Resonating Valence Bond Theory of Coupled Heisenberg Chains

S. R. White and R. M. Noack
Department of Physics, University of California, Irvine, California 92717

D. J. Scalapino
Department of Physics, University of California, Santa Barbara, California 93106
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Using numerical results from a density matrix renormalization group study as a guide, we develop a resonating valence bond (RVB) theory for coupled Heisenberg chains. We argue that simple topological effects mandate a short-range RVB description of systems with an even number of chains n_c, with a spin gap, short-range correlations, and confinement of topological spin defects. Odd-n_c systems have long-range RVB ground states, no gap, and power-law correlations.

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The discovery of materials such as $(VO)_2P_2O_7$ [1] and $Sr_2Cu_4O_6$ [2], which contain weakly coupled arrays of metal-oxide-metal ladders, has stimulated interest in coupled-chain Heisenberg, Hubbard, and t-J systems. A number of studies [3–7] have provided strong evidence that at half-filling the two-chain ladder systems are spin liquids, with a spin gap and finite spin-spin correlation length. It has been proposed that the system can be described in terms of a short-range resonating valence bond (RVB) picture [6,7], and mean field treatments with Gutzwiller renormalization of the matrix elements have supported this conclusion. Based on these results, it has been suggested that systems with an even number of chains n_c are gapped spin liquids, while odd-n_c systems are gapless [6,7]. This idea was supported by limited exact diagonalization results for three chains [8], and additional mean field results for two and four chains [7].

In this Letter we summarize results of a density matrix renormalization group (DMRG) study [9] of isotropic Heisenberg coupled-chain systems with $n_c = 1$, 2, 3, and 4. We find that the $n_c = 2$ and $n_c = 4$ systems have a spin gap, while the $n_c = 1$ and $n_c = 3$ systems are gapless. Based on these results, we discuss how a variational RVB wave function, originally introduced by Liang *et al.* [10] to describe the 2D antiferromagnetic Heisenberg system, provides an intuitive picture for understanding the results and suggests behavior for larger n_c than can be studied numerically. We conclude that, indeed, all even n_c systems are spin liquids, and we give a simple explanation for the difference between even and odd n_c systems based on confinement of topological defects.

We consider the Heisenberg Hamiltonian

$$H = J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j \qquad (1)$$

defined on an $L \times n_c$ lattice with $S = \frac{1}{2}$. We will also consider the anisotropic system where the exchange along the chains is J and between the chains is J', but unless otherwise noted, $J' = J = 1$. We begin by calculating the spin gap Δ defined by

$$\Delta(L) = E_0(L, 1) - E_0(L, 0). \qquad (2)$$

Here $E_0(L, S_z)$ is the ground state energy for an $L \times n_c$ lattice with open boundary conditions and z component of total spin S_z. For a single chain we expect that the finite size corrections scale as L^{-1}, and we have plotted $\Delta(L)$ versus L^{-1} in Fig. 1 for $n_c = 1$–4. The solid curves are fits to the data of the form

$$\Delta(L) = \Delta + a_1 L^{-1} + a_2 L^{-2} + \cdots . \qquad (3)$$

For both $n_c = 1$ and $n_c = 3$, an accurate fit is obtained with $\Delta = 0$. For $n_c = 2$ and $n_c = 4$, the data are fit very well with $a_1 = 0$, which is the expected form for an $S = 1$ Heisenberg chain [11]. For $n_c = 2$, we find $\Delta = 0.504$, and for $n_c = 4$, we find $\Delta = 0.190$. The spin-spin correlation functions $\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle$ are shown in Fig. 2. Here, because of the open boundary conditions, we have chosen i and j so that they are as symmetrically located about the center of the lattice as possible. The semilog plot in the inset of Fig. 2(a) shows the exponential decay of the spin correlations for the two and four chain systems. The correlation length for $n_c = 2$ is $\xi = 3.19(1)$, and for $n_c = 4$, $\xi \sim 5$–6. The spin-spin correlations for $n_c = 3$ decay as a power law, similar to those for a single ($n_c = 1$) chain, as shown in the inset of Fig. 2(b).

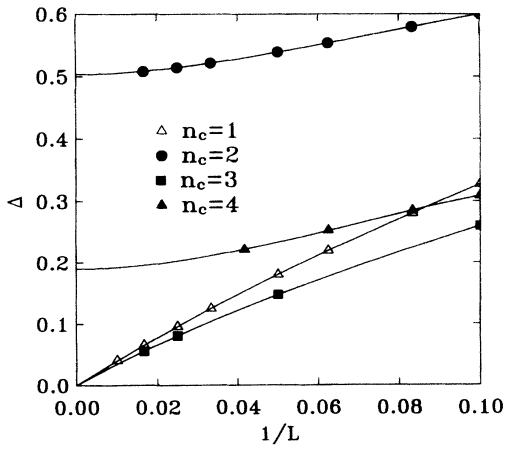

FIG. 1. Spin gaps as a function of system size L for open $L \times n_c$ coupled chain Heisenberg systems.

