. A "site" can be a collection of any number of atomic sites, provided that the Hamiltonian on the "site" has a unique ground state.

iv) *Strong Magnetic Field.* Let H_0 be any finite range translation invariant Hamiltonian. Then the Hamiltonian

$$H = h \sum_i S_i^z + H_0$$

falls into class A if we regard H_0 as a perturbation. The rigorous perturbation converges for sufficiently large magnetic field h, and we can show that the model has a unique ground state and a gap. Note that we do not have to make any technical assumptions (other than finite range) on the unperturbed Hamiltonian H_0.

4.3. Polymer Expansion. To prove the theorems, we first develop a polymer expansion. Our expansion is based on the standard idea [8, 18, 44, 53, 61] of expanding the exponential of an operator by using the Lie product formula. We first develop the expansion for a finite volume Λ. All the estimates will be uniform in the volume. An orthonormal basis for the state space of Λ is given by $\bigotimes_{i \in \Lambda} e_{\mu_i}^{(i)}$ with $1 \leqq \mu_i \leqq d$. We will use ϕ to denote elements of this basis.

Consider a model in class B. In the following H will denote the sum of the terms in the Hamiltonian whose support lies entirely in Λ. A model in class A can be

treated in a similar (and simpler) manner. A simple variant of the Lie product formula says that

$$\begin{aligned}\mathrm{Tr}(\exp(-\beta H)) &= \lim_{N\to\infty} \mathrm{Tr}\left\{\left[\left(1-\frac{\varepsilon}{N}P\right)e^{-(1/N)V}\right]^{N\beta}\right\} \\ &= \lim_{N\to\infty}\sum_{\phi}\prod_{t}\left(\phi_{t-1/N},\left(1-\frac{\varepsilon}{N}P\right)e^{-(1/N)V}\phi_t\right) \\ &= \lim_{N\to\infty}\sum_{\phi}\prod_{t}\left(\phi_{t-1/N},\left(1-\frac{\varepsilon}{N}P\right)\phi_t\right)(\phi_t, e^{-(1/N)V}\phi_t)\,.\end{aligned}$$

Here ϕ is shorthand for $\phi_{1/N}, \phi_{2/N}, \ldots, \phi_\beta$. Each $\phi_{k/N}$ is summed over the orthonormal basis defined above in which the V_i or V_{ij} are all diagonal. Because of the trace we have $\phi_0 = \phi_\beta$. The product over t is over the values $1/N, 2/N, \ldots \beta$. (We assume for convenience that $N\beta$ is an integer.)

We further expand this expression by expanding the $1-(\varepsilon/N)P$ term. At each time t we can either take one of the terms in $-(\varepsilon/N)\sum_i P_i$ or simply the 1. So for each time t we can either choose a site i (which labels P_i) or no site at all. Let n be the number of times at which we choose a site, let $t_1, t_2, \ldots, t_n$ be the times and let $i_1, i_2, \ldots, i_n$ be the sites. We refer to a choice of ϕ, $t_1, \ldots, t_n, i_1, \ldots, i_n$ as a configuration and denote it by C. The weight of C is zero unless $\phi_{t-1/N} = \phi_t$ for $t \notin \{t_1, t_2, \ldots, t_n\}$. In this case the weight is

$$W(C) = \prod_t (\phi_t, e^{-(1/N)V}\phi_t)\prod_{j=1}^{n}\left(\phi_{t_j-1/N}, -\frac{\varepsilon}{N}P_{i_j}\phi_{t_j}\right). \tag{4.5}$$

We now have

$$\mathrm{Tr}(\exp(-\beta H)) = \lim_{N\to\infty}\sum_C W(C)\,.$$

Next we define the support, $s(C)$, of a configuration C. Loosely speaking, the support is the part of the space time picture that is not in the ground state. To get an expansion in the $N\to\infty$ limit, and to take advantage of the usual polymer expansion methods, we introduce a "blocking" in the time direction. τ is a time scale that will be chosen later. We divide the time axis $[0,\beta]$ into intervals $[(l-1)\tau, l\tau]$. For convenience we assume that β is a multiple of τ. P_i has finite support, i.e., it acts nontrivially only on a finite set of sites. For each of these sites we take the unit hypercube in the spatial lattice which is centered at the site, and define S_i to be the union of these hypercubes. So S_i is a "thickened" version of the support set of P_i. For a model from class B, the support set will consist of plaquettes of the form $(i,j)\times[(l-1)\tau, l\tau]$ and "boxes" of the form $S_i\times[(l-1)\tau, l\tau]$.

Given a configuration C, the plaquette $(i,j)\times[(l-1)\tau, l\tau]$ is in $s(C)$ if ϕ_t restricted to sites i and j is never in any of the m ground states of $V_{i,j}$ for $(l-1)\tau \leqq t \leqq l\tau$. The box $S_i\times[(l-1)\tau, l\tau]$ is in $s(C)$ if i equals one of the i_j with $t_j \in [(l-1)\tau, l\tau]$, i.e., if the operator P_i appears during the time interval. (In a model in class A, we replace plaquettes by (time-like) bonds of the form $\{i\}\times[(l-1)\tau, l\tau]$. The bond is in $s(C)$ if ϕ_t at site i is never in the ground state for $(l-1)\tau \leqq t \leqq l\tau$.)

The most important property of the above construction is the following.

Lemma 4.4. *If the space time site (i,t) is not in $s(C)$ then ϕ_t at site i is in one of the ground states.*

Proof. Let l be such that $t \in [(l-1)\tau, l\tau]$. The plaquette $(i,j) \times [(l-1)\tau, l\tau]$ is not in $s(C)$ since $(i,t) \notin s(C)$, so ϕ_t at site i must be in a ground state for at least part of the interval $[(l-1)\tau, l\tau]$. But to excite ϕ_t out of this ground state into one of the excited states, one must hit it by an off-diagonal element of the Hamiltonian, which is the perturbation εP. This is impossible because no boxes intersect with the bond $i \times [(l-1)\tau, l\tau]$. ∎

In a model in class B, a space time point not in $s(C)$ is in one of the ground states, $\mu = 1, \ldots, m$. It is clear from the definition that two space time points not in $s(C)$ with different μ are separated by a wall of $s(C)$. Thus all the space time sites in the same connected component of the complement of $s(C)$ have the same ground state. Therefore (in class B) we extend the definition of the support set $s(C)$ so that it also specifies the ground state indices μ for each connected component of the lattice sites not in $s(C)$. We will refer to this as simply a "ground state assignment."

Let X be a possible support set, i.e., a set which equals $s(C)$ for some C. Define the weight of X to be

$$W(X) = \lim_{N \to \infty} \sum_{C : s(C) = \chi} W(C) . \tag{4.6}$$

Then we have

$$\mathrm{Tr}(\exp(-\beta H)) = \sum_{X} W(X) .$$

The following two properties of the weight $W(X)$ enable us to use the standard machinery of convergent polymer expansions.

Lemma 4.5. (factorization): *Let X be a possible support set and let $X = \chi_1 \cup \chi_2 \cup \ldots \cup \chi_n$ be the decomposition of X into connected components. (We regard two elements in X as connected whenever they share a common space-time site.) A connected component χ_i is called a polymer. In class B, a polymer carries information about the ground state assignment. Then*

$$W(X) = \prod_{i=1}^{n} W(\chi_i) . \tag{4.7}$$

Proof. Let C be a configuration with $s(C) = X$. Let C_i be the configuration which agrees with C on χ_i and equals the appropriate ground state off of χ_i. Then $s(C_i) = \chi_i$. Thus there is a one to one correspondence between C with $s(C) = X$ and $C_1, C_2, \ldots, C_n$ with $s(C_i) = \chi_i$. Furthermore, since we have normalized V so that the ground state energy is zero,

$$W(C) = \prod_{i=1}^{n} W(C_i) .$$

This proves the lemma. ∎

Lemma 4.6. *Given $\mu > 0$ we can choose τ and ε_0 so that $|\varepsilon| \leqq \varepsilon_0$ implies*

$$|W(\chi)| \leqq e^{-\mu|\chi|} . \tag{4.8}$$

For a model in class A, *$|\chi|$ is the number of bonds and boxes that make up χ. For a model in class* B, *$|\chi|$ is the number of plaquettes and boxes in χ plus the number of bonds in χ which are associated with sites in the boundary of Λ.*

We will prove Lemma 4.6 in Sect. 4.5. Here we give a heuristic explanation of why it should be true. If a plaquette $(i,j)\times[(l-1)\tau, l\tau]$ is in $s(C)$ then the part of $W(C)$ that comes from the diagonal terms in the Hamiltonian should contain a factor at least as small as $e^{-g\tau}$. This is small if we take τ large enough. If a box appears in $s(C)$, then there is a corresponding factor of ε in $W(C)$. Thus there is a small factor associated with each plaquette and box in $s(C)$. We still must control the sum over all C such that $s(C)=\chi$. In particular the factor of ε associated with a box can occur anywhere in the box, so it is really a factor of $\varepsilon\tau$. Thus we will have to first choose τ large enough that $e^{-g\tau}$ is small, and then choose ε small enough that $\varepsilon\tau$ is small.

