Equivalence of the antiferromagnetic Heisenberg ladder to a single $S = 1$ chain

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Abstract

I introduce two continuous transformations between the $S = 1$ Heisenberg chain and the antiferromagnetic $S = 1/2$ Heisenberg ladder. Both transformations couple diagonally situated next nearest neighbor $S = 1/2$'s to form each $S = 1$. Using the density matrix renormalization group, I demonstrate that the two systems are in the same phase. Furthermore, I find that the hidden topological long-range order characterizing the $S = 1$ system is even stronger in the isotropic two-chain system.

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In the dozen years since Haldane’s conjecture \cite{1} that antiferromagnetic Heisenberg chains with integral spin are gapped, while half-integral spin chains are gapless, our understanding of these systems has increased tremendously. New analytical approaches, exactly soluble models, experimental systems and techniques, and numerical techniques have provided convincing evidence in support of the conjecture \cite{2}. One of the most instructive developments was the discovery of the AKLT model \cite{3}, an exactly soluble, gapped $S = 1$ chain system, differing from the Heisenberg system only by the addition to the Hamiltonian of a biquadratic term $-\frac{1}{3}(S_i \cdot S_j)^2$. The AKLT state is now believed to be an ideal example of the “Haldane” state of the $S = 1$ system. It has a hidden form of topological long-range order \cite{4,5}, measured by a “string” correlation function, which has been determined to be present in the Heisenberg $S = 1$ chain \cite{5,6}.

More recently, attention has been focused on the problem of the antiferromagnetic Heisenberg ladder (AFHL), two antiferromagnetically coupled antiferromagnetic $S = 1/2$ chains \cite{7–10}. There is now evidence that this system has a gap for all nonzero interchain couplings $J_\perp$ \cite{9}. It has been suggested that the AFHL system and the $S = 1$ Heisenberg system may be in the same phase \cite{11}. I consider two systems to be in the same phase if there is a continuous path through model parameter space from one system to the other, without crossing any phase boundaries or critical points, and consequently without change in any broken symmetries or disappearance or appearance of gaps. The ferromagnetically coupled Heisenberg ladder (FHL), for sufficiently strong interchain coupling, has been known for some time to be in the same phase as a single $S = 1$ chain; in the limit $J_\perp \rightarrow -\infty$, the two models are identical. For the AFHL case, the origin of the gap is clear in the large $J_\perp$ limit, where a single “rung” of the ladder has a gap of size $J_\perp$ between the singlet and triplet states. This origin for the gap seems completely different from the origin in the Haldane case, and it is natural to assume that there are two distinct phases. Furthermore, the most obvious path connecting the systems, varying $J_\perp$ from positive to negative values, passes through the gapless point $J_\perp = 0$. Xian has proposed \cite{12} that for a region of large $J_\perp$, the system is in a dimerized phase consisting primarily of singlets on each rung, while for smaller
$J_\perp > 0$, the system is either in a Haldane phase or in another gapped phase which has no topological long-range order. A useful example of such a gapped, orderless state has been thought to be the dimer resonating valence bond (RVB) state \cite{13}, which has been used to describe the qualitative features of the AFHL system \cite{14,10}. However, in the RVB picture there is no distinction between the rung-singlet dimerized phase and the gapped, orderless phase.

In this letter I show that the AFHL system does belong to the same phase as the $S = 1$ chain, the Haldane phase, for all values of $J_\perp > 0$. The dimerized phase, the Haldane phase, and the dimer RVB phase are all identical. These surprising results are possible because, unlike the FHL case, diagonally-situated next-nearest neighbor spins couple to form an effective $S = 1$, rather than two spins on the same rung. The AFHL and FHL systems belong to the same phase in a slightly more limited sense, in that a shift of one chain relative to the other by one lattice spacing is necessary in constructing the path connecting the systems. I demonstrate these results by constructing explicit paths, and calculating the properties of the system to high accuracy, as the parameters are varied, using the density matrix renormalization group (DMRG) \cite{15}. In addition to calculating the gap, I calculate the limiting value of the string correlation function. Surprisingly, the hidden topological order is stronger in two isotropically coupled chains than in the $S = 1$ chain. Furthermore, I show that the dimer RVB state on two coupled chains has “perfect” topological order, just like the AKLT state. In fact, in the composite spin model \cite{16}, which can be thought of as both a single chain $S = 1$ system and a $S = 1/2$ ladder, the dimer RVB state is the AKLT state.

I consider the Heisenberg Hamiltonian

$$H = \sum_{i,j} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j.$$  \hspace{1cm} (1)

Figure 1 illustrates the various models considered. In all cases, the intrachain coupling is taken as $J_{ij} = J = 1$, while additional interchain couplings are as shown. The mapping used for the FHL system, which has been studied in some detail \cite{17}, is shown in Fig. 1(a).
Figure 1(b) shows a mapping for the AFHL case. Here next-nearest neighbor spins, which because of the antiferromagnetic order tend to be in a triplet state, are grouped in pairs to form \( S = 1 \) spins. For \( J_2 = 0 \), we have the AFHL system. In the limit \( J_2 \to -\infty \), the singlet states of the spins coupled by \( J_2 \) are pushed to \( \infty \), and the system is identical to an \( S = 1 \) single chain, with effective coupling \( J_{\text{eff}} = 3/4J \).