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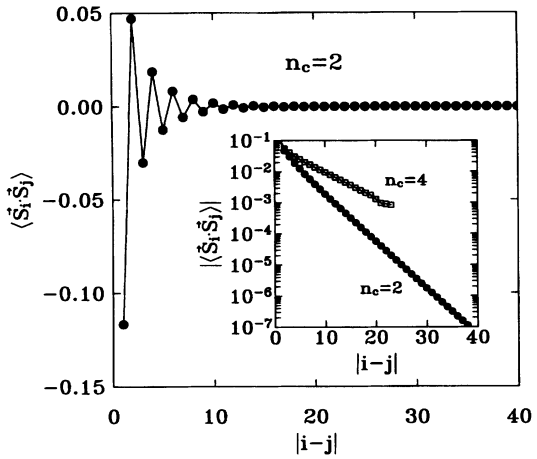
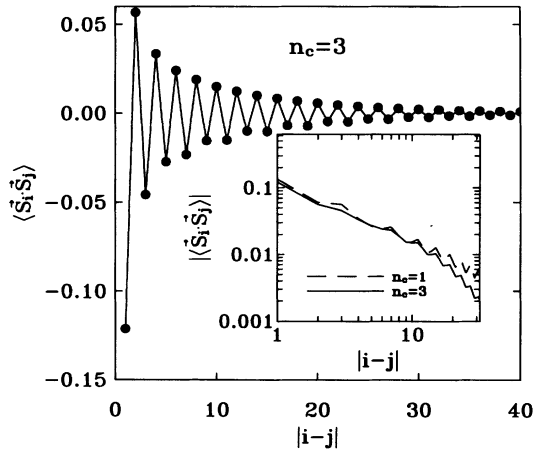


(a)



(b)

FIG. 2. Spin-spin correlations $\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle$ versus $|i - j|$ with i and j located on the top chain for (a) n_c even. The semilog plot in the inset shows the exponential decay of the correlations. (b) n_c odd. The log-log plot in the inset shows that the correlations for $n_c = 3$ and $n_c = 1$ decay with similar power laws. The deviation from pure power-law behavior visible for the largest values of $|i - j|$ is due to finite-size effects from the open boundaries.

The Lieb-Shultz-Mattis (LSM) theorem states that a half-integer spin chain, with a Hamiltonian that has local couplings and rotational and translational symmetry, either has gapless excitations or else has degenerate ground states. Affleck proved a similar statement for coupled spin chains with odd n_c [12]: An isotropic coupled-chain system with half-integer spin and a finite, odd number of chains either has gapless excitations or else has degenerate ground states. For even-n_c systems, the theorem does not apply.

Haldane's conjecture [13] that single Heisenberg spin chains containing integer spins have gaps, while those containing half-integer spins do not, has by now been fairly well established. This property of single chains undoubtedly helped prompt the suggestion that a similar property holds for coupled chains [6,7]: for odd n_c the spin gap vanishes, while for even n_c there is a spin gap. The generalized LSM theorem and our DMRG results for $n_c = 2$ and 4 provide strong support for this idea. To obtain a more intuitive picture, we examine an RVB variational wave function [14,15]. We consider both short-range and long-range RVB states and conclude that a short-range RVB picture applies for even n_c, whereas a long-range RVB picture describes systems with odd n_c.

The RVB states we consider are specific to bipartite lattices, and contain only bonds connecting one sublattice (A) to the other (B). We consider wave functions of the form [10]

$$|\psi\rangle = \sum_{\substack{i_\alpha \in A \\ j_\alpha \in B}} h(i_1 - j_1) \cdots h(i_n - j_n)\, (i_1 j_1) \cdots (i_n j_n)\,. \tag{4}$$

Here (ij) represents a singlet bond between sites i and j, and the non-negative bond amplitude h can be chosen variationally. We consider a short-range RVB wave function to be one with a bond amplitude $h(l)$ which decays exponentially in l or faster, while a long-range RVB wave function will typically have a power-law decay, $h(l) \sim l^{-p}$. The state with the shortest possible range is the dimer RVB state, for which $h(i - j) = 1$ for i and j nearest neighbors, and is zero otherwise.