Lemma 4.5 implies that

$$\mathrm{Tr}(e^{-\beta H}) = \sum_{\chi_1,\ldots,\chi_n} \prod_{i=1}^{n} W(\chi_i)\,. \tag{4.9}$$

The sum is over polymers χ_i which do not overlap with each other. For a model in class A, (4.9) is the desired polymer expansion. For a model in class B there are constraints on the χ_i arising from the ground state assignments. We return to the expansion for these models later.

We can develop a similar polymer expansion for the (unnormalized) expectation value of an arbitrary local operator A. For a model in class A this is given by

$$\mathrm{Tr}(A\exp(-\beta H)) = \sum_X W_A(X)\,.$$

$W_A(X)$ can be decomposed as

$$W_A(X) = W_A(\chi(A))\prod_{i=1}^{n} W(\chi_i)\,,$$

where $\chi(A)$ is the collection of polymers (in X) that overlap with the support of A at time $t=0$, and $\chi_1,\ldots,\chi_n$ are the rest of the polymers in X. The weight $W(\chi_i)$ is the same as that appearing in (4.7). Corresponding to the bound (4.8), the weight $W_A(\chi(A))$ satisfies

$$|W_A(\chi(A))| \leqq \|A\| e^{-\mu(|\chi(A)|-v_A)} \tag{4.10}$$

with the same μ, where v_A is the number of sites in the support of A. Suppose that A is a product of two local operators B, C whose supports do not overlap. If $\chi(B)$ unioned with the support of B and $\chi(C)$ unioned with the support of C are disjoint, then we have

$$W_A(\chi(A)) = W_B(\chi(B))\,W_C(\chi(C))\,.$$

Now let us discuss a model in class B. In the polymer expansion (4.9), there is the global constraint that the ground state assignments of the χ_i must be compatible. We will eliminate this constraint by introducing equivalence classes of polymers. We will construct the m different ground states by modifying the Hamiltonian at the boundary. Define for a volume Λ

$$H_\Lambda^\mu = \sum_{i,j\in\Lambda} V_{i,j} + \varepsilon \sum_{i:\,\mathrm{supp}(P_i)\subset\Lambda} P_i + \sum_{i\in\partial\Lambda} P_i^\mu\,.$$

The sum over i, j is over nearest neighbor pairs in Λ. $\partial\Lambda$ denotes the sites in Λ which have a nearest neighbor that is not in Λ. P_i^μ denotes the orthogonal projection whose kernel consists of the states which are in the ground state μ on site i. We let

$$\omega_{\Lambda,\beta}^{\mu}(O) = \mathrm{Tr}(O \exp(-\beta H_\Lambda^\mu))/\mathrm{Tr}(\exp(-\beta H_\Lambda^\mu))$$

and $\omega^\mu(O) = \lim_{\Lambda\to\infty} \lim_{\beta\to\infty} \omega_{\Lambda,\beta}^{\mu}(O)$. Note that we let $\beta \to \infty$ first. (The existence of the limits will follow from the expansion.) For models in class B we modify the definition of the support, $s(C)$, of a configuration C. If a site at the boundary of Λ is never in ground state μ during the time interval $[(l-1)\tau, l\tau]$, then we include the line segment $i \times [(l-1)\tau, l\tau]$ in $s(C)$.

Let X be a support set including the ground state assignment, and let $X = \chi_1 \cup \chi_2 \cup \ldots \cup \chi_n$ be its decomposition into a union of polymers. Each χ_i inherits a ground state assignment from X in a natural way. We think of the configuration as being in ground state μ outside of Λ. Then each polymer χ has a unique exterior component; we will refer to its ground state as the exterior ground state. If χ_i completely encloses χ_j then the exterior ground state of χ_j is determined by χ_i. This forces us to introduce equivalence classes in the following way.

The symmetry group acts transitively on the m ground states, so there are unitary operators U_μ which leave V and P invariant and send ground state 1 into ground state μ. If χ and χ' do not intersect $\partial\Lambda$, then we define χ and χ' to be equivalent if the following are true. First χ and χ' must be identical as geometric objects. Let μ and μ' be the exterior ground states of χ and χ'. Second, the ground state assignment of χ' must be equal to that obtained by applying $U_{\mu'} U_\mu^{-1}$ to the ground state assignment of χ. This definition is an equivalence relation since $U_{\mu_1} U_{\mu_2}^{-1} U_{\mu_2} U_{\mu_3}^{-1} = U_{\mu_1} U_{\mu_3}^{-1}$. The key point is that if we are given an equivalence class $\tilde{\chi}$ and a ground state for the exterior of $\tilde{\chi}$, then there is a unique element of $\tilde{\chi}$ whose ground state on the exterior is the specified one. If either of χ or χ' intersects $\partial\Lambda$, then we define them to be equivalent only if they are identical.

To eliminate the global constraint from (4.9), we must show that two support sets from the same equivalence class have the same weight. At first glance this may appear to be a trivial consequence of the symmetry assumptions. (In the classical case it is.) However, we had to choose a basis to do the path space expansion and that breaks the symmetry. If we can find a basis for which the action of the unitary operators from the symmetry group is simply to permute the basis vectors among themselves, then the desired equality is indeed trivial. Unfortunately, in the example we are most interested in, the Haldane phase studied in Sect. 5, this is not the case. We prove the following lemma in Subsect. 4.6.

Lemma 4.7. *If χ and χ' belong to the same equivalence class, then*

$$W(\chi) = W(\chi') .$$

Let X be a support set which appears in the expansion of $\mathrm{Tr}(\exp(-\beta H_\Lambda^\mu))$. Let $X = \chi_1 \cup \ldots \cup \chi_n$ be its decomposition into connected components. As before we let $\tilde{\chi}_i$ denote the equivalence class of χ_i. Recall that the equivalence class $\tilde{\chi}_i$ and the exterior ground state of χ_i together determine χ_i. Since the ground state outside of Λ is fixed to be μ, $\tilde{\chi}_1, \ldots, \tilde{\chi}_n$ determines $\chi_1, \ldots, \chi_n$. The $\chi_1, \ldots, \chi_n$ had to satisfy the global constraint that their ground state assignments were compatible. There is

no such constraint on the equivalence classes. Using Lemma 4.7 we get the desired polymer expansion

$$\mathrm{Tr}(\exp(-\beta H_\Lambda^n)) = \sum_{\tilde{\chi}_1, \ldots, \tilde{\chi}_n} \prod_{i=1}^{n} W(\tilde{\chi}_i) ,$$

where the only constraint on the $\tilde{\chi}_i$ is that they are disjoint.

For a model from class B, the expansion for the expectation value of an observable A is a little trickier than in class A. As above we picture the support of A as being at $t = 0$. The observable A need not be invariant under the symmetries. Thus the weight of a polymer that intersects the support of A will depend on the exterior ground state of the polymer. If there is another polymer that completely encloses the first polymer and the support of A, then removing this polymer could change the weight of the first polymer. We define $\chi(A)$ to be the union of the polymers that intersect the support of A and any polymers which completely enclose the support of A. The weight $W_A(\chi(A))$ is then well defined since the ground state outside of the space time lattice is fixed. It is important to note that if the polymer χ encloses the support of A and it also encloses the polymer χ', but χ' does not intersect the support of A or enclose the support of A, then we do not include χ' in $\chi(A)$. (To do so would be a disaster when we tried to bound $W_A(\chi(A))$.)

We must check that we have not enlarged $\chi(A)$ so much that we cannot bound $W_A(\chi(A))$ as before. For any integer n the number of polymers with $|\chi| = n$ which enclose a fixed site is bounded by $c_1 n c_2^n$ for constants c_1 and c_2. (To see this fix a line of sites which goes through the fixed site. Any such polymer much contain at least one site on this line within a distance n of the fixed site.) Thus a bound similar to (4.10) holds.

4.4. Proofs of Theorems. Let us now outline how to prove the main theorems. We shall be rather sketchy here because most of the arguments are standard.

A standard combinatoric argument shows that the number of all the possible polymers which include the origin 0 of the space-time lattice is bounded from above by $c^{|\chi|}$ with some finite constant c. It then follows from the bound (4.8) that, for a given positive constant $q < 1$, there is ε_0 such that the following bound holds in a model with $\varepsilon \leqq \varepsilon_0$.

$$\sum_{\chi \ni 0} |W(\chi)| e^{|\chi|} \leqq q . \tag{4.12}$$

We rewrite the polymer expansion in the last section as

$$\mathrm{Tr}(\exp(-\beta H)) = 1 + \sum_{n \geqq 1} \sum_{\chi_1, \ldots, \chi_n} W(\chi_1) \ldots W(\chi_n) ,$$

where the second sum is over the polymers that satisfy the "hard core condition" $\chi_i \cap \chi_j = \emptyset$ for $i \neq j$. Then a standard result in rigorous statistical mechanics is that, when we have the condition (4.12), we can take the logarithm of the above expansion [14, 31],

$$\log \mathrm{Tr}(\exp(-\beta H)) = \sum_{n \geqq 1} \sum_{\chi_1, \ldots, \chi_n} W(\chi_1) \ldots W(\chi_n) \psi_c(\chi_1, \ldots, \chi_n) , \tag{4.13}$$

$\psi_c(\chi_1, \ldots, \chi_n)$ is the connected part of the hard core interaction. The definition of ψ_c can be found in [14]. $\psi_c(\chi_1, \ldots, \chi_n)$ is nonvanishing only when the union of the

polymers $\chi_1, \ldots, \chi_n$ is connected. If we denote by I_n the n^{th} term in (4.13), it satisfies the bound

$$|I_n| \leqq \frac{1}{n} q^n |\Lambda| \beta \,, \tag{4.14}$$

where $|\Lambda|$ is the number of sites in the (space) lattice Λ.

