An Impurity Driven Phase Transition in the Antiferromagnetic Spin-1 Chain

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Abstract

Using an asymptotically exact real space renormalization procedure, we find that the Heisenberg antiferromagnetic spin-1 chain undergoes an impurity driven second order phase transition from the Haldane phase to the random singlet phase, as the bond distribution is broadened. In the Haldane phase and near the critical point, there is a Griffiths region in which the gap is filled and the susceptibility diverges in a non-universal manner. The correlation length critical exponent is $\nu \approx 2.3$.

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Recently, there has been tremendous interest in the antiferromagnetic (AF) spin-1 chain, inspired by the famous conjecture by Haldane [1] that integer-spin chains behave quite differently from half-odd-integer-spin chains. For example, in the absence of disorder, the spin-1 chain has short-range spin-spin correlations in the ground state and an excitation gap [1] whereas the spin-1/2 chain is critical. The ground state of the spin-1 chain also has a novel string-topological order [2]. Some of these results have been experimentally confirmed [3].

Randomness is always present in real materials. Theoretical work has demonstrated that randomness dramatically affects the physical properties of the AF spin-1/2 chain [4,5] and other random one-dimensional magnetic systems [6–9]. In this letter we report a systematic theoretical study on the effects of bond randomness on the AF spin-1 chain, based on the real space renormalization group scheme developed by Ma et al. [4] (see also Ref. [10]) and extended by Fisher [5].

Our main result is that in the presence of bond randomness, there are two distinct phases in the AF Heisenberg spin-1 chain, separated by a second order critical point. The nature of these two phases are described below.

The ground state in the Haldane phase in the absence of randomness is well described by the valence bond solid (VBS) state [11]. In the VBS state each spin-1 is composed of two symmetrized spin-1/2 objects. The spin-1/2 objects form singlets with spin-1/2 objects on neighboring sites. This state resembles the ground state of a dimerized spin-1/2 chain. The ground state is nondegenerate, there is an excitation gap, as well as a very stable topological structure. Thus we expect the Haldane phase and its topological structure to be stable against weak bond randomness [8]. On the other hand, when the randomness is strong and the distribution of bond strength is broad, the original spin-1 objects coupled by strong bonds form inert singlet pairs and generate effective further neighbor AF couplings. An asymptotically exact real space renormalization group (RG) analysis [4,5] shows that in this case the system flows toward a random singlet (RS) phase [5] with universal thermodynamic properties and power law behavior in averaged spin-spin correlations. In order to study the
transition from the Haldane phase to the random singlet (RS) phase, we have extended this RG scheme so that it may be used in both phases. We find the transition between these two phases is second order. The extended RG scheme becomes asymptotically exact in the low energy limit at the critical point, as well as in the RS phase. Thus we are able to extract exact information about the critical point. For examples, we find as the randomness strength approaches the critical point from the Haldane phase, the average spin-spin correlation length diverges in a power law manner with exponent \( \nu = \frac{6}{\sqrt{13} - 1} \approx 2.3 \). The string-topological order parameter vanishes with a power law exponent \( \gamma = 2\nu \approx 4.6 \).

Consider the Hamiltonian

\[
H = \sum_i J_i \mathbf{S}_i \cdot \mathbf{S}_{i+1},
\]