We first consider the dimer wave function for the two-chain system. A valence bond configuration for this state is formed by drawing dimer bonds connecting pairs of adjacent sites, with every site part of one bond. The resonance between different valence bond configurations leads to a substantial lowering of the energy. The simplest and perhaps most important type of resonance consists of a square of four adjacent sites fluctuating between two adjacent vertical bonds and two adjacent horizontal bonds [15]. For a ladder system, there are two types of bond configurations, "resonating" and "staggered," as shown in Figs. 3(a) and 3(b), respectively. The staggered type of configuration is incapable of resonance, and thus has higher energy. It is possible to form a local region of staggered bond order only by placing soliton spin defects at the edges of the region, as shown in Fig. 3(c). Ignoring staggered configurations, the dimer ansatz gives an energy per site of –0.556 029 [16,17]. Compared with the essentially exact result from the DMRG calculations of –0.578 043 140, the simple dimer RVB energy differs by less than 4%. While the variational energy is reasonable, the spin-spin correlation length $\xi = 0.238\,012$ calculated with this dimer RVB state is more than an order of magnitude smaller than our DMRG result of $\xi = 3.19$. This implies that $h(l)$ has a larger range. However, as discussed for the 2D lattice in Ref. [10], as long as $h(l)$ falls off exponentially one finds an exponential decay of spin correlations and a spin gap.

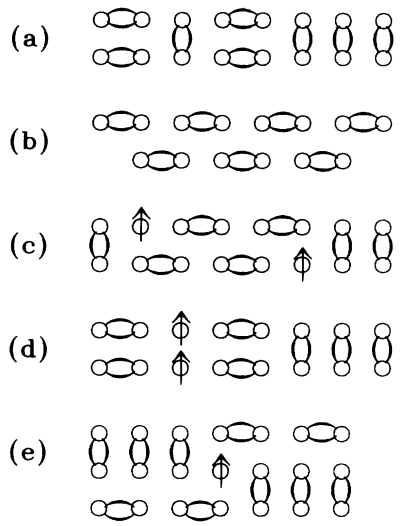


FIG. 3. Various dimer valence bond configurations, with and without topological spin defects present.

Although, as we have seen, the correlation length is poorly determined with the dimer RVB ansatz, a variety of qualitative features predicted by the ansatz are indeed present. For example, the variational state has a greater bond strength for interchain nearest-neighbor bonds compared to intrachain bonds [c.f. Fig. 4(b)]. Most importantly, within the short-range RVB picture one expects to find that pairs of topological spin defects are bound. We see from Fig. 3(c) that two spin defects produce a region of staggered bond order between them if they are separated. Furthermore, one expects from this picture that the pair of defects should reside predominantly on a single rung, as in Fig. 3(d), rather than on adjacent sites on a single chain, in order to maximize resonance. Each of these predictions is supported by the DMRG calculations.

If we remove one of the sites of the lattice from both the first and last rungs, as shown in Fig. 3(b), in order to *force* the system to have staggered bond order, we expect a topological spin defect to appear at each end to remove the staggering effect. The resulting spin defects are confined to the ends of the lattice, and are similar to the effective $S = \frac{1}{2}$ spins on the ends of open $S = 1$ chains [9,18]. As in that case, instead of an isolated ground state, we have a singlet and a triplet of states with a separation in energy which falls off exponentially with L. Figure 4 shows DMRG results for the local spin moment and nearest-neighbor bond strengths in the vicinity of a modified end of an $n_c = 2$ lattice. A localized spin defect is clearly present.

Now, it is possible to represent *any* singlet state as an RVB state [10], provided long-range singlet bonds are allowed. The crucial point in considering such an RVB representation is whether the amplitude for long-range bonds decays exponentially or algebraically, and if algebraically, with what exponent. Our DMRG results indicate that for the $n_c = 2$ and $n_c = 4$ systems the