Therefore we get an expansion for the specific free energy.

$$-\frac{1}{|\Lambda|\beta} \log \mathrm{Tr}(\exp(-\beta H)) = -\sum_{n \geqq 1} \frac{I_n}{|\Lambda|\beta} \,,$$

which is uniformly absolutely convergent in the limits $\Lambda, \beta \to \infty$ because of the bound (4.14). This proves the analyticity of the energy stated in part i) of Theorem 4.3.

The rest of the statements are proved by developing similar convergent expansions for various expectation values. For the finite volume Gibbs state

$$\omega_{\Lambda,\beta}(A) = \frac{\mathrm{Tr}(A \exp(-\beta H))}{\mathrm{Tr}(\exp(-\beta H))} \,,$$

we have the expansion

$$\omega_{\Lambda,\beta}(A) = \sum_{n \geqq 0} \sum_{\chi(A), \chi_1, \ldots, \chi_n} W_A(\chi(A)) W(\chi_1) \ldots W(\chi_n) \psi_c(\tilde{\chi}, \chi_1, \ldots, \chi_n) \,,$$

where the n^{th} term in the sum is bounded from above by $C_A q^n / n$, where C_A is a finite constant independent of Λ and β. Therefore we get a uniformly absolutely convergent expansion for the expectation value in the $\Lambda, \beta \to \infty$ limits. The existence of an infinite volume ground state in Theorem 4.1 and the analyticity of the expectation value in Theorem 4.3 ii) follow. We construct the m infinite volume ground states of Theorem 4.2 by using the Hamiltonian which includes the boundary term H_Λ^μ. The proof of part iii) of Theorem 4.3 using the convergent expansion is standard.

To prove part iv) of Theorem 4.3 we first consider the finite volume Hamiltonian H_Λ^μ. Let $E_0, E_1, E_2, \ldots$ be its eigenvalues counted according to multiplicity. Then

$$\mathrm{Tr} \exp(-\beta H_\Lambda^\mu) = \sum_{n=0}^{\infty} \exp(-\beta E_n) \,.$$

The expansion implies that

$$\mathrm{Tr} \exp(-\beta H_\Lambda^\mu) = \exp(-\beta f + O(e^{-\gamma\beta}))$$

for some constants f and γ. γ is positive and does not depend on Λ. (The terms in $O(e^{-\gamma\beta})$ come from terms in the expansion that go all the way around the periodic time axis.) Comparing these two expressions for the trace, we see that E_0 is a simple eigenvalue and $E_1 - E_0 \geqq \gamma$. Let $\omega_\Lambda^\mu = \lim_{\beta \to \infty} \omega_{\Lambda,\beta}^\mu$, so ω_Λ^μ is just expectation in the ground state of H_Λ^μ. By expanding in eigenstates of H_Λ^μ, it is easy to show that $E_1 - E_0 \geqq \gamma$ implies

$$\omega_\Lambda^\mu(A^*[H_\Lambda^\mu, A]) \geqq \gamma [\omega_\Lambda^\mu(A^*A) - |\omega_\Lambda^\mu(A)|^2]$$

for any local observable A. Letting $\Lambda \to \infty$ we obtain part iv) of Theorem 4.3.

Finally we show how to prove the uniqueness of the translation invariant ground state mentioned in Theorem 4.1. Let Q_0 be an arbitrary local observable, and Q_i its translation. We consider the translation invariant Hamiltonian

$$H(\delta) = H + \delta \sum_i Q_i \,.$$

Let $E(\delta)$ be the ground state energy per spin defined as in (4.4). The main ingredient of the proof is the following "Feynman's relation" proved in [37] by using a theorem of Bratteli, Kishimoto and Robinson [13].

Lemma 4.8. *Let $\omega(\cdot)$ be an arbitrary translation invariant ground state of the Hamiltonian H. When $E(\delta)$ is differentiable in δ at $\delta = 0$, we have*

$$\omega(Q_0) = \frac{d}{d\delta} E(\delta) \,.$$

We will prove the differentiability of $E(\delta)$ for an *arbitrary* local observable Q_0. Then the lemma implies the uniqueness of the translation invariant ground state. To prove the differentiability, we note that the Hamiltonian $H(\delta)$ is in class A if we think of δQ_i as part of the perturbation εP_i. So we have a convergent expansion for $E(\delta)$ if δ is sufficiently small. It follows as above that $E(\delta)$ is analytic in a neighborhood of $\delta = 0$.

4.5. Convergence Estimates. To facilitate the control of the sum over all C such that $s(C) = \chi$ in the definition of $W(\chi)$, we introduce a "comparison Hamiltonian"

$$\hat{H} = -\frac{1}{\tau} \sum_i \hat{P}_i \,. \tag{4.15}$$

$\hat{P}_i$ is obtained by replacing the matrix elements of P_i by their absolute values. For a configuration C we let $\hat{W}(C)$ be the weight we get by using $\hat{H}$ in place of H in Eq. (4.5). Clearly, $\hat{W}(C) \geqq 0$. It is important to note that $\hat{H}$ contains a factor of $1/\tau$ rather than the ε found in H.

Lemma 4.9.

$$\sum_{C:\, s(C) = \chi} \hat{W}(C) \leqq e^{k|\chi|} \,,$$

k is a constant that depends on the operator P_i, but not on ε or τ.

Proof of Lemma 4.6 given Lemma 4.9. In the proof we assume we have a model from class B. A model from class A requires some trivial changes in notation and terminology in the proof. Let C be a configuration with $s(C) = \chi$. Let $p(C)$ be the number of plaquettes in $s(C)$, $b(C)$ the number of boxes in $s(C)$ and $d(C)$ the number of bonds in $s(C)$ which are associated with boundary sites. (So $|\chi| = p(C) + b(C) + d(C)$). Recall that a plaquette $(i, j) \times [(l-1)\tau, l\tau]$ is included in the support set if V_{ij} is never in one of its ground states during the time interval. A bond $i \times [(l-1)\tau, l\tau]$ with $i \in \partial\Lambda$ is in $s(C)$ if the state at i is never in ground state μ during the time interval. These definitions, hypothesis (4.3) and the addition of the boundary term $\sum_{i \in \partial\Lambda} P_i^{\mu}$ to the Hamiltonian imply

$$\prod_t \left(\phi_t, \exp\left[-\frac{1}{N}(V + P_{\partial\Lambda}^{\mu}) \right] \phi_t \right) \leqq e^{-g\tau p(C) - \tau d(C)} \,. \tag{4.16}$$

We also have

$$\left| \prod_{j=1}^{n} \left(\phi_{t_j - 1/N}, -\frac{\varepsilon}{N} P_{i_j} \phi_{t_j} \right) \right| = (|\varepsilon|\tau)^n \prod_{j=1}^{n} \left(\phi_{t_j - 1/N}, \frac{1}{\tau N} \hat{P}_{i_j} \phi_{t_j} \right). \tag{4.17}$$

Noting that $n \geqq b(C)$ and assuming that $|\varepsilon|\tau \leqq 1$ and $g \leqq 1$, we conclude that

$$|W(C)| \leqq \varepsilon^{-g\tau(p(C)+d(C))} (|\varepsilon|\tau)^{b(C)} \hat{W}(C) .$$

We now take

$$\varepsilon_0 = \frac{1}{\tau} e^{-g\tau} \tag{4.18}$$

so $|\varepsilon| \leqq \varepsilon_0$ implies $|\varepsilon|\tau \leqq e^{-g\tau}$, and thus

$$|W(C)| \leqq \varepsilon^{-g\tau|\chi|} \hat{W}(C) .$$

Using Lemma 4.9 this implies

$$|W(\chi)| \leqq e^{-g\tau|\chi| + k|\chi|} .$$

If we take $\tau \geqq (k + \mu)/g$ and define ε_0 as in (4.18), then this proves the lemma. ∎

Proof of Lemma 4.9. Consider the restriction of χ to $t = 0$. This gives us a subset χ_0 of the spatial lattice. χ also gives us an assignment of a ground state to each connected component of the complement of χ_0. Let $\Pi(\chi_0)$ be the projection onto the states which are in the ground state specified by χ_0 outside of χ_0. Let

$$I_l(\chi) = \{i : S_i \times [(l-1)\tau, l\tau] \subset \chi\} .$$

So $I(\chi)$ is the set of sites which are in X at time 0. $I_l(\chi)$ specifies the boxes which are in X during the time interval $[(l-1)\tau, l\tau]$. Let

$$H_l = \sum_{i \in I_l(\chi)} \hat{P}_i .$$

We claim that

$$\sum_{C : s(C) = \chi} \hat{W}(C) \leqq \mathrm{Tr}(\Pi(\chi_0) e^{-H_1} e^{-H_2} \ldots e^{-H_{\beta/\tau}}) . \tag{4.19}$$

In the path space expansion of the right side, every term is nonnegative. Each term in the left side appears in this expansion, so the claim follows.

