Hidden $Z_2 \times Z_2$ symmetry breaking in Haldane-gap antiferromagnets

Tom Kennedy
Department of Mathematics, University of Arizona, Tucson, Arizona 85721

Hal Tasaki
Department of Physics, Gakushuin University, Mejiro, Toshima-ku, Tokyo 171, Japan
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We show that the Haldane phase of the $S=1$ antiferromagnetic chain is closely related to the breaking of a hidden $Z_2 \times Z_2$ symmetry. When the chain is in the Haldane phase, this $Z_2 \times Z_2$ symmetry is fully broken, but when the chain is in a massive phase other than the Haldane phase, e.g., the Ising phase or the dimerized phase, this symmetry is broken only partially or not at all. The hidden $Z_2 \times Z_2$ symmetry is revealed by introducing a nonlocal unitary transformation of the chain. This unitary transformation also leads to a simple variational calculation which qualitatively reproduces the phase diagram of the $S=1$ chain.

INTRODUCTION

Quantum spin systems are full of fascinating surprises. In 1983 Haldane argued that the spin S Heisenberg antiferromagnetic chain has a ground state with 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 a power-law decay when S is half integral.[1] This conclusion has been examined by various numerical, experimental, and rigorous studies.[2] In this paper we will show that the appearance of the Haldane gap in the $S=1$ chain corresponds to the breaking of a hidden $Z_2 \times Z_2$ symmetry.

A rigorous example of disordered ground state in an integer spin model was provided by Affleck, Kennedy, Lieb, and Tasaki.[3] They studied an $S=1$ spin chain with a specific biquadratic Hamiltonian [see (5) below], and proved that the model has a unique infinite volume ground state with a gap and exponentially decaying correlation functions.

Despite the exponential decay of the correlations in the Haldane phase of the spin-1 chain, there is a form of hidden antiferromagnetic order in this phase. Den Nijs and Rommelse[4] proposed a nonlocal string order parameter to detect this hidden order and suggested that the existence of such a hidden order is essential to the basic mechanism of the Haldane gap. This order parameter was studied further by Girvin and Arovas.[5] The connection between the hidden order and the mechanism of the Haldane gap was further addressed by Tasaki.[6] The expectation of this order parameter can be calculated explicitly for the solvable model of Ref. 3, and is nonzero.

Another interesting feature of the exact solution of Ref. 3 is that the model 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. In general in the Haldane phase the ground state of the open chain is not exactly fourfold degenerate, but the four lowest eigenvalues are very close. The separation of these eigenvalues converges to zero exponentially fast as the length of the chain goes to infinity. This phenomenon was studied by Kennedy[7] and by Affleck and Halperin.[8] The geometric picture in Ref. 6 also suggests this phenomenon. Experimental consequences of this fourfold near degeneracy of the ground states in a finite open chain have been studied by Hagiwara, Katsumata, Affleck, Halperin, and Renard.[9]

The hidden antiferromagnetic order and the near degeneracy of the ground state are two distinctive properties of the Haldane gap systems. In this paper we show that both of them can be regarded as consequences of the hidden $Z_2 \times Z_2$ symmetry breaking. We introduce a nonlocal unitary transformation of the $S=1$ chain which makes this symmetry breaking quite explicit. We also use this transformation to do a simple variational calculation that yields a qualitatively correct picture of the phase diagram of the $S=1$ chain. We can prove rigorously that the $Z_2 \times Z_2$ symmetry is broken for the exactly solvable model of Ref. 3 and in an open region of the parameter space of Hamiltonians for the $S=1$ chain. (Unfortunately, this region does not include the usual Heisenberg Hamiltonian.)

Des Nijs and Rommelse[4] argued that the spin-1 chain is equivalent to a two-dimensional RSOS model. Den Nijs[10] then argued that the Coulomb-gas representations for the long-distance behavior of this RSOS model and the Ashkin-Teller model are the same. This is interesting since the latter model also has a $Z_2 \times Z_2$ symmetry which is spontaneously broken.

THE MODEL AND THE ORDER PARAMETERS

We consider a quantum spin chain with $S=1$. The Hamiltonian is

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

where we assume the model to be antiferromagnetic, i.e., $\lambda > 0$. The Hamiltonian is invariant under rotations about the z axis and under the spin flip with respect to this axis, so it has a global O(2) symmetry. At the Heisenberg point $\lambda=1$, $D=0$, the Hamiltonian has the full SU(2) symmetry. We denote by $\langle \cdots \rangle_H$ the expectation value in the infinite volume ground state of H.

