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

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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.

In the dozen years since Haldane's conjecture[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.[2] One of the most instructive developments was the discovery of the Affleck-Kennedy-Lieb-Tasaki (AKLT) model,[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 $-\frac{1}{3}(\mathbf{S}_i\cdot\mathbf{S}_j)^2$. The AKLT ''valence bond solid'' 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,[4,5] measured by a ''string'' correlation function, which is also found in the Heisenberg $S=1$ chain.[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.[7–10] There is now evidence that this system has a gap for all nonzero interchain couplings $J_\perp$.[9] This raises an important question: is the AFHL system in a fundamentally new state, or is it in the same phase as another, more familiar system, namely, the $S=1$ Heisenberg chain? 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 $J_\perp\to-\infty$, 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 $J_\perp=0$.

Evidence in favor of a Haldane phase in the AFHL is provided indirectly by the work of Hida,[11] who studied the dimerized $S=1/2$ chain. In the fully dimerized limit this system is identical to the fully dimerized ladder, $J_\perp\to\infty$, with singlets on each rung. Primarily using exact diagonalization, Hida gave evidence that the dimerized $S=1/2$ chain is in the $S=1$ Haldane phase.[11] This implies a Haldane phase region for the AFHL for large $J_\perp$. Numerical results for the AFHL have not shown any evidence for a change in phase as a function of $J_\perp$,[9] indicating that perhaps the AFHL is in the Haldane phase for all $J_\perp$. In contrast, Xian has proposed several alternative possibilities,[12] such as that there may be two separate phases for small and large $J_\perp>0$, and that for small $J_\perp>0$, the system may be in a non-Haldane gapped phase which has no topological long-range order.

Hida also argued that the topological long-range order, which he showed is present in the dimerized $S=1/2$ chain, indicates the presence of short-range *static* valence-bond order. In contrast, it has been generally presumed that a short-range *resonating* valence bond (RVB)[13] state describes a ''featureless'' gapped state without topological long-range order. The RVB ansatz has proven to be a useful qualitative picture for the AFHL,[14,10] and has been argued to apply for all $J_\perp>0$. However, if the RVB picture is valid for all $J_\perp>0$, and if for large $J_\perp$ the system is in a Haldane phase, then the RVB state must have topological long-range order. Indeed, I find that this is the case.

In this article 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).[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

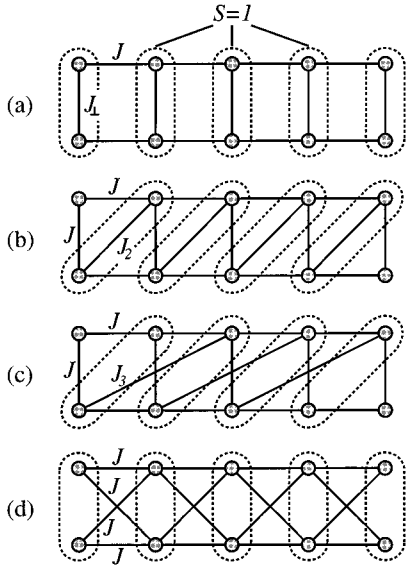

FIG. 1. Several mappings between two coupled $S=1/2$ Heisenberg chains and a single $S=1$ chain.

model,[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

$$H=\sum_{i,j} J_{ij}\mathbf{S}_i\cdot\mathbf{S}_j\,. \tag{1}$$

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,[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 correlations 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 $J_2\rightarrow-\infty$, the singlet states of the spins coupled by J_2 are pushed to ∞, and the system is identical to an $S=1$ single chain, with effective coupling $J_{\rm eff}=3/4J$.

Figure 2 shows the evolution of the gap as J_2 is varied for the system shown in Fig. 1(b). The gap is plotted as a function of $x_0^{1/2}$, where x_0 is the probability (and $x_0^{1/2}$ the amplitude) that a pair of spins i,j coupled by J_2 are in a singlet state, $x_0=1/4-\langle\mathbf{S}_i\cdot\mathbf{S}_j\rangle$. 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 2×10^{-6}. The point at $x_0=0$ is taken from previous results for the $S=1$ chain, $\Delta\cong0.41050(2)\times3/4$. The line is a fourth-order polynomial fit to the data. The typical deviation of the points from the fit is $\cong10^{-4}$. 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 correlations, indicating that even at $J_2=0$, the system is not too far (in this sense) from the $S=1$ system.