We now bound the right side of (4.19) by using

$$\mathrm{Tr}(AB) \leqq \|B\| \mathrm{Tr}(A) ,$$

where A is a positive operator. We take $A = \Pi(\chi_0)$ and $B = e^{-H_1} e^{-H_2} \ldots e^{-H_{\beta/\tau}}$. $\mathrm{Tr}(\Pi(\chi_0))$ is just the dimension of the range of this projection, which equals d^n, where n is the number of sites in χ_0 and d is the dimension of the state space at a single site. To bound $\|B\|$ we use $\|H_l\| \leqq |I_l(\chi)| \, \|\hat{P}_0\|$, to conclude

$$\|e^{-H_1} e^{-H_2} \ldots e^{-H_{\beta/\tau}}\| \leqq \exp\left[\sum_{l=1}^{\beta/\tau} \|H_l\| \right] \leqq \exp(|\chi| \, \|\hat{P}_0\|) .$$ ∎

4.6. Symmetry. In this subsection we prove Lemma 4.7. In many models in class B we can choose the basis $\{e_\mu^{(i)}\}$ so that the elements of the symmetry group merely permute the basis vectors. In this case Lemma 4.7 is trivial. To handle the general case we develop a representation for the weight that does not involve a choice of basis.

For a set I of sites in Λ, define

$$H(I) = \sum_{i,j} V_{ij} + \varepsilon \sum_{i \in I} P_i \,.$$

The sum over i, j is still over all nearest neighbor pairs in Λ. Next we define

$$(e^{-\tau H(I)})_c = \sum_{J: J \subset I} (-1)^{|I|-|J|} e^{-\tau H(J)} \,. \tag{4.20}$$

Lemma 4.10. *For vectors ϕ and ψ the path space expansion of $(\phi, (e^{-\tau H(I)})_c \psi)$ is given by taking the expansion of $(\phi, e^{-\tau H(I)}\psi)$ and only keeping the configurations in which the number of times P_i appears is zero if $i \notin I$ and is at least one if $i \in I$.*

Proof. (This is a standard inversion trick.) Define $L(I)$ to be the sum of the configurations in the path space expansion of $(\phi, e^{-\tau H(I)}\psi)$ in which the number of times P_i appears is zero if $i \notin I$ and is at least one if $i \in I$. We must prove that $(\phi, (e^{-\tau H(I)})_c \psi) = L(I)$. Clearly we have

$$(\phi, e^{-\tau H(I)}\psi) = \sum_{K: K \subset I} L(K) \,.$$

Thus

$$\begin{aligned}(\phi, (e^{-\tau H(I)})_c \psi) &= \sum_{J: J \subset I} (-1)^{|I|-|J|} (\phi, e^{-\tau H(J)}\psi) \\ &= \sum_{J: J \subset I} (-1)^{|I|-|J|} \sum_{K: K \subset J} L(K) \\ &= \sum_{K: K \subset I} L(K) \sum_{J: K \subset J \subset I} (-1)^{|I|-|J|} \,.\end{aligned}$$

A little thought shows that the sum over J vanishes unless $K = I$, and so the above just equals $L(I)$. ∎

Using the above definition and lemma we can write down an expression for $W(\chi)$ which does not involve an explicit path space expansion. Let l be an integer. Define $I(\chi, l)$ to be the set of sites i such that the "box" $S_i \times [(l-1)\tau, l\tau]$ is in χ. So $I(\chi, l)$ tells you where the operator P_i appeared during the time interval $(l-1)\tau$ to $l\tau$. If $i \notin \bigcup_{j \in I(\chi, l)} S_j$, then the state at site i during $[(l-1)\tau, l\tau]$ is unchanged. Define $E(\chi, l)$ to be the set of these sites i such that the state is not a ground state and $G_\mu(\chi, l)$ to be the set of these sites such that the state is ground state μ. Now let

$$H(\chi, l) = H(I(\chi, l))$$

$$P(\chi, l) = \prod_{i:\, i \in E(\chi, l)} P_i^E \prod_{\mu=1}^{m} \prod_{i \in G_\mu(\chi, l)} P_i^{G,\mu} \,, \tag{4.21}$$

where $P_i^{G,\mu}$ and P_i^E are the projections onto the μ^{th} ground state subspace at site i and onto the subspace of excited states at site i respectively.

Lemma 4.11.

$$W(\chi) = \mathrm{Tr}\,[P(\chi, 0)(e^{-H(\chi,1)})_c P(\chi, 1)(e^{-H(\chi,2)})_c \ldots P(\chi, \beta/\tau - 1)(e^{-H(X,\beta/\tau)})_c] \,.$$

Proof. The equation for $W(\chi)$ follows from the previous lemma and the definitions. ∎

Proof of Lemma 4.7. The operators P_i^E and $(e^{-H(\chi,l)})_c$ are invariant under the symmetries $U_v U_\rho^{-1}$. The operators $P_i^{G,\mu}$ transform according to $U_v U_\rho^{-1} P_i^{G,\mu} (U_v U_\rho^{-1})^{-1} = P_i^{G,\sigma}$ with $\sigma = v$ if $\mu = \rho$. Lemma 4.7 now follows easily from Lemma 4.11. ∎

5. Perturbation Theory About Diagonally Dominant Hamiltonians

5.1. Statement of Results. In this section we will do rigorous perturbation theory for a third class of Hamiltonians. This class will include the dimerized Hamiltonian H_2 in the shaded portion of region H of the phase diagram in Fig. 1.2. The results of this section will prove Theorem 2.6. In particular we show that in this region of the phase diagram all of the string order parameters are nonzero in the ground state of the original Hamiltonian, and the transformed Hamiltonian has at least four infinite volume ground states. Thus the full $Z_2 \times Z_2$ symmetry is broken.

In the previous section we perturbed Hamiltonians that were completely trivial in the sense that we could choose a basis in which all the eigenstates of the unperturbed Hamiltonian were simple tensor products. In this section we will perturb Hamiltonians for which the ground state(s) are simple tensor products, but the excited states need not be. Of course, we require some condition on the unperturbed Hamiltonian. The condition we assume, which we refer to as diagonal dominance, says roughly that each diagonal entry of the unperturbed Hamiltonian is greater than the sum of the absolute values of the off diagonal entries in the same column.

The models we perturbed in Sect. 4 had a correlation length of zero. In this section, the models we perturb may have a correlation length of order one. We will introduce a blocking in the space direction(s), with the scale for the blocking chosen much larger than the correlation length. Using the diagonal dominance condition and the comparison Hamiltonian technique introduced in the previous section we will prove that the polymer expansion for this blocked system converges.

C: Diagonally Dominant Hamiltonians. This class of models has a translation invariant Hamiltonian of the form

$$H = V + \varepsilon P$$
$$V = \sum_{i,j} V_{i,j}, \quad P = \sum_i P_i \,. \tag{5.1}$$

The sum over i, j is over pairs of nearest neighbor sites. Here $V_{i,j}$ acts nontrivially only on sites i and j. The perturbation P_0 acts nontrivially only on a finite set containing the origin 0, and P_i is the translation of P_0 by i. The diagonal dominance condition will only involve V. Note that the perturbation P is essentially arbitrary (except for the symmetry requirement described below), but of course ε must be small.

We assume that there is a basis $\{e_\mu^{(i)}\}_{\mu=1}^d$ for the state space at a single site and an integer $m \leqq d$ such that the ground state subspace of $V_{i,j}$ is spanned by $e_\mu^{(i)} \otimes e_\mu^{(j)}$ for $\mu = 1, 2, \ldots, m$. It is important to note that we do not require that this basis be orthogonal or normalized. We normalize V so that its ground state energy is zero.

Fix a nearest neighbor pair i, j and let $v_{\mu\nu,\rho\sigma}$ be the matrix of $V_{i,j}$ with respect to the basis $e_\mu^{(i)} \otimes e_\nu^{(j)}$. More precisely,

$$V_{i,j} e_\rho^{(i)} \otimes e_\sigma^{(j)} = \sum_{\mu,\nu=1}^{d} v_{\mu\nu,\rho\sigma}\, e_\mu^{(i)} \otimes e_\nu^{(j)} . \tag{5.2}$$

Since the ground state energy is zero, we have $v_{\mu\nu,\rho\rho} = 0$ for $\rho = 1, 2, \ldots, m$ and any μ, ν. We say that V is diagonally dominant if

$$\sum_{\mu\nu:\ \mu\nu \neq \rho\sigma} |v_{\mu\nu,\rho\sigma}| < v_{\rho\sigma,\rho\sigma} \tag{5.3}$$

for any $\rho\sigma$ except $\rho\sigma = 11, 22, \ldots, mm$. (For these exceptional values of $\rho\sigma$, both sides of the inequality are zero.) This condition depends on the basis chosen, so it may hold in one basis but not in another.