We define the Néel order parameter, ferromagnetic order parameter, and the string order parameter in the α direction (where $\alpha = x, y$, or z) as follows:

$$\begin{aligned} O^{\alpha}_{\text{Néel}}(H) &= \lim_{|i-j| \to \infty} (-1)^{|i-j|} \langle S^{\alpha}_i S^{\alpha}_j \rangle_H , \\ O^{\alpha}_{\text{ferro}}(H) &= \lim_{|i-j| \to \infty} \langle S^{\alpha}_i S^{\alpha}_j \rangle_H , \\ O^{\alpha}_{\text{string}}(H) &= \lim_{|i-j| - \infty} \langle \sigma^{\alpha}_{ij} \rangle_H . \end{aligned} \tag{2}$$

Here σ^{α}_{ij} is the string operator of den Nijs and Rommelse[4] defined by

$$\sigma^{\alpha}_{ij} = -S^{\alpha}_i \exp\left[i\pi \sum_{l=i+1}^{j-1} S^{\alpha}_l \right] S^{\alpha}_j . \tag{3}$$

In Ref. 11 we prove[12] that $O^{\alpha}_{\text{string}}(H) \geq O_{\text{Néel}}(H)$ for $\alpha = x, y$ or z.

THE UNITARY

For a finite chain with open boundary conditions we define a unitary operator U as follows. We work in the usual basis in which all the operators S^z_l are diagonal. A state in this basis may be represented by a string of 0's, $+$'s, and $-$'s corresponding to the eigenvalues 0, $+1$, and -1 for S^z_i. The unitary U will map each basis state onto some other basis state or onto a basis state times -1. Let A be a string of 0's $+$'s and $-$'s. The action of U on A is defined as follows. All the 0's in A are left unchanged. Suppose there is a $+$ at site l in A. We count the number of $+$'s and $-$'s in A which are to the left of the site l. If this number is odd then we replace the $+$ by a $-$. If this number is even we leave the $+$ alone. Similarly, if there is a $-$ at site l and the number of $+$'s and $-$'s to the left of site l is odd, then we replace this $-$ with a $+$. If this number is even then we leave the $-$ at site l alone. Finally we count the number of 0's that sit at odd sites anywhere in the finite chain. If this number is odd we multiply the state constructed above by -1. Here are a few examples of the action of U:

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

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

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

It is immediate from the definition of U that U is unitary and $U^{-1} = U$.

Applying the unitary to the string operators, we find $U \sigma^{\alpha}_{ij} U^{-1} = S^{\alpha}_i S^{\alpha}_j$ for $\alpha = x$ or z. (Unfortunately the result of applying U to the string observable σ^{y}_{ij} is not simply $S^y_i S^y_j$). This leads us to the following important relations between the order parameters:

$$O^{\alpha}_{\text{string}}(H) = O^{\alpha}_{\text{ferro}}(\tilde{H}) \text{ for } \alpha = x \text{ or } z , \tag{4}$$

where $\tilde{H} = UHU^{-1}$ is the Hamiltonian we obtain by applying the unitary to the original Hamiltonian.

To see how the Hamiltonian transforms we note that $U(S^{\alpha}_i S^{\alpha}_{i+1})U^{-1} = -S^{\alpha}_i S^{\alpha}_{i+1}$ for $\alpha = x$ or z, $U(S^y_i S^y_{i+1})U^{-1} = S^y_i \exp[i\pi(S^z_i + S^x_{i+1})] S^y_{i+1}$, and $U(S^z_i)^2 U^{-1} = (S^z_i)^2$. The symmetry of the original Hamiltonian H is destroyed by the unitary. We find that $\tilde{H} = UHU^{-1}$ is only invariant under rotations of π about each of the three coordinate axes. It is not invariant under a rotation of π about an arbitrary axis. These three rotations generate the discrete group $Z_2 \times Z_2$. Of course, the transformed Hamiltonian $\tilde{H}$ will have the same symmetries as the original Hamiltonian H since these two operators are related by a unitary, but in general these symmetries for $\tilde{H}$ 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 of π around the x and the z axes, i.e., $\Phi \to \exp(i\pi \sum_j S^x_j)\Phi$ and $\Phi \to \exp(i\pi \sum_j S^z_j)\Phi$. Possible spontaneous breaking of these symmetries may be measured by the order parameters $O^z_{\text{ferro}}(\tilde{H})$ and $O^x_{\text{ferro}}(\tilde{H})$, respectively.