where \( \mathbf{S}_i \) are spin-S operators and \( J_i \) are random coupling constants (assumed positive unless otherwise specified). Let us begin with the case that randomness is strong and the width of the distribution of \( J \) is very broad (on a logarithmic scale). In this case we can use the decimation renormalization group procedure developed by Ma, Dasgupta, and Hu [4] (MDH) for the special case of \( S = 1/2 \). We first pick the largest bond in the system, say \( J_2 \) between spins 2 and 3. Since this is such a strong bond, and the width of the bond distribution is broad, bonds \( J_1 \) and \( J_3 \) will likely be much weaker than \( J_2 \). Thus to lowest order in \( J_1 \) and \( J_3 \), spins 2 and 3 form a singlet pair and become unimportant at low energies (on scales much smaller than \( J_2 \)). The major physical effect of the existence of spins 2 and 3 is to generate an induced coupling between neighboring spins 1 and 4. \( \tilde{H}_{1-4} = \tilde{J}_{14} \mathbf{S}_1 \cdot \mathbf{S}_4 \) where \( \tilde{J}_{14} = \frac{2}{3} S(S + 1) J_1 J_3 / J_2 + O(1/J_2^2) \). This formula is correct even if \( J_1 \) and/or \( J_3 \) are ferromagnetic (F) as long as their magnitude is much less than \( J_2 \). The generated bond is typically much weaker than all three original bonds. Thus the effect of this decimation procedure is to get rid of the strongest bond (and also its two neighbors) in the system, generate a weaker bond between the spins neighboring the decimated ones, and lower the overall energy scale. Fisher [5] has shown rigorously that as one proceeds with the RG scheme the width of bond distribution broadens and the accuracy of the procedure improves.
as the energy scale is lowered. It becomes *asymptotically exact* in the long-distance, low-energy limit where the bond distribution flows toward an energy scale dependent stable fixed point distribution. Fisher names the phase characterized by this universal bond distribution the random singlet (RS) phase. Thus in the presence of strong enough bond randomness, a spin-$S$ Heisenberg AF chain will be in the RS phase, irrespective of the size of $S$ and independent of $S$ being an integer or a half-odd-integer.

The above real space RG procedure may not be accurate when the initial bond distribution is not very broad. In this case there is a finite probability that $J_1$ and/or $J_3$ is of similar strength as $J_2$, in which case the lowest order perturbation is not sufficient. What one needs to do in this case is to pick the segment in the chain in which all spins are coupled by strong bonds (while the segment itself is only weakly coupled to the rest of the chain), solve the spectrum of the segment, and keep only the low energy states, and consider their coupling to the rest of the chain. In the case of a spin-1/2 chain, the ground state for a segment is either a singlet (for even segments) or a doublet (for odd segments), which are separated from higher energy states by a gap. In the former case the segment will be inert, and merely mediates a weak effective AF coupling between the two spins neighboring the segment, while in the latter case the segment may be modeled by an effective spin-1/2 at low energy which is coupled to the rest of the chain antiferromagnetically. Thus the structure of the RG scheme remains the same as the MDH procedure, even if greater care is necessary in the beginning. It is therefore believed that the RS phase correctly describes the long-distance, low-energy physics of the spin-1/2 chain, even if there is only *weak* randomness.

The situation is very different in the case of the spin-1 chain. For a finite segment of the spin-1 chain with no disorder, there are two effective *half* spins localized near the two edges of the segment, and the coupling between them is $g(l) \sim (-1)^l J a^l$, where $l$ is the length of the segment and $a < 1$. Thus the coupling between the two half spins in the same segment may be either ferromagnetic or antiferromagnetic, and decays *exponentially* with the length of the segment. The coupling of an edge spin to the rest of the chain, however, remains antiferromagnetic. The low energy states of a segment are the singlet
and triplet states formed by these two edge spins (and both of them must be kept); other
states will be separated from them by the Haldane gap of order $J$. We expect this scenario
to remain correct even when there is weak randomness in the bond strength in such finite
segments. Thus even though the spin chain is composed of spin-1 objects, the effective
degrees of freedom at low energies are actually half spins. This is also true when there is
no randomness. The valence bond solid state is also composed of half spins. We may
describe the low energy physics of a random spin-1 chain using an an effective Hamiltonian
in terms of these half spins, with the following structure: the chain consists of half spins only;
the even bonds are taken from an antiferromagnetic bond distribution, and odd bonds are
taken from a distribution containing antiferromagnetic and ferromagnetic bonds. Physically
the even bonds are couplings between edge half spins of neighboring segments (which are
always AF), and odd bonds are the coupling between edge spin in the same segment. Such
a effective description is particularly accurate for the special case of a spin-1 chain with a
bimodal bond distribution: most of the bonds are of strength $J$, while a small but finite
fraction of bonds have a much smaller strength $J'$. In this case the system can indeed be
viewed as a collection of weakly coupled segments of uniform chains. The couplings between
edge half spins are random because the length of the segments are random. We believe this
model correctly describes the long-distance, low-energy physics of a random spin-1 chain.
In particular, the original spin-1 Hamiltonian may be recovered by setting all odd bonds
strongly ferromagnetic.