Finally we require that V and P are invariant under a symmetry group that acts transitively on the ground states of the models.

It is not hard to see that every Hamiltonian in class B of the previous section is in class C. In this section we will prove for Hamiltonians in class C all the results that we proved for Hamiltonians in class B in the previous section.

Theorem 5.1. *Consider a model in class* C. *Then there is a positive constant* ε_0 *such that for* $|\varepsilon| \leqq \varepsilon_0$ *all the conclusions of Theorems* 4.2 *and* 4.3 *hold.*

5.2. Applications. Our main interest in this class of Hamiltonians is that it includes Hamiltonians which are in the Haldane phase. Before considering this application we will present a simpler application that is of interest in its own right.

i) *The Spin* 1/2 *Anisotropic Heisenberg Ferromagnet.* In this application we take the spin to be 1/2. The unperturbed Hamiltonian is

$$V_{i,j} = -[\lambda(\sigma_i^z \sigma_j^z - 1) + \sigma_i^x \sigma_j^x + \sigma_i^y \sigma_j^y]$$

with $\lambda > 1$. This Hamiltonian has two ground states: $(+\,+)$ and $(-\,-)$. Their energy is zero. The nonzero matrix elements of $V_{i,j}$ are

$$\langle +- | V_{i,j} | +- \rangle = \langle -+ | V_{i,j} | -+ \rangle = 2\lambda ,$$

$$\langle +- | V_{i,j} | -+ \rangle = \langle -+ | V_{i,j} | +- \rangle = -2 .$$

Thus this Hamiltonian is diagonally dominant if $\lambda > 1$. Note that the excited states cannot be written as simple tensor products. The perturbation P is arbitrary with the obvious caveat that the closer λ is to 1, the smaller we require ε to be. For example, we could take the perturbation to be $S_i^x S_j^x$ so that the total Hamiltonian becomes a completely anisotropic Heisenberg Hamiltonian in which all three coupling constants are different.

ii) *The Haldane Phase.* The unperturbed Hamiltonian we consider is the Hamiltonian we obtain by applying the unitary transformation of Sect. 2 to the

Hamiltonian H_2 with $\beta = -1/3$ and δ small but nonzero. (If δ equals zero, then the model is trivial but the ground state is highly degenerate. The perturbation theory we are considering cannot be regarded as a perturbation around $\delta = 0$.) To put this model in the general framework above, we think of two adjacent sites $2i$ and $2i+1$ that are strongly coupled as a single site. Site i in the general framework of class C will correspond to sites $2i$ and $2i+1$ in the Hamiltonian H_2. So the dimension d is 9 rather than 3.

By changing the Hamiltonian in some trivial ways we can take the unperturbed Hamiltonian to be given by

$$V_{i,i+1} = \frac{1}{2}\hat{P}^{S=2}_{2i,2i+1} + \delta\hat{P}^{S=2}_{2i+1,2i+2} + \frac{1}{2}\hat{P}^{S=2}_{2i+2,2i+3}, \tag{5.4}$$

where $\hat{P}^{S=2}_{j,j+1} = U^{-1}P^{S=2}_{j,j+1}U$ with $P^{S=2}_{j,j+1}$ denoting the projection onto the states whose restriction to sites j and $j+1$ has total spin 2. The nontrivial numerical fact is that for $\delta \leqq 0.033$ we can find a basis in which this Hamiltonian is diagonally dominant. We show this in the appendix.

The perturbation can be anything which preserves the $Z_2 \times Z_2$ symmetry of the transformed Hamiltonian. In particular the shaded portion of region H of the phase diagram in Fig. 1.2 is covered. We can also add a small amount of the crystal field term $(S^z_j)^2$ or make the isotropic terms $\mathbf{S}_i \cdot \mathbf{S}_{i+1}$ and $(\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2$ slightly anisotropic.

Note that the region of the Haldane phase in which we have rigorous control does not include any translation invariant Hamiltonians. For $\delta = 1$ and $\beta = -1/3$ the ground states of the transformed Hamiltonian are simple tensor products, but we have not been able to find a basis in which the Hamiltonian is diagonally dominant. (If we could then the results of this section would allow us to conclude that the translation invariant Hamiltonian was in the Haldane phase for β in a small neighborhood of $-1/3$.)

5.3. Development of the Expansion. The tensor products $\bigotimes_{i\in\Lambda} e^{(i)}_{\mu_i}$ with $1 \leqq \mu_i \leqq d$ form a basis for the state space for the finite volume Λ. We denote a choice of $\{\mu_i\}_{i\in\Lambda}$ by K, and the corresponding basis vector by e_K. For an operator O we define its matrix elements, $O(K, K')$, with respect to this basis in the usual way, $Oe_K = \sum_{K'} O(K', K)e_{K'}$. For reasons having to do with the convergence of the expansion, we will construct the ground states in a slightly different way from the previous section. If K_0 is a basis state which has nonzero overlap with the ground state, then we can compute the ground state expectation of O by

$$\langle O\rangle = \lim_{\beta\to\infty} \frac{[\exp(-\beta H/2)O\exp(-\beta H/2)](K_0, K_0)}{\exp(-\beta H)(K_0, K_0)}. \tag{5.5}$$

Our basis is not orthonormal, but we can still develop the path space expansion as we did in the last section. We must simply interpret expressions like $(\phi_t, O\phi_{\tau'})$ as the $\phi_t, \phi_{\tau'}$ matrix element of the operator O.

Let $D_{i,j}$ be the diagonal part of $V_{i,j}$ and $O_{i,j}$ the off diagonal part of $V_{i,j}$. Let $D = \sum_{i,j} D_{i,j}$, $O = \sum_{i,j} O_{i,j}$. The sums are over nearest neighbor pairs. Using

$$e^{-\beta H} = \lim_{N\to\infty}\left[1 - \frac{1}{N}(O + \varepsilon P)e^{-(1/N)D}\right]^{N\beta}$$

we obtain

$$e^{-\beta H}(K_0, K_0) = \lim_{N\to\infty} \sum_{K_{1/N}, K_{2/N}, \ldots K_{\beta-1/N}} \prod_t \left\{\left[1 - \frac{1}{N}(O + \varepsilon P)\right] e^{-(1/N)D}\right\}(K_{t-1/N}, K_t)$$

$$= \lim_{N\to\infty} \sum_{K_{1/N}, K_{2/N}, \ldots K_{\beta-1/N}} \prod_t \left[1 - \frac{1}{N}(O + \varepsilon P)\right](K_{t-1/N}, K_t) e^{-(1/N)D}(K_t, K_t) .$$

Each of $K_{1/N}, K_{2/N}, \ldots K_{\beta-1/N}$ is summed over the basis. The product over t is over the values $1/N, 2/N, \ldots, \beta$. We take $K_\beta = K_0$ in the above. Keeping in mind that $1 - 1/N(O + \varepsilon P) = 1 - 1/N \sum_{i,j} O_{i,j} - \varepsilon/N \sum_i P_i$, we continue the expansion by choosing for each time t either the 1 term, one of the $O_{i,j}$ terms or one of the εP_i terms. Let n be the number of times we choose an $O_{i,j}$ term and m the number of times we chose an εP_i term. Let $t_1, t_2, \ldots, t_n$ be the times at which we choose an $O_{i,j}$ term, and let $(i_1, j_1), (i_2, j_2), \ldots, (i_n, j_n)$ be the particular terms chosen at these times. Likewise let $s_1, s_2, \ldots, s_m$ be the times at which we choose an εP_i term and let $k_1, k_2, \ldots, k_n$ be the terms chosen. A choice of $K_{1/N}, K_{2/N}, \ldots, K_\beta, t_1, \ldots, t_n, (i_1, j_1), \ldots, (i_n, j_n), s_1, \ldots, s_m, k_1, \ldots, k_m$ will be referred to as a configuration and denoted simply by C. The weight, $W(C)$, of the configuration is zero unless $K_{t-1/N} = K_t$ for all t other than $t_1, \ldots, t_n, s_1, \ldots, s_m$. In this case

$$W(C) = \prod_t e^{-(1/N)D}(K_t, K_t) \prod_{p=1}^{n} -\frac{1}{N} O_{i_p, j_p}(K_{t_p - 1/N}, K_{t_p})$$

$$\times \prod_{r=1}^{m} -\frac{1}{N} \varepsilon P_{k_r}(K_{s_r - 1/N}, K_{s_r}) . \tag{5.6}$$

We divide the space time lattice into large blocks that are L units wide in each of the space directions and τ units long in the time direction. We take the block boundaries to run through lattice sites. This means that some lattice sites are on the block boundaries, but all the bonds in the space direction will lie in exactly one block. (τ is the length in physical units, not the length in terms of the number of lattice sites. As always, the lattice sites should be thought of as being separated by $1/N$ in the time direction.) The constants L and τ will be chosen later. (They will be large.)