THE HALDANE GAP AND THE $Z_2 \times Z_2$ SYMMETRY BREAKING

We will now consider what happens to the $Z_2 \times Z_2$ symmetry in various regions of the parameter space of Hamiltonian (1). We will show that this symmetry may be broken fully, partially, or not at all. First suppose that the original Hamiltonian H has strong Ising-like anisotropy, i.e., $\lambda \gg 1$. Then it is well known that H has two infinite-volume ground states with long-range Néel order. The ground states are characterized by a nonvanishing Néel order parameter $O^z_{\text{Néel}}(H) > 0$. We also have $O^z_{\text{string}}(H) > 0$ and $O^{\alpha}_{\text{Néel}}(H) = O^{\alpha}_{\text{string}}(H) = 0$ for $\alpha = x, y$. Then by the relation (4) we have $O^z_{\text{ferro}}(\tilde{H}) > 0$ and $O^x_{\text{ferro}}(\tilde{H}) = 0$ for the order parameters of the transformed Hamiltonian. This is consistent with the fact that the transformed Hamiltonian $\tilde{H}$ describes a ferromagnetic Ising chain with a small perturbation when $\lambda \gg 1$. One can prove that such a Hamiltonian has two infinite-volume ground states where the Z_2 symmetry corresponding to the π rotation around the x axis is spontaneously broken, but the other Z_2 symmetry is unbroken.[11]

Next consider the case where the anisotropy parameter D in H is very large. The infinite-volume ground state of H is then unique, has exponentially decaying correlation functions and has a finite excitation gap. All the order parameters are vanishing in this ground state. The ground state of the corresponding $\tilde{H}$ has similar properties. It is unique, disordered, and breaks no symmetry at all.[11] Similar conclusions hold for a Hamiltonian with strong dimerization.[11]

Finally we consider the Haldane phase which is believed to take place in a region of parameter space including the isotropic Heisenberg point $\lambda=1$, $D=0$. Here the infinite-volume ground state of H is also unique, has exponentially decaying correlation functions, and has a finite excitation gap. In particular we have $O^{\alpha}_{\text{Néel}}=0$ for $\alpha=x,y,z$. However the ground state is believed[13] to have a hidden antiferromagnetic order characterized by $O^{\alpha}_{\text{string}}(H)>0$ for $\alpha=x,y,z$. Then from relation (4) we find that the order parameters for the unitary transformed Hamiltonian $\tilde{H}$ must satisfy $O^{x}_{\text{ferro}}(\tilde{H})>0$ and $O^{z}_{\text{ferro}}(\tilde{H})>0$. Therefore the full $Z_2\times Z_2$ symmetry of $\tilde{H}$ is spontaneously broken.

This observation leads us to the somewhat puzzling conclusion that in the Haldane phase $\tilde{H}$ has four distinct infinite-volume grounds states, while H has a unique infinite-volume ground state. Recall that the numbers of infinite-volume ground states are unchanged by the unitary when we are in the Néel, the large-D, or the dimerized phases. Of course our unitary is nonlocal, so the number of infinite-volume ground states of H does not have to equal the number of infinite-volume ground states for $\tilde{H}$. The four infinite-volume ground states of $\tilde{H}$ when we are in the Haldane phase do have an important consequence for the original Hamiltonian H. For a finite open chain the Hamiltonian $\tilde{H}$ must have at least four eigenstates with very low energies. For a finite open chain H and $\tilde{H}$ have the same eigenvalues, so the Hamiltonian H must also have four eigenstates with very low energies. We conclude that the near degeneracy in the Haldane phase is an inevitable consequence of the $Z_2\times Z_2$ symmetry breaking.

A VARIATIONAL CALCULATION

The above picture can be recovered by a surprisingly simple variational analysis. We consider states which can be written as $\Phi=\phi\otimes\phi\otimes\cdots\otimes\phi$ where ϕ is a state on a single site, and minimize the expection value $\langle\Phi|\tilde{H}|\Phi\rangle$ of the transformed Hamiltonian.