To study this model, we develop an extended version of the MDH real space renormal-
ization scheme, which properly accounts for strong ferromagnetic bonds. In our scheme, at
any stage of RG, the energy scale $\Omega$ is set by the strongest antiferromagnetic bond in the
system. All even bonds, which are all AF, will be weaker than $\Omega$. We separate the odd
bonds, which can be either F or AF, into two groups: group A consists of all AF bonds and
those F bonds that are weaker than $\Omega$, while group B consists of F bonds that are stronger
than $\Omega$. The new spin decimation procedure works in the following way. Find the strongest
AF bond in the system, say $J_i$. If $i$ is odd, then its neighbors are both weaker AF bonds.
We just follow the usual MDH decimation procedure. If \( i \) is even and both neighbors belong to group A we can again follow the MDH decimation procedure. If one of the bonds, say \( J_{i+1} \), belongs to group B, we solve the 3-spin cluster problem of \( S_i, S_{i+1} \) and \( S_{i+2} \), and keep the low energy states, which are a doublet. The doublet may be modeled by a new spin-1/2, which couples to the rest of the chain. If both neighbors of \( J_i \) belong to group B, we solve the 4-spin cluster including spin \( i-1, i, i+1 \) and \( i+2 \). The ground state is a singlet, with an excitation gap of order \( J_i \). Thus it drops out at low energy and mediates an effective AF coupling between spins \( i-2 \) and \( i+3 \). It is easy to show that this procedure keeps the original structure of the system; i.e., even bonds AF and odd bonds F or AF.

The flow equations for the distributions of bonds in this approximate RG scheme are

\[
\frac{-dP_e(J, \Omega)}{d\Omega} = \left[ P_o(\Omega, \Omega) + N^2(\Omega)P_e(\Omega, \Omega) \right] \\
\cdot \int_{-\Omega}^{\Omega} dJ_1 P_e(J_1, \Omega) \int_{-\Omega}^{\Omega} dJ_2 P_e(J_2, \Omega) \delta \left( J - \frac{J_1 J_2}{\Omega} \right) \\
+ \left[ P_e(\Omega, \Omega)(1 - N^2(\Omega)) - P_o(\Omega, \Omega) \right] P_e(J) \\
- \delta(\Omega - J)P_e(\Omega, \Omega), \quad (2)
\]

\[
\frac{-dP_o(J, \Omega)}{d\Omega} = P_e(\Omega, \Omega) \int_{-\Omega}^{\Omega} dJ_1 P_o(J_1, \Omega) \\
\cdot \int_{-\Omega}^{\Omega} dJ_2 P_o(J_2, \Omega) \delta \left( J - \frac{J_1 J_2}{\Omega} \right) \\
- \delta(\Omega - J)P_o(\Omega, \Omega) + 2P_e(\Omega, \Omega)N(\Omega)P_o(-J, \Omega) \\
+ \left[ P_o(\Omega, \Omega) - P_e(\Omega, \Omega)(1 - N^2(\Omega)) \right] P_o(J), \quad (3)
\]

\[
\frac{-dN(\Omega)}{d\Omega} = \left[ P_o(\Omega, \Omega) - P_e(\Omega, \Omega)(1 - N^2(\Omega)) \right] N(\Omega) \\
+ P_o(-\Omega, \Omega). \quad (4)
\]

Here \( P_e(J, \Omega) \) is the (normalized) probability distribution of even bonds with \( \Omega > J > 0 \), \( P_o(J, \Omega) \) is the probability distribution of odd bonds with \( \Omega > J > -\Omega \), and \( N(\Omega) \) is the fraction of odd bonds that are strongly ferromagnetic \( J < -\Omega \). \( P_o(J, \Omega) \) and \( N(\Omega) \) are related by the normalization condition \( \int_{-\Omega}^{\Omega} dJ P_o(J, \Omega) + N(\Omega) = 1 \). Anticipating that the
bond distribution will become very broad in the low energy limit, we have neglected factors of order 1 in the strength of generated bonds. They become irrelevant in the asymptotic limit \[5\]. We have also assumed that the ferromagnetic bonds that are stronger than \(\Omega\) are much stronger than \(\Omega\), so that two spin-1/2 objects connected by a strong ferromagnetic bond form a spin-1 object. Again this assumption is valid in the asymptotic limit \((\Omega \to 0)\), and simplifies the solution of clusters including strong F bonds.