Figure 2 shows the evolution of the gap as \( J_2 \) is varied for the system shown in Fig. 1b. The gap is plotted as a function of \( x_{1/2} \), where \( x_0 \) is the probability (and \( x_{1/2} \) the amplitude) that a pair of spins \( i,j \) coupled by \( J_2 \) are in a singlet state, \( x_0 = 1/4 - \langle S_i \cdot S_j \rangle \). The results were obtained by extrapolating from three system sizes, \( L = 19, 31, 39 \), using open boundary conditions. The extrapolation used a polynomial fit in \( 1/L^n \), with the \( 1/L \) term excluded. The finite system version of DMRG was used, keeping 60 states, with a typical discarded weight of \( 2 \times 10^{-6} \). The point at \( x_0 = 0 \) is the taken from previous results for the \( S = 1 \) chain, \( \Delta \approx 0.41050(2) \times 3/4 \). The line is a fourth-order polynomial fit to the data. The typical deviation of the points from the fit is \( \approx 10^{-4} \). At \( J_2 = 0 \), the probability of finding a diagonally situated pair of spins in a triplet state is 96.2%, a surprisingly high number reflecting the short-range antiferromagnetic order, indicating that even at \( J_2 = 0 \), the system is not too far (in this sense) from the \( S = 1 \) system.

Figure 1(c) shows another mapping between the AFHL system and a single \( S = 1 \) chain. In this case a finite antiferromagnetic coupling \( J_3 = 1 \) turns two chains into the composite spin model shown in Fig. 1(d), if one shifts the upper chain to the left by one spacing. The composite spin model is identical to a \( S = 1 \) chain, except for some extra excited states involving singlet modes of a rung. The total spin of each rung commutes with the Hamiltonian, so the eigenstates can all be classified by the total spin on each rung. The set of eigenstates with no singlet modes on any rungs corresponds to the spectrum of the \( S = 1 \) Heisenberg chain.

Figure 3 shows the gap as \( J_3 \) is varied from 0 to 1. In this case the results for finite \( L \) as well as the extrapolation to \( L \to \infty \) are shown. To demonstrate conclusively the robustness of this mapping, large systems were used (up to \( L = 100 \)). Again the finite system version
of DMRG was used, this time keeping up to 100 states, for a typical discarded weight of $10^{-8}$. The data was fit very well with a 14 parameter polynomial function with terms of the form $J^n_3/L^n$, excluding $n = 1$. The resulting gap for $L \to \infty$ as a function of $J_3$, accurate to four or five digits, is

$$\Delta = 0.50249 - 0.227786J_3 + 0.074252J_3^2 + 0.067215J_3^3 - 0.005681J_3^4$$  \hspace{1cm} (2)$$

This very smooth evolution of the gap shows that no phase transitions of either first or second order occur along this path.

Given these results, the AFHL system must exhibit the same topological order known to exist for Haldane chains. This broken symmetry is measured by the string correlation function \[4,12\]

$$g(\ell) = \langle S_0^z(\prod_{k=1}^{\ell-1} e^{i\pi S_k^z})S_\ell^z \rangle.$$  \hspace{1cm} (3)$$

For coupled chains, the expression for $g(\ell)$ is the same as for a single $S = 1$ chain if we take

$$S_k = S_{k,1} + S_{k,2},$$  \hspace{1cm} (4)$$

where the indices 1, 2 indicate the two $S = 1/2$ spins which we expect to combine to form a single effective $S = 1$ spin. If sites 1 and 2 are taken from the same rung, as would be appropriate for the FHL system, the string correlation function decays very rapidly to zero, with a decay length of about 1. Figure 4 shows $g(\infty)$ when sites 1 and 2 are next-nearest neighbors, as shown in Fig. 1(c), as $J_3$ is varied from 0 to 1. As many as 108 states were kept in the calculations, for which no finite-size extrapolation is necessary. Details of the procedure are described in Ref. \[8\]. The result at $J_3 = 0$, $g(\infty) = -0.38010765$ is larger in magnitude than the result for the $S = 1$ chain ($J_3 = 1$) \[6\], $g(\infty) = -0.374325096(2)$.

I have also calculated $g(\infty)$ as a function of $J_\perp$ with $J_3 = 0$. Fig. 5 shows the results, plotted as a function of $J_\perp/(1 + J_\perp)$. Near $J_\perp = 0$, I find $g(\infty) \sim J_\perp^{1/2}$. At the maximum point shown, $J_\perp = 1.3$, $g(\infty) = -0.387263374$. At $J_\perp = \infty$, I find $g(\infty) = 1/4$.