Next we define the support $s(C)$ of a configuration C. It will be made up of a subset of the blocks introduced above. First we look at the off diagonal operators O_{i_p, j_p} and P_{k_r} which appear at times t_p and s_r, respectively. Any block which contains part of the support of one of these operators is included in $s(C)$. In the remaining blocks the basis state at each site must be constant as a function of time. Any of these blocks which contains a nearest neighbor pair of sites that are not in one of the ground states of V is added to $s(C)$.

To construct the m different ground states, we add the boundary term $\sum_{i \in \partial\Lambda} P_i^\mu$ to the Hamiltonian as we did in the previous section. As before P_i^μ is the orthogonal projection whose kernel consists of the states which equal $e_\mu^{(i)}$ on site i. Since the basis is not orthogonal, the matrix of P_i^μ need not be diagonal. The action of P_i^μ in our basis is given by

$$P_i^\mu e_\nu^{(i)} = \begin{cases} 0 & \text{if } \nu = \mu \\ e_\nu^{(i)} - \alpha_{\mu,\nu} e_\mu^{(i)} & \text{if } \nu \neq \mu \end{cases},$$

where $\alpha_{\mu,\nu} = (e_\nu^{(i)}, e_\mu^{(i)})/(e_\mu^{(i)}, e_\mu^{(i)})$. By the symmetry, $\|e_\mu^{(i)}\| = \|e_\nu^{(i)}\|$, and so $\alpha_{\mu,\nu} < 1$. Thus P_i^μ is diagonally dominant in the basis. We treat P_i^μ in the expansion just as we do the $V_{i,j}$ terms. If a block which includes sites in $\partial\Lambda$ has not already been included in $s(C)$ and one of the boundary sites is in a state other than the ground state μ for the entire time interval, then we include this block in $s(C)$.

As in the previous section the weight of a possible support set is defined to be the sum of the weights of all the configurations that have that support set. We decompose the support set into its connected components as we did in Sect. 4.3. In the next section we will prove that the weight of a connected component χ is exponentially small in the number of blocks in χ. Given this estimate the development of the expansion and the proof of Theorem 5.1 proceed as in the previous section with one small twist.

In the proof of part iv) of Theorem 4.3 we made use of the expansion for $\mathrm{Tr}\exp(-\beta H_\Lambda^\mu)$. In this section we only develop expansions for $\exp(-\beta H_\Lambda^\mu)(K_0, K_0)$ for any basis element K_0. For a fixed volume Λ these expansions imply

$$\mathrm{Tr}\exp(-\beta H_\Lambda^\mu) = \sum_{K_0} \exp(-\beta H_\Lambda^\mu)(K_0, K_0) = c\exp(-\beta f + O(e^{-\gamma\beta}))$$

for some constants f, γ, c with $\gamma > 0$. We cannot conclude that $c = 1$ as we had in Sect. 4, and so we cannot conclude that the ground state eigenvalue is simple. However, the above estimate shows that for small ε there is a gap between the ground state eigenvalue and the next eigenvalue. When $\varepsilon = 0$ we know the ground state eigenvalue is simple, so it must remain simple for small ε. The proof of the existence of the gap now proceeds as in the previous section.

5.4. Proof of Convergence. The convergence of the expansion will be established by comparing things with what we would get if we used the following "comparison Hamiltonian." The diagonally dominant assumption implies that we can find constants $g > 0$ and $0 < \rho < 1$ such that

$$\rho^{-1} \sum_{\mu,\nu:\ \mu\nu \neq \rho\sigma} |v_{\mu\nu,\rho\sigma}| \leqq v_{\rho\sigma,\rho\sigma} - g \tag{5.7}$$

for any $\rho\sigma$ except $\rho\sigma = 11, 22, \ldots, mm$. Let $\hat{V}_{i,j}$ be the Hamiltonian we get from $V_{i,j}$ as follows. Replace the off diagonal matrix elements by $-\rho^{-1}$ times their absolute value. Subtract g from the diagonal elements except for the diagonal elements that are 0. Note that the choice of g and ρ insures that $\hat{V}$ is diagonally dominant. Let $\hat{P}_i$ be the Hamiltonian we get from P_i by replacing every matrix element by its absolute value times $-\rho^{-1}$. Finally, let

$$\hat{H} = \sum_{i,j} \hat{V}_{i,j} + \sum_i \frac{1}{\tau L} \hat{P}_i \,. \tag{5.8}$$

It is important to note that there is a $1/\tau L$ in front of the $\hat{P}_i$ term, rather than an ε. (ε will be small compared to $1/\tau L$.)

Lemma 5.2. *Given $\mu > 0$ we can find τ, L and ε_0 such that for $|\varepsilon| < \varepsilon_0$,*

$$|W(\chi)| \leqq \exp(-\mu|\chi|) \,. \tag{5.9}$$

Here χ is any connected support set, $W(\chi)$ is its weight, and $|\chi|$ is the number of blocks in χ.

How large we must make τ and L and how small we must make ε_0 depends on the constants g and ρ which we chose above using the definition of diagonal dominance. This lemma with large enough μ implies that the usual polymer expansion converges.

Proof of Lemma 5.2. For a configuration C we let $n(C)$ be the number of off diagonal matrix elements in C which come from $V_{i,j}$ terms, and let $m(C)$ be the number of off diagonal elements which come from P_i terms. We let $t(C)$ be $1/N$ times the number of nearest neighbor pairs i, j such that the configuration is not in a ground state of $V_{i,j}$ at time t. Then we let

$$\mu(C) = (\varepsilon\tau L)^{m(C)} \rho^{n(C)} \exp(-gt(C)) . \tag{5.10}$$

Let $\hat{W}(C)$ be the weight of C we get using the Hamiltonian $\hat{H}$. Then we have

$$|W(C)| = \mu(C)\hat{W}(C) .$$

The proof of the lemma follows fairly easily from the following two lemmas.

Lemma 5.3. *Given $\alpha > 0$ we can choose τ and L large enough and ε_0 small enough so that for any configuration C with $s(C) = \chi$, we have*

$$\mu(C) \leqq \exp(-\alpha|\chi|) . \tag{5.11}$$

Lemma 5.4.

$$\sum_{C:\ s(C)=\chi} \hat{W}(C) \leqq \exp(k|\chi|) , \tag{5.12}$$

where k is a constant that depends only on the perturbation P_0. In particular it does not depend on ε, L or τ.

Proof of Lemma 5.3. The key to the proof, and to the expansion of this section, is the following fact. The operator $V_{i,j}$ has no matrix elements between the ground state and the excited states. Thus if a region of the space-time picture is in the ground state, it can go into an excited state only by a matrix element from P_i or by an excitation moving in from the right or the left. In other words, every connected component of the excited region of a configuration C must have a factor of ε associated with it. If one of these connected components extends a distance of at least L in the space direction then $\mu(C)$ will contain a factor of ρ^L. If it extends a distance of at least τ in the time direction, then $\mu(C)$ will contain a factor of $e^{-\tau g}$. Since $\rho < 1$, $g > 0$ and τ and L are both large, ρ^L and $e^{-\tau g}$ are both small.

For a block b, we let $\bar{b}$ denote the union of b and the blocks that touch it in the sense of having at least one space time point in common with it. (Note that the number of such blocks depends only on the dimension of the lattice.) Let $b_1, b_2, \ldots, b_n$ be blocks in χ such that $\bar{b}_1, \bar{b}_2, \ldots, \bar{b}_n$ do not have any blocks in common. We will show later that we can choose these blocks so that $n \geqq (1/M)|\chi| + 1$, where M is an integer that depends only on the number of dimensions of the lattice. First we will show that we can associate a factor of $(\varepsilon\tau L)^{1/q}$, ρ^L or $e^{-g\tau}$ from $\mu(C)$ with each $\bar{b}_i$. The integer q is the maximum number of blocks that the support of a single P_i can intersect. This will prove the lemma with α given by

$$e^{-M\alpha} = \max\{(\varepsilon_0\tau L)^{1/q}, \rho^L, e^{-g\tau}\} .$$

We can make α as large as we like by first choosing L and τ and then choosing ε_0. Consider $\bar{b}_i$. If it contains a matrix element from some P_i, then there is a factor of $\varepsilon\tau L$ in $\mu(C)$. Each factor of $\varepsilon\tau L$ is associated with at most q blocks, so we have a factor of $(\varepsilon\tau L)^{1/q}$ for $\bar{b}_i$. If there is no matrix element from some P_i in $\bar{b}_i$, then the excited part of C must have a connected piece extending between b_i and the exterior of $\bar{b}_i$. Thus the part of $\mu(C)$ that is associated with $\bar{b}_i$ must be at least as small as the larger of ρ^L and $e^{-\tau g}$.