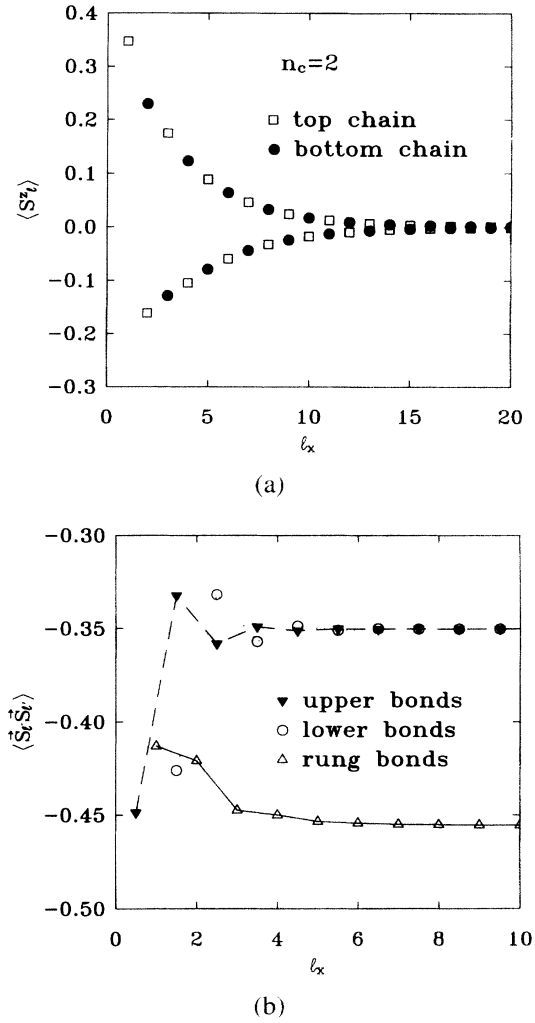


FIG. 4. One end of a long ($L = 50$) $n_c = 2$ chain with the first site of the bottom chain missing. A topological spin defect (an $S = \frac{1}{2}$ up spin) is trapped near the end of the chain. The defect "heals" the staggered bond order imposed by the modified chain end. In (a) we show the local magnetization, and in (b) we show the nearest-neighbor bond strengths.

universality class is that of the short-range RVB. The generalization of the LSM theorem, plus our results for $n_c = 3$, indicate that the universality class for odd n_c is the long-range RVB state.

What is the behavior for even $n_c > 4$, and why is there different behavior for odd and even n_c? We believe the answer to this can be understood in terms of the confinement of topological defects present within a dimer RVB state with even n_c. The confinement for $n_c = 2$ is represented in Fig. 3(c), and the lack of confinement for $n_c = 3$ is shown in Fig. 3(e). In general, for even n_c, the presence of a single defect puts the system into a generalized form of staggered order characterized by an odd number of bonds crossing any vertical line separating rungs. We expect that this staggered order, although still capable of resonance for $n_c \geq 4$, is higher in energy than

the "resonating" type of order. Thus defects are confined for an even number of chains, just as for the $n_c = 2$ case illustrated in Fig. 3(c). For odd n_c, there is only one type of order, characterized by an alternation as one moves along the chains of an odd number and an even number of bonds crossing a vertical line. A defect shifts the alternation by one lattice spacing, but with no cost in energy away from the defect.

The confinement of defects relates to the presence of long-range bonds in the ground state because a long-range bond can be considered to be a pair of separated topological defects. Thus considering a single long bond in a background of dimer bonds, we expect "confinement" of the long bond for even n_c; in other words, we expect it to be suppressed exponentially with the separation, since the energy difference grows linearly with the size of the staggered region. (In making this argument, we are allowing the region between the two sites connected by the long bond to resonate between different valence bond configurations, while holding the long bond fixed. The same conclusion is obtained if we instead consider the *number* of valence bond configurations which have such a long bond.) Note also that the presence of nondimer, but still short-ranged bonds does not heal the staggered order induced by the long-range bond. Such a short-range bond only heals the staggered order within the region of the bond. The presence of these short-range nondimer bonds can be considered as "dressing" the dimer state, lowering the energies of regions with resonant bond order and with staggered order, but not changing the result that the staggered-order region is higher in energy. If a sufficiently high density of nondimer bonds were present, the confinement picture might not be valid, but variational calculations for the 2D Heisenberg model show that even in long-range, low-energy RVB states, dimer bonds are much more probable than any other type of bond [10].

Since the characteristic size for this confinement mechanism is the system width n_c, we expect that for even n_c, the spin-spin correlation length varies as $\xi \sim n_c$, corresponding to a spin gap varying as $1/n_c$. For odd n_c, no confinement occurs, and the system is free to have long-range bonds. Although this, in itself, does not show that bond amplitudes decay as a power-law, both our numerical results and the generalization of the LSM theorem provide evidence that they do. The results suggest that in general, unless there is some mechanism to suppress long-range bonds, such as the confinement mechanism, we should expect power-law decay of bond amplitudes.

The confinement argument applies also to the anisotropic case, with $J' \neq J$. The most interesting case is $J' < J$. From our RVB picture we expect a gap to be present for all finite J'/J. As $J' \longrightarrow 0$, the number of vertical bonds decreases, and the difference in energy between the staggered and resonant types of bond configurations decreases. Nevertheless, the energy difference should be nonzero for all finite J', and confinement should cause exponential falloff of the bond amplitudes $h(l)$, giving exponential spin-spin correlations and a finite gap. We expect similar behavior for any system with an even number of chains. This prediction is in agreement with the conclusions for $n_c = 2$ of Strong and Millis [4] and the numerical evidence of Barnes *et al.* [5].

For even n_c, we expect that the confinement mechanism applies also to charge defects. In particular, for $n_c = 2$ we expect that a single hole will consist primarily of an empty site and a spin defect located on the same rung, in agreement with the results of Tsunetsugu *et al.* [19], for the t-J model. Similarly, two holes will be bound, and will primarily consist of two empty sites on the same rung. For odd n_c, the lack of confinement of long-range bonds does not necessarily imply spin-charge separation, although it does occur for $n_c = 1$.

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