Resonating Valence Bond Theory of Coupled Heisenberg Chains

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Abstract

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 \((\text{VO})_2\text{P}_2\text{O}_7\) \(^1\) and \(\text{Sr}_2\text{Cu}_4\text{O}_6\) \(^2\), 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 \(^3\)–\(^8\) 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 \(^4\)–\(^8\), and mean field treatments with Gutzwiller renormalization of the matrix elements have supported this conclusion. It has also been suggested that in contrast, systems with an odd number of chains \(n_c\) are gapless \(^7\)–\(^8\).

In this paper 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. Furthermore, Affleck’s generalization \(^10\) of the Lieb-Shultz-Mattis (LSM) theorem for coupled chain systems shows that all odd-\(n_c\) systems are gapless. Based on these results, we discuss how a variational RVB wave function, originally introduced by Liang et. al. \(^12\) 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 consider the Heisenberg Hamiltonian

\[
H = J \sum_{\langle i,j \rangle} S_i \cdot S_j
\]

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, \(J' = J\). We begin by calculating the spin gap \(\Delta\) defined by

\[
\Delta(L) = E_0(L, 1) - E_0(L, 0).
\]

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

$$\Delta(L) = \Delta + a_1 L^{-1} + a_2 L^{-2} + \ldots$$

(3)

For $n_c = 1$, we use $\Delta = 0$, $a_1 = 4.09$, $a_2 = -11.2$. For $n_c = 2$, the data is fit very well with $a_1 = 0$, which is the expected form for an $S = 1$ Heisenberg chain [13]: we find $\Delta = 0.5037$, $a_2 = 21.24$, $a_3 = -162.8$, $a_4 = 470.8$. For $n_c = 3$, we have $\Delta = 0$, $a_1 = 2.61$, $a_2 = 4.11$. For $n_c = 4$, we have $\Delta = 0.209$, $a_1 = 0$, $a_2 = 10.1$. The spin-spin correlation functions $\langle S_i \cdot S_j \rangle$ 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).

The 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 [10]: 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 [11] that single Heisenberg spin chains containing integer spins have gaps, while those containing half-integer spin do not, has by now been fairly well established. The inapplicability of the generalized LSM theorem for even-$n_c$ systems, and our DMRG results for $n_c = 2$ and 4 (along with other $n_c = 2$ results [3,4,11]) suggest that a similar statement may be true for coupled Heisenberg $S = \frac{1}{2}$ chain systems: for odd $n_c$ the spin gap vanishes, while for even $n_c$ there is a spin gap. To obtain a more intuitive picture, we examine an RVB variational wavefunction [17,18]. Previous descriptions of the spin-liquid state of the $n_c = 2$ ladder have used a mean field approach which represents spins in terms of bond
operators for the rungs \[8\]. Here, in contrast, we consider variational RVB wavefunctions for the ground state 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 \([12]\)

\[
|\psi\rangle = \sum_{i_\alpha \in A} \sum_{j_\alpha \in B} h(i_1 - j_1) \ldots h(i_n - j_n)(i_1 j_1) \ldots (i_n j_n),
\]

(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 wavefunction 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, \(h(l) \sim l^{-p}\).

For the \(n_c = 2\) system, we first consider a specific dimer RVB ansatz, such that \(h(i - j) = 1\) for \(i\) and \(j\) nearest neighbors, and is zero otherwise. A variety of properties of the system are qualitatively, although not quantitatively predicted by this simple variational state. Unlike the equivalent two-dimensional system \([12]\), where a Monte Carlo calculation is necessary, for the ladder the properties of the system can be calculated analytically. However, its most appealing feature is that many of its most important characteristics can be understood without the need of detailed calculations.

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 \([18]\). Consider the possible resonances for a ladder system. The two types of bond configurations, “resonating” and “staggered”, are shown in Fig. 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). Hence to lowest order the staggered bond configurations
can be ignored. We assume that all resonating configurations are equally likely, and the
ground state, within this variational estimate, is taken as the sum of all such configurations.
The properties of this state can be obtained using the loop-covering method developed by
Sutherland [14,12]. We use a recursion relation for the normalization of $\psi$ as a function of
the ladder length $L$; from this, we can find spin-spin correlation functions and the energy of
the system. The derivation will be published elsewhere. One obtains an average energy per
site of -0.556029. Compared with the essentially exact result from the DMRG calculations
of -0.578043140, the simple dimer RVB energy differs by less than 4%. While the variational
energy is reasonable, the spin-spin correlation length $\xi = 0.238012$ 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.
[12], as long as $h(l)$ falls off exponentially one finds an exponential decay of spin correlations
and a spin gap.

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 nearest-neighbor intrachain bonds. 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 [21,13]. 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 which contains one of these localized spin defects. Both the staggered bond order and localized spin defect are clearly visible. The greater bond strength for rung bonds in the center of the system is also apparent.

Now, it is possible to represent any singlet state as an RVB state \([12]\), provided long-range singlet bonds are allowed. (In order to represent any singlet state, Eq. (2) must be generalized somewhat. Nevertheless, Eq. (2) has been shown to work extremely well for the ground state of the 2D system \([12]\).) In 2D, even when the probability amplitude of a long-range bond decays as a power-law with the separation, one can still obtain a finite staggered magnetization, provided the power is sufficiently small \([12]\). For a finite number of coupled chains, however, it seems more likely that power law decay of bond amplitudes always gives power law decay of spin-spin correlations. 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 universality class is that of the short-range RVB, i.e. exponential decay of bond amplitudes. For quantitative results from the variational state, we expect that we must include some longer bonds and optimize over the bond amplitudes, but for qualitative results, the dimer state is adequate. 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) \cite{21}. 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 non-dimer, 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 non-dimer 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 non-dimer 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 \cite{12}. Thus it appears that this confinement mechanism is very effective at suppressing long-range bonds.

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
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 $J' \to 0$, 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]. In addition, using the DMRG method, we have calculated the gap as a function of system length $L$ for $J' = 0.1$, $J = 1$, and $n_c = 2$ for $L$ as large as 100. We find a gap of 0.05988 for the infinite system.

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. [22], 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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FIGURES

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

FIG. 2. Spin-spin correlations $\langle S_i \cdot S_j \rangle$ 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.

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

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.
Fig. 1

White, Noack, and Scalapino
Fig. 2(a)

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Fig. 2(b)

White, Noack, and Scalapino
Fig. 3

White, Noack, and Scalapino
Fig. 4(a)

White, Noack, and Scalapino
Fig. 4(b)

White, Noack, and Scalapino