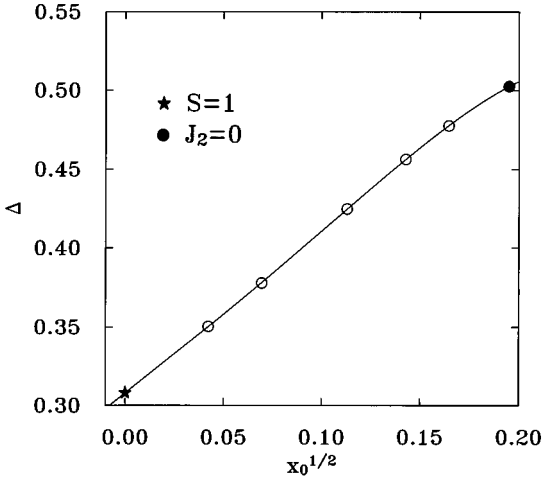

FIG. 2. Gap between the ground state and first excited state of the ladder system shown in Fig. 1(b) as J_2 is varied, plotted as a function of $x_0^{1/2}$, where $x_0=1/4-\langle\mathbf{S}_i\cdot\mathbf{S}_j\rangle$, with i and j coupled by J_2.

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 $L\rightarrow\infty$ 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

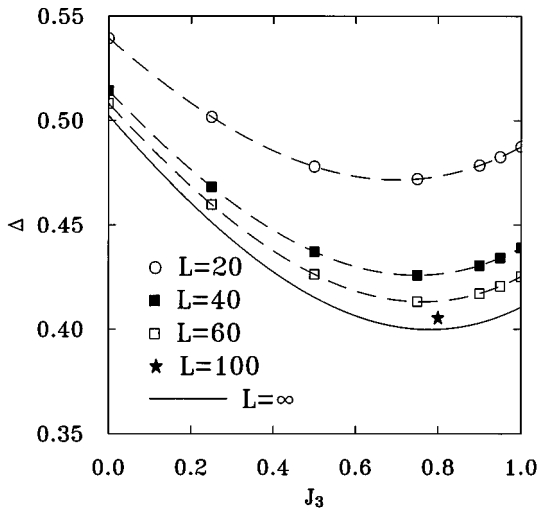

FIG. 3. Gap as a function of J_3 for the ladder system shown in Fig. 1(c). The $S=1$ chain corresponds to $J_3=1$.

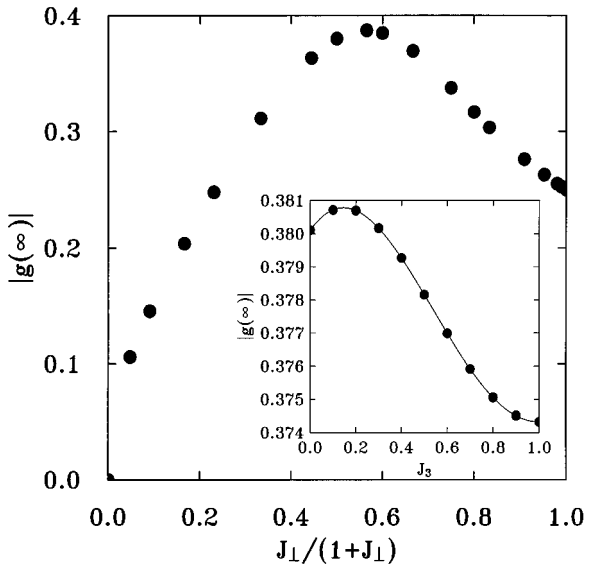

FIG. 4. Limiting value of the string correlation function as a function of $J_\perp$ for the AFHL system (with $J_2=J_3=0$). The inset shows $g(\infty)$ as a function of J_3 for the system of Fig. 1(c).

parameter polynomial function with terms of the form J_3^m/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

$$\Delta = 0.50249 - 0.227786J_3 + 0.074252J_3^2 + 0.067215J_3^3 - 0.005681J_3^4. \quad (2)$$

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]

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

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

$$\mathbf{S}_k = \mathbf{S}_{k,1} + \mathbf{S}_{k,2}, \quad (4)$$

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 for $J_\perp=J$. The inset of Fig. 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. 6. The result at $J_3=0$, $g(\infty)=-0.38010765$ is *larger* in magnitude than the result for the $S=1$ chain ($J_3=1$) (Ref. 6), $g(\infty)=-0.374325096(2)$.

I have also calculated $g(\infty)$ as a function of $J_\perp$ with $J_3=0$, again with next-nearest neighbors combined to form $S=1$'s. The main part of Fig. 4 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 $S_i^z+S_j^z=0$. Using this, all but a few of the $e^{i\pi S_k^z}$ 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

$$\tilde{g}(\ell) = \frac{-g(\ell)}{\langle (S_{k,1}^z + S_{k,2}^z)^2 \rangle^2}, \quad (5)$$

where k is any $S=1$ "site." The denominator in (5) is simply the probability that neither endpoint, $k=0$ and $k=\ell$, is in a $S_{k,1}^z+S_{k,2}^z=0$ configuration. Since these configurations give no contribution to $g(\ell)$, the normalized function shows more clearly whether there are defects in the topological order *between* sites 0 and ℓ. For $J_\perp=\infty$, $\tilde{g}(\infty)=1$, indicating perfect topological order. 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 presence of a maximum in the main part of Fig. 4 is entirely due to a maximum in the denominator of (5); $\tilde{g}(\infty)$ is monotonic as a function of $J_\perp$. In contrast, the maximum in the inset of Fig. 4 reflects nonmonotonic behavior in $\tilde{g}(\infty)$.