The behavior of $g(\infty)$ at $J_\perp = \infty$ is easily understood. In this limit, the ground state consists of singlets on each rung. If sites $i$ and $j$ are part of such a singlet, then necessarily
all but a few of the \( e^{i\pi S^z_k} \) terms in (3) cancel, leaving a factor of \(-i/2\) for each of the two ends. Hence \( g(\infty) = -1/4 \) at \( J_\perp = \infty \), in agreement with our results. It is useful also to consider a “normalized” string correlation function, defined by

\[
\tilde{g}(\ell) = \frac{-g(\ell)}{\langle (S^z_{k,1} + S^z_{k,2})^2 \rangle^2},
\]

where \( k \) is any \( S = 1 \) “site”. In \( \tilde{g}(\ell) \), one obtains contributions only from those spin configurations for which \( S^z_{k,1} + S^z_{k,2} = \pm 1 \) for the endpoints \( k = 0 \) and \( k = \ell \). The normalized function shows more clearly whether there are defects in the string order between sites 0 and \( \ell \).

For \( J_\perp = \infty \), \( \tilde{g}(\infty) = 1 \), indicating perfect order within the string. For a \( S = 1 \) single chain, the denominator of (5) is 4/9, and the AKLT model also has perfect order, \( \tilde{g}(\infty) = 1 \). For the Heisenberg \( S = 1 \) chain \( \tilde{g}(\infty) = 0.84 \). For the AFHL system with \( J_\perp = 1 \), \( \tilde{g}(\infty) = 0.924 \).

The rung-singlet ground state of \( J_\perp = \infty \) can be considered a limiting case of a more general set of wavefunctions, dimer RVB states, which are themselves limiting cases of the set of short-range RVB states. A dimer RVB state also has perfect string order. The proof is straightforward and similar to that of the strong coupling case: pairs of spins which are parts of singlets cancel in their effect on \( \tilde{g}(\ell) \). Valence bond configurations for which the contribution to \( \tilde{g}(\ell) \) is not 1 are either “staggered” configurations [14], which are negligible in the thermodynamic limit, or they have at least one long-range (non-dimer) bond, with exactly one end within the region 0 and \( \ell \). This means that the confinement of long range bonds within the RVB picture [14] is directly measured by the string correlation function. Probably any short-range RVB state has nonzero string order. Note also that staggered configurations in the two-chain system corresponds to spin-Peierls order in the \( S = 1 \) chain, which has been known to be forbidden [18].

The AKLT state of the \( S = 1 \) chain is constructed within the composite spin model (Fig. 1(d)) by first making intrachain near-neighbor singlets so that each rung has two singlets attached, one to the left and one to the right. Then, one symmetrizes the spins on each rung. It has apparently not been noticed before that this state is also the dimer RVB state for the composite spin model, provided that one eliminates the two spin-Peierls valence bond
configurations, which are negligible in the thermodynamic limit. (Also, no single-rung dimers are allowed.) The symmetrizing operation corresponds to summing over all dimer valence bond configurations, which have an especially simple structure in the composite spin model. Note that the lattice of the composite spin model is symmetrical with respect to interchange of the sites on any rung. Consequently, there is only one reasonable dimer state that can be constructed, as opposed to the AFHL system, for which an infinite number of dimer states can be constructed, corresponding to different amplitudes for horizontal and vertical bonds and to different correlations between horizontal and vertical bonds.

The mappings discussed here also explain the relationship between the $S = 1/2$ end states seen at open ends of $S = 1$ chains [19, 20, 15] and later also on AFHL systems with an extra site on the end of one of the chains [14]. Because of the shift of one chain relative to the other implicit in the transformation of one system to the other, an open $S = 1$ end is equivalent to a ladder with an extra site on one chain.

An important consequence of these results concerns doped ladders and chains. Recent studies of Hubbard and $t$-$J$ ladders have found evidence for a spin-liquid phase with strong pairing correlations for moderate doping [21]. It may be possible to dope ladder compounds to form a physical analog of such a system. Our results suggest that doped Haldane chains may also exhibit a spin-liquid phase with strong pairing correlations.

After this work was finished, I received a preprint by H. Watanabe which comes to some of the same conclusions reached here. I thank Ian Affleck for helpful conversations, and Y. Xian and H. Watanabe for sending preprints of their work. I acknowledge support from the Office of Naval Research under grant No. N00014-91-J-1143. This work was supported in part by the University of California through an allocation of computer time.
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FIGURES

FIG. 1. Several mappings between two coupled $S = \frac{1}{2}$ Heisenberg chains and a single $S = 1$ chain.

FIG. 2. Gap between the ground state and first excited state of the ladder system shown in Fig. 1(b) as $J_2$ is varied, plotted as a function of $x_0^{1/2}$, where $x_0 = 1/4 - \langle S_i \cdot S_j \rangle$, with $i$ and $j$ coupled by $J_2$.

FIG. 3. Gap as a function of $J_3$ for the ladder system shown in Fig. 1(c).

FIG. 4. Limiting value of the string correlation function as a function of $J_3$ for the system of Fig. 1(c).

FIG. 5. Limiting value of the string correlation function as a function of $J_\perp$ for the AFHL system (with $J_2 = J_3 = 0$).
Fig. 1

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Fig. 3

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Fig. 4
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Fig. 5

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