In the parameter region $D<4$, $2\lambda-D<4$, $\lambda>0$, we find that the minimum is attained at four different variational states: $\phi=\alpha|0\rangle\pm\beta|+\rangle$, $\phi=\alpha|0\rangle\pm\beta|-\rangle$ where $\alpha=\sqrt{(4+D-2\lambda)/(8-2\lambda)}$, $\beta=\sqrt{(4-D)/(8-2\lambda)}$. (Surprisingly, these states at the Heisenberg point $\lambda=1$, $D=0$ are the exact ground states of the solvable model discussed below.) Figure 1 shows the energy landscape for the Heisenberg model in this simple variational approach. As we increase λ with $D<4$ fixed we see α vanishes at a critical value. For λ larger than this critical value the minimum is attained at the two variational states $\phi=|+\rangle$ and $\phi=|-\rangle$. These states, which break only half of the $Z_2\times Z_2$ symmetry, are the minimizers in the region $2\lambda-D>4$, $\lambda>D,\lambda>0$. Finally, in the region $D>4$, $D>\lambda>0$, none of the $Z_2\times Z_2$ symmetry is broken. The minimum is attained at one state, $\phi=|0\rangle$. Thus our variational calculation qualitatively recovers the phase diagram of the model.

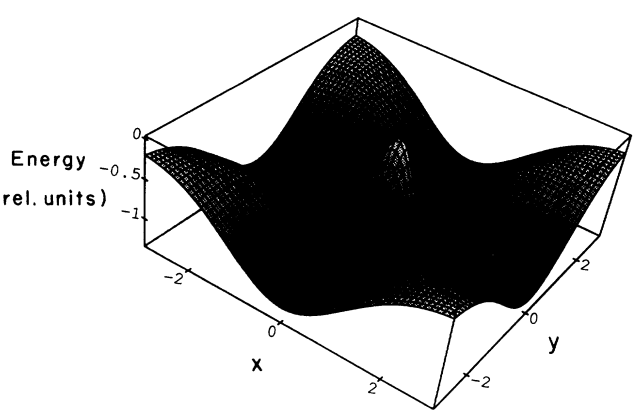

FIG. 1. The energy for the Heisenberg model ($\lambda=1$, $D=0$) is plotted as a function of the variational parameters x and y. The variational state is $\phi=|0\rangle+x|+\rangle+y|-\rangle$. The minimum is attained at four points, indicating the full $Z_2\times Z_2$ symmetry is broken.

THE SOLVABLE MODEL AND RIGOROUS RESULTS

The SU(2)-invariant biquadratic Hamiltonian

$$H=\sum_{i=1}^{L-1} J_i[\mathbf{S}_i\cdot\mathbf{S}_{i+1}-\beta(\mathbf{S}_i\cdot\mathbf{S}_{i+1})^2] , \tag{5}$$

with $J_i>0$ is solvable for $\beta=-\frac{1}{3}$. The above scenario can be rigorously verified in this case. In Ref. 3 it was proved that the infinite-volume ground state of this Hamiltonian is unique, has exponentially decaying correlations and a finite excitation gap. However, it was also found that in a finite open chain there are four distinct ground states. We will not need explicit formulas for these ground states here, but we should emphasize that none of these ground states can be written as a single tensor product of states at each site. As we will now show the ground states of $\tilde{H}=UHU^{-1}$ can be written as a simple tensor product. (If $\beta=-\frac{1}{3}$ and the J_i's are all positive then the ground state is independent of the J_i's. We include them for later use.)

One can easily diagonalize the two-site Hamiltonian corresponding to $\tilde{H}$. The ground state subspace is four dimensional and is spanned by $\phi_\nu\otimes\phi_\nu$ with $\nu=1,2,3,4$, where

$$\begin{aligned}\phi_1&=\sqrt{1/3}|0\rangle+\sqrt{2/3}|+\rangle ,\\ \phi_2&=\sqrt{1/3}|0\rangle-\sqrt{2/3}|+\rangle ,\\ \phi_3&=\sqrt{1/3}|0\rangle+\sqrt{2/3}|-\rangle ,\\ \phi_4&=\sqrt{1/3}|0\rangle-\sqrt{2/3}|-\rangle .\end{aligned} \tag{6}$$