To complete the proof we must find $b_1, b_2, \ldots, b_n$ such that $n \geqq 1/M|\chi| + 1$ and $\bar{b}_i$ and $\bar{b}_j$ have no block in common. Pick b_1 in χ. Let $\bar{\bar{b}}_1$ be $\bar{b}_1$ unioned with the blocks that touch $\bar{b}_1$. Let M be the number of blocks in $\bar{\bar{b}}_1$. (If we have one spatial dimension, $\bar{\bar{b}}_1$ is a five block by five block rectangle centered at b_1, and $M = 25$.) Now pick a block b_2 in $\chi \backslash \bar{\bar{b}}_1$. Continuing, we let b_i be a block in $\chi \backslash \bigcup_{l=1}^{i-1} \bar{\bar{b}}_l$. Since $\bar{\bar{b}}_l$ contains M blocks, $\chi \backslash \bigcup_{l=1}^{i-1} \bar{\bar{b}}_l$ cannot be empty until $i - 1$ is at least $(1/M)|\chi|$. If $i > j$, then b_i is not in $\bar{\bar{b}}_j$. Hence $\bar{b}_i$ and $\bar{b}_j$ cannot have any blocks in common. ∎

Proof of Lemma 5.4. Throughout the proof we let n denote β/τ. Let $I_m(\chi)$ be the set of sites i such that the support of P_i during the time interval $((m-1)\tau, m\tau)$ lies entirely in χ. We then let

$$H_m = \tau \sum_i \hat{V}_{i,j} + \frac{1}{L} \sum_{i \in I_m(\chi)} \hat{P}_i \,. \tag{5.13}$$

Note that H_m contains a factor of τ compared to $\hat{H}$. We claim that

$$\limsup_{N \to \infty} \sum_{C:\, s(C) = \chi} \hat{W}(C) \leqq (e^{-H_1} e^{-H_2} \ldots e^{-H_n})(K_0, K_0) \,.$$

The claim follows from observing that every term in the left side appears in the path space expansion of the right side, and all the terms in this expansion are nonnegative. We can bound the above by

$$\sum_K (e^{-H_1} e^{-H_2} \ldots e^{-H_n})(K, K_0)$$

since each term in this sum is nonnegative.

Let $\hat{D}_{i,j}$ and $\hat{O}_{i,j}$ be the diagonal and off diagonal parts of $\hat{V}_{i,j}$, respectively. The definition of diagonal dominance and the choice of the constants g and ρ, i.e., inequality (5.7), imply that for any K',

$$\begin{aligned}
&\sum_K \left[1 - \frac{1}{N} \sum_{i,j} \hat{O}_{i,j}\right](K, K') e^{-(1/N)\sum_{i,j} \hat{D}_{i,j}(K',K')} \\
&= \left[1 - \frac{1}{N} \sum_{i,j} \sum_K \hat{O}_{i,j}(K, K')\right] e^{-(1/N)\sum_{i,j} \hat{D}_{i,j}(K',K')} \\
&\leqq \left[1 + \frac{1}{N} \sum_{i,j} \hat{D}_{i,j}(K', K')\right] e^{-(1/N)\sum_{i,j} \hat{D}_{i,j}(K',K')} \leqq 1 \,.
\end{aligned} \tag{5.14}$$

Defining

$$M = \sup_{K'} \sum_K \hat{P}_i(K, K') \,,$$

we have

$$\sum_K \left[1 - \frac{1}{N}\left(\sum_{i,j} \hat{O}_{i,j} + \frac{1}{L}\sum_{i \in I_m(\chi)} \hat{P}_i\right)\right](K, K') e^{-(1/N)\sum_{i,j}\hat{D}_{i,j}(K',K')}$$

$$\leqq 1 + \frac{1}{NL}|I_m(\chi)|M \leqq \exp\left(\frac{1}{NL}|I_m(\chi)|M\right)$$

for any K'. Repeated applications of this bound to the usual path space expansion lead to

$$\sum_K (e^{-H_1} e^{-H_2} \ldots e^{-H_n})(K, K_0) \leqq \prod_{m=1}^{n} \exp\left(\frac{1}{L}|I_m(\chi)|M\right).$$

Now $(1/L)\sum_m |I_m(\chi)| \leqq c|\chi|$, where c is a constant that depends only on the size of the support set of P_0. ∎

Appendix

In this appendix we will give a basis in which the Hamiltonian H_2 with $\beta = -1/3$ and δ sufficiently small is diagonally dominant. We start by defining nine states on two sites. For $i = 1, 2, 3, 4$ we let

$$\psi_i = \phi_i \otimes \phi_i ,$$

where ϕ_i are the states on the site defined in Sect. 2.3. We then let

$$\psi_5 = |+-\rangle ,$$

$$\psi_6 = |-+\rangle ,$$

$$\psi_7 = [|+0\rangle + |0+\rangle]/\sqrt{2} ,$$

$$\psi_8 = [|-0\rangle + |0-\rangle]/\sqrt{2} ,$$

$$\psi_9 = [2|00\rangle + |++\rangle + |--\rangle]/\sqrt{6} .$$

Note that these states are not all orthogonal. The first four states are just the ground states of the transformed Hamiltonian on two sites with $\beta = -1/3$. Thus these states are the states one obtains by applying the unitary transformation of Sect. 2 to the four states on two sites which have total spin equal to 0 to 1. The last five states above are the states one obtains by applying this unitary transformation to the states on two sites which have total spin 2. Thus they too are eigenstates of the transformed Hamiltonian on two sites. Finally we define $e_k = c\psi_k$ for $k = 1, \ldots 4$ and $e_k = \psi_k$ for $k = 5, \ldots 9$. Since the basis does not have to be normalized we are free to choose the constant c as we like. To test for diagonal dominance we must compute the matrix of $V_{i,i+1}$ as defined in Eq. (5.4) in Sect. 5.2. V is diagonally dominant if inequality (5.3) holds. We find that with $c = 0.161$, V is diagonally dominant for $\delta \leqq 0.033$.

Acknowledgements. T.K. was supported in part by N.S.F. grant DMS-8902248. H.T. was supported in part by Grant-in-Aid for Encouragement of Young Scientists from the Japanese

Ministry of Education, Science and Culture. The authors thank Tohru Koma and Elliott Lieb for useful discussions, and Bruno Nachtergaele for valuable comments on the manuscript. H.T. thanks the Meson Science Laboratory at the University of Tokyo for generously providing access to their computer network.

References

1. Albanes, C.: On the spectrum of the Heisenberg Hamiltonian. J. Stat. Phys. **55**, 297 (1989)
2. Affleck, I.: Quantum spin chains and the Haldane gap. J. Phys.: Condensed Matter **1**, 3047 (1989)
3. Affleck, I., Halperin, B.I.: private communication
4. Affleck, I., Kennedy, T., Lieb, E.H., Tasaki, H.: Rigorous results on valence-bond ground states in antiferromagnets. Phys. Rev. Lett. **59**, 799 (1987); Valence-bond ground states in isotropic quantum antiferromagnets. Commun. Math. Phys. **115**, 477 (1988)
5. Affleck, I., Lieb, E.H.: A proof of part of Haldane's conjecture on spin chains. Lett. Math. Phys. **12**, 57 (1986)
6. Ajiro, Y., Goto, T., Kikuchi, H., Sakakibara, T., Inami, T.: High-field magnetization of a quasi-one-dimensional $S = 1$ antiferromagnet $Ni(C_2H_8N_2)_2NO_2(ClO_4)$: Observation of the Haldane gap. Phys. Rev. Lett. **63**, 1424 (1989)
7. Arovas, D.P., Auerbach, A., Haldane, F.D.M.: Extended Heisenberg models of antiferromagnetism: Analogies to the fractional quantum Hall effect. Phys. Rev. Lett. **60**, 531 (1988)
8. Asano, T.: Theorems on the partition functions of the Heisenberg ferromagnets. J. Phys. Soc. Jpn. **29**, 350 (1970)
9. Babudjian, H.M.: Exact solutions of the one-dimensional isotropic Heisenberg chain with arbitrary S. Phys. Lett. **90A**, 479 (1982); Exact solutions of the isotropic Heisenberg chain with arbitrary spins: Thermodynamics of the model. Nucl. Phys. **B215**, 317 (1983)
10. Barber, M.N., Batchelor, M.T.: Spectrum of the biquadratic spin-1 antiferromagnetic chain. Phys. Rev. **B40**, 4621 (1989)
11. Borgs, C.: Confinement, deconfinement and freezing in lattice Yang Mills theories with continuous time. Commun. Math. Phys. **116**, 309 (1988)
12. Botet, R., Julien, R., Kolb, M.: Finite-size scaling study of the spin-1 Heisenberg-Ising chain with uniaxial anisotropy. Phys. Rev. **B28**, 3914 (1983)
13. Bratteli, O., Kishimoto, A., Robinson, D.: Ground states of quantum spin systems. Commun. Math. Phys. **64**, 41 (1978)
14. Brydges, D.: A short course on cluster expansions. In: Critical Phenomena, Random Systems, Gauge Theories. Osterwalder, K., Stora, R. (eds.), Amsterdam: Elsevier 1986
15. Buyers, W., Morra, R., Armstrong, R., Hogan, M., Gerlack, P., Hirakawa, K.: Experimental evidence for the Haldane gap in a spin-1, nearly isotropic, antiferromagnetic chain. Phys. Rev. Lett. **56**, 371 (1986)
16. den Nijs, M., Rommelse, K.: Preroughning transitions in crystal surfaces and valence-bond phases in quantum spin chains. Phys. Rev. **B40**, 4709 (1989)
17. Fannes, M., Nachtergaele, B., Werner, R.F.: Exact antiferromagnetic ground states of quantum spin chains. Europhys. Lett. **10**, 633 (1989); Finitely correlated states on quantum spin chains. Commun. Math. Phys. **144**, 443 (1992)
18. Ginibre, J.: Existence of phase transitions for quantum lattice system. Commun. Math. Phys. **14**, 205 (1969)
19. Girvin, S.M., Arovas, D.: Hidden topological order in integer quantum spin chains. Physica Scripta **T27**, 156 (1989)
20. Glarum, S.H., Geschwind, S., Lee, K.M., Kaplan, M.L., Michel, J.: Observation of fractional spin $S = 1/2$ on open ends of $S = 1$ linear antiferromagnetic chains: Nonmagnetic doping. Phys. Rev. Lett. **67**, 1614 (1991)
21. Hagiwara, M., Katsumata, K., Affleck, I., Halperin, B.I., Renard, J.P.: Observation of $S = 1/2$ degrees of freedom in an $S = 1$ linear-chain Heisenberg antiferromagnet. Phys. Rev. Lett. **65**, 3181 (1990)
22. Haldane, F.D.M.: Continuum dynamics of the 1-D Heisenberg antiferromagnet: Identification with the $O(3)$ nonlinear sigma model. Phys. Lett. **93A**, 464 (1983); Nonlinear field theory