The rung-singlet ground state of $J_\perp=\infty$ can be considered a limiting case of a more general set of wave functions, dimer RVB states, which are themselves limiting cases of the set of short-range RVB states. A dimer RVB state also has perfect topological 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 neglible in the thermodynamic limit, or they have at least one long-range (nondimer) bond, with exactly one end within the region between 0 and ℓ. This means that the confinement of long-range bonds within the RVB picture[14] is directly measured by the string correlation function; consequently, we expect any short-range RVB state to have nonzero topological order. In particular, we expect any Heisenberg ladder with an even number of legs to have topological long-range order, while a ladder with an odd number of legs does not.

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 neglible in the thermodynamic limit. (Also, no single-rung dimers are allowed.) The symmetrizing operation corresponds to summing over all dimer valence bond configura-

tions, 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[18,19,15] 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.[20] 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 two independent reports,[21,22] each of which partially overlaps this work. Watanabe[21] emphasizes the new form of the string correlation function, while Nishiyama, Hatano, and Suzuki[22] emphasize the relevance of the RVB theory to the topological order and perform an interesting analysis of the $J_\perp=0$ critical point. I thank Ian Affleck for helpful conversations. 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.

[1] F. D. M. Haldane, Phys. Lett. **93A**, 464 (1983).
[2] For an early review, see I. Affleck, J. Phys. Condens. Matter **1**, 3047 (1989).
[3] I. Affleck, T. Kennedy, E. H. Lieb, and H. Tasaki, Phys. Rev. Lett. **59**, 799 (1987).
[4] K. Rommelse and M. den Nijs, Phys. Rev. Lett. **59**, 2578 (1987).
[5] S.M. Girvin and D. P. Arovas, Physica Scripta **T**27, 156 (1989).
[6] S.R. White and D.A. Huse, Phys. Rev. B **48**, 3844 (1993).
[7] E. Dagotto, J. Riera, and D.J. Scalapino, Phys. Rev. B **45**, 5744 (1992).
[8] S.P. Strong, and A.J. Millis, Phys. Rev. Lett. **69**, 2419 (1992).
[9] T. Barnes *et al.*, Phys. Rev. B **47**, 3196 (1993).
[10] T.M. Rice, S. Gopalan, and M. Sigrist, Europhys. Lett. **23**, 445 (1993); M. Sigrist, T.M. Rice, and F.C. Zhang, *Phys. Rev.* B **49**, 12 058 (1994).
[11] K. Hida, Phys. Rev. B **45**, 2207 (1992); K. Hida and S. Takada, J. Phys. Soc. Jpn. **61**, 1879 (1992).
[12] Y. Xian (unpublished).
[13] S.A. Kivelson, D.S. Rokhsar, and J.P. Sethna, Phys. Rev. B **35**, 8865 (1987).
[14] S.R. White, R.M. Noack, and D.J. Scalapino, Phys. Rev. Lett. **73**, 886 (1994).
[15] S.R. White, Phys. Rev. Lett. **69**, 2863 (1992), Phys. Rev. B **48**, 10 345 (1993).
[16] M. den Nijs, Physica **111A**, 237 (1982); J. Timonen and A. Luther, J. Phys. C **18**, 1439 (1985); H. J. Schuz, *ibid*. **34**, 6372 (1986); J. Solyom and J. Timonen, *ibid.* **34**, 487 (1986); **39**, 7003 (1989); **40**, 7150 (1989).
[17] See, for example, H. Watanabe, Phys. Rev. B **50**, 13 442 (1994).
[18] T. Kennedy, J. Phys. Condens. Matter **2**, 5737 (1990).
[19] M. Hagiwara, K. Katsumata, I. Affleck, B.I. Halperin, and J.P. Renard, Phys. Rev. Lett. **65**, 3181 (1990).
[20] See R.M. Noack, S.R. White, and D.J. Scalapino, Phys. Rev. Lett. **73**, 882 (1994), and references therein.
[21] H. Watanabe, Phys. Rev. B **52**, 12 508 (1995).
[22] Y. Nishiyama, N. Hatano, and M. Suzuki, J. Phys. Soc. Jpn. **64**, 1967 (1995).