It is clear that the four states

$$\Psi_\nu\equiv\phi_\nu\otimes\phi_\nu\otimes\cdots\otimes\phi_\nu\otimes\phi_\nu \quad \text{for } \nu=1,2,3,4 , \tag{7}$$

are ground states for $\tilde{H}$. It is easy to prove that they are the only ground states. As was discussed in Ref. 3, the corresponding four ground states of the original Hamiltonian H converge to a single infinite-volume ground state. The four states above will converge to four distinct ground states. One can easily show this by computing the expectations of some local observables, e.g., S_i^x,S_i^y,S_i^z, in these four states. In Ref. 11 we prove that these four infinite-volume ground states are the only infinite-volume ground states of $\tilde{H}$. Of course we have nonvanishing order parameters, $O^{x}_{\text{ferro}}(\tilde{H})=O^{z}_{\text{ferro}}(\tilde{H})=\frac{4}{9}$, in these states.

For the dimerized chain in which $J_i=1$ for even i and

$J_i=\delta>0$ for odd i, we have obtained rigorous results for small δ in a neighborhood of $\beta=-\frac{1}{3}$. The precise statement is as follows. There is a constant c such that if δ is sufficiently small and $|\beta+\frac{1}{3}|<c\delta$, then the order parameters $O^x_{\text{ferro}}(\tilde{H})$ and $O^z_{\text{ferro}}(\tilde{H})$ are nonzero and the transformed Hamiltonian $\tilde{H}$ has four infinite-volume ground states. Furthermore in the original system the truncated correlation functions decay exponentially and there is a gap. We stress that the ground states of the models with $\beta\neq-\frac{1}{3}$ are not as simple as those for $\beta=-\frac{1}{3}$. Unlike the VBS states they cannot be written in the form of Eq. (7).

CONCLUSION

We have argued that the appearance of the Haldane gap corresponds to the full breaking of a hidden $Z_2\times Z_2$ symmetry. The hidden antiferromagnetic order and the fourfold near degeneracy of the ground state can be regarded as consequences of this hidden symmetry breaking. By introducing a nonlocal unitary transformation of the $S=1$ chain we have made the hidden $Z_2\times Z_2$ symmetry explicit and given a simple variational calculation that predicts the Haldane phase.

One might further conclude that the $Z_2\times Z_2$ symmetry breaking is the origin of the Haldane gap phenomena since a breaking of a discrete symmetry usually leads to a gap and exponentially decaying correlation functions. We stress that the relation between this symmetry breaking and the appearance of the Haldane phase is not that simple since the unitary we have used is highly nonlocal. Exponential decay of the correlations in the transformed system has, *a priori*, nothing to do with exponential decay of the correlations in the original system. A gap in the transformed system might seem to imply a gap in the original system since their energy spectra for a finite chain must be the same. However, a proper definition of the existence of an energy gap must be done in the infinite-volume setting and involves the local observables of the system. The set of local observables for the original system is not the same set of operators as the set of local observables for the transformed system, so there is no immediate connection between a gap in the original and transformed systems. However we will present[11] an argument (not yet rigorous) that the $Z_2\times Z_2$ symmetry breaking in the transformed system should lead to a unique ground state and a gap in the original system.

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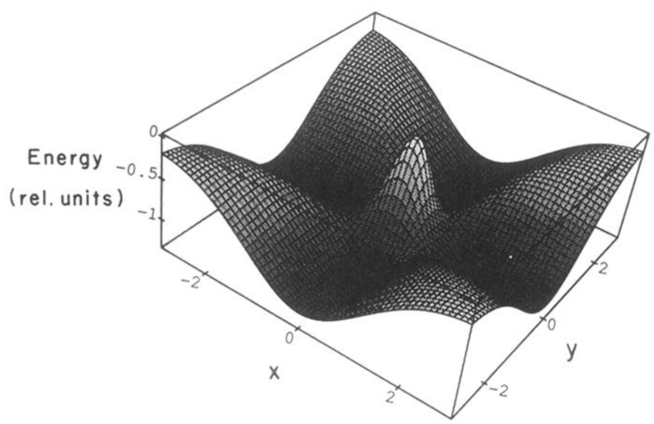
[12]If we use the open boundary conditions then the only constraint on the parameters is that $\lambda\geq 0$.
[13]At the isotropic point $\lambda=1$, $D=0$, the order parameters $O^{\alpha}_{\text{string}}(H)$ should have the same value for $\alpha=x,y,z$ since the ground state is rotation invariant. It is natural to expect that they all take nonvanishing values throughout the Haldane phase.



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