of large-spin Heisenberg antiferromagnets: Semiclassically quantized solitons of the one-dimensional easy-axis Néel state. Phys. Rev. Lett. **50**, 1153 (1983)
23. Hatsugai, Y., Kohmoto, M.: Numerical study of hidden antiferromagnetic order in the Haldane phase. Phys. Rev. B **44**, 11789 (1991)
24. Katsumata, K., Hori, H., Takeuchi, T., Date, M., Yamagishi, A., Renard, J.P.: Magnetization process of an $S = 1$ linear-chain Heisenberg antiferromagnet. Phys. Rev. Lett. **63**, 86 (1989)
25. Kennedy, T.: Exact diagonalization of open spin 1 chains. J. Phys.: Condens. Matter **2**, 5737–5745 (1990)
26. Kennedy, T., Tasaki, H.: Hidden $Z_2 \times Z_2$ symmetry breaking in Haldane gap antiferromagnets. Phys. Rev. B (to appear)
27. Kirkwood, J.R., Thomas, L.E.: Expansions and phase transitions for the ground state of quantum Ising lattice systems. Commun. Math. Phys. **88**, 569 (1983)
28. Klümper, A.: The spectra of q state vertex models and related antiferromagnetic quantum spin chains. J. Phys. A.: Math. Gen. **23**, 809 (1990)
29. Knabe, S.: Energy gap and elementary excitations for certain VBS quantum antiferromagnets. J. Stat. Phys. **52**, 627 (1988)
30. Kolb, M.: Symmetry and boundary condition of planar spin systems. Phys. Rev. **B31**, 7494 (1985)
31. Kotecký, R., Preiss, D.: Cluster expansion for abstract polymer models. Commun. Math. Phys. **103**, 491 (1986)
32. Kulish, P., Reshtikhin, N. Yu, Sklyanin, E.: Yang-Baxter equation and representation theory. Lett. Math. Phys. **5**, 393 (1981); Quantum spectral transform method: Recent developments. In: Integrable quantum field theories. Ehlers, J., Hepp, K., Kippenhahn, R., Weidenmüllen, H.A., Zittartz, J. (eds.). Lecture Notes in Physics, Vol. 151, pp. 61. Berlin, Heidelberg, New York: Springer 1982
33. Lai, J.K.: Lattice gas with nearest neighbor interaction in one dimension with arbitrary statistics. J. Math. Phys. **15**, 1675 (1974)
34. Liang, S.: Monte Carlo calculation of the correlation functions for Heisenberg Spin Chains at $T = 0$. Phys. Rev. Lett. **64**, 1597 (1990)
35. Lieb, E.H., Mattis, D.: Ordering energy levels in interacting spin chains. J. Math. Phys. **3**, 749–751 (1962)
36. Lieb, E., Schultz, T., Mattis, D.: Two soluble models of an antiferromagnetic chain. Ann. Phys. (NY) **16**, 407 (1961)
37. Matsui, T.: Uniqueness of the translationally invariant ground state in quantum spin systems. Commun. Math. Phys. **126**, 453 (1990)
38. Matsui, T.: Remarks on the duality of 1 dimensional quantum spin models (preprint)
39. Nightingale, M.P., Blöte, H.W.J.: Gap of the linear spin-1 Heisenberg antiferromagnet: A Monte Carlo calculation. Phys. Rev. **B33**, 659 (1986)
40. Oitmaa, J., Parkinson, J.B., Bonner, J.C.: Crossover effects in a general spin-1-bilinear-biquadratic exchange Hamiltonian. J. Phys. C **19**, L595 (1986)
41. Oshikwa, M.: Hidden $Z_2 \times Z_2$ symmetry in arbitrary integer S quantum spin chains. J. Phys.: Condens. Matter (to appear)
42. Perk, J.H.H., Schultz, C.L.: Diagonalization of the transfer matrix of a nonintersecting string model. Physica **122A**, 50 (1983)
43. Renard, J.P., Verdaguer, M., Regnault, L.P., Erkelens, W.A.C., Rossat-Mignod, J., Ribas, J., Stirling, W.G., Vettier, C.: Quantum energy gap in two quasi-one-dimensional $S = 1$ Heisenberg antiferromagnets. J. Appl. Phys. **63**, 3538 (1988)
44. Robinson, D.: A new proof of the existence of phase transitions in the anisotropic Heisenberg model. Commun. Math. Phys. **14**, 195 (1969)
45. Sakai, T., Takahashi, M.: Energy gap of $S = 1$ antiferromagnetic Heisenberg chain. Phys. Rev. **42**, 1090 (1990)
46. Schorr, A.J.: Antiferromagnetic quantum spin chains with an anisotropic coupling. Princeton University senior thesis, 1987 (unpublished)
47. Schulz, H.J.: Phase diagrams and correlation exponents for quantum spin chains of arbitrary spin quantum number. Phys. Rev. **B34**, 6372 (1986)
48. Schulz, H.J., Ziman, T.: Finite-length calculation of η and phase diagrams of quantum spin chains. Phys. Rev. **B33**, 6545 (1986)
49. Singh, R.P.R., Gelfand, M.P.: Order and criticality in spin-1 chains. Phys. Rev. Lett. **61**, 2133 (1988)

50. Sólyom, J.: Competing bilinear and biquadratic exchange couplings in spin 1 Heisenberg chains. Phys. Rev. **B36**, 8642 (1987)
51. Steiner, M., Kakurai, K., Kjems, J.K., Petitgrand, D., Pynn, R.: Inelastic neutron scattering studies on 1D near-Heisenberg antiferromagnets: A test of the Haldane conjecture. J. Appl. Phys. **61**, 3953 (1987)
52. Sutherland, B.: Model for a multi component quantum system. Phys. Rev. **B12**, 3795 (1975)
53. Suzuki, M., Fisher, M.E.: Zeros of the partition function for the Heisenberg, ferroelectric, and general Ising models. J. Math. Phys. **12**, 235 (1971)
54. Takada, S., Kubo, K.: Nonlocal unitary transformation on $S = 1$ antiferromagnetic spin chains. J. Phys. Soc. Jpn. **60**, 4026 (1991)
55. Takahashi, M.: Monte Carlo calculation of elementary excitation of spin chains. Phys. Rev. Lett. **62**, 2313 (1989)
56. Takhatajan, L.: The picture of low-lying excitations in the isotropic Heisenberg chain of arbitrary spins. Phys. Lett. **87A**, 479 (1982)
57. Tasaki, H.: Haldane gap in three dimensions: A rigorous example. Phys. Rev. Lett. **64**, 2066 (1990)
58. Tasaki, H.: Quantum liquid in antiferromagnetic chains: A stochastic geometric approach to the Haldane gap. Phys. Rev. Lett. **66**, 798 (1991)
59. Tasaki, H.: Haldane gap antiferromagnets in transverse magnetic field. J. Phys.: Condens. Matter **3**, 5875 (1991)
60. Tasaki, H.: Haldane gap in quantum spin chains. A geometric approach. (in preparation)
61. Thomas, L.E., Yin, Z.: Low temperature expansions for the Gibbs states of weakly interacting quantum Ising lattice systems. Commun. Math. Phys. **91**, 405 (1983); Low temperature expansions for the Gibbs states of quantum Ising lattice systems. J. Math. Phys. **25**, 3128 (1984)
62. Uimin, G.V.: One-dimensional problem for $S = 1$ with modified antiferromagnetic Hamiltonian. J.E.T.P. Lett. **12**, 225 (1970)

Communicated by M. Aizenman

Note added in proof. The details of the proof for the final bound of Theorem 2.6 (the exponential decay of the usual two point correlation) are not given in this paper. A sketch of the proof can be found in [38]. In [38], Matsui proves that the model treated in Theorem 2.6 has a unique ground state and a gap, results that we do not prove in the present paper.