The density, \(\rho(\Omega)\), of spins that have not yet paired into singlets at scale \(\Omega\) satisfies

\[
-\frac{d\rho(\Omega)}{d\Omega} = - \left\{ P_e(\Omega, \Omega) \left[ 1 + N^2(\Omega) \right] + P_o(\Omega, \Omega) \right\} \rho(\Omega).
\]

(5)

These spins are essentially free at temperatures that are higher than \(\Omega\). All thermodynamic quantities can be determined from \(\rho(\Omega)\) \[5,14,15\].

It is natural to combine the distributions in the following way

\[
Q_+(J, \Omega) = \frac{1}{1 - N(\Omega)} [P_o(J, \Omega) + P_o(-J, \Omega)],
\]

\[
P_-(J, \Omega) = P_o(J, \Omega) - P_o(-J, \Omega),
\]

(6)

so that \(Q_+(J, \Omega)\) is normalized. We find that fixed point solutions to the flow equations are power laws \(P_e(x) = P e^{-Px}\) and \(Q_+(x) = Q e^{-Qx}\) where \(x = \log(\Omega/J)\) and \(P_+ = 0\) \[14,15\]. The variables \(P, Q, N,\) and \(\rho\) obey

\[
\frac{dP}{d\Gamma} = -N^2P^2 - \frac{(1 - N)}{2}QP \\
\frac{dQ}{d\Gamma} = -(1 - N)QP \\
\frac{dN}{d\Gamma} = (1 - N^2)(\frac{Q}{2} - NP) \\
\frac{d\rho}{d\Gamma} = -[(1 + N^2)P + \frac{1 - N}{2}Q]\rho,
\]

(7)

where \(\Gamma = \log(\Omega_i/\Omega)\) (\(\Omega_i\) is the initial cutoff of AF bonds). We find there are two classes of stable fixed points, corresponding to two stable phases. They are the random singlet phase \((P = \Gamma^{-1}, Q = Q_0, N = 1, \rho \propto \Gamma^{-2})\), and the Haldane phase \((P = P_0, Q = 0, N = 0, \rho \propto \Omega^{P_0}\), where \(0 < P_0 < 1\) is a nonuniversal number). There is also an unstable fixed
point (near which there is a single relevant operator): \( (P = Q = 2\Gamma^{-1}, N = \frac{1}{2}, \rho \propto \Gamma^{-3}) \). It describes the critical point. In the following we describes the physical nature of these fixed points.

In the random singlet phase, all the odd bonds become F bonds much stronger than the AF even bonds. All the spin-1/2’s are ferromagnetically combined into spin-1’s. The spin-1’s then couple into singlets over all length scales. The ground state and thermodynamic properties are the same as for the spin-1/2 random singlet state studied previously [4,5]. The disorder averaged spin-spin correlation function \( C(r) \) decays as \( r^{-2} \), and the susceptibility take the universal form in the low temperature limit: \( \chi \sim [T \log^2 T]^{-1} \). There is no gap because the bond distribution has weight at \( J = 0 \).

In the Haldane phase all odd bonds (F and AF) become much weaker than the even bonds, only spin-1/2’s remain in the system and they form singlets only over even bonds. The system may be viewed as a set of uncoupled dimers. The spin-spin correlations decay exponentially with a finite correlation length. There is also long range string-topological order [8]. This phase is analogous to the random dimer phase in random dimerized AF spin-1/2 chains [8] and the ground state resembles the valence bond solid state. The flow equations describe the Griffiths region of the Haldane phase where there is no gap and the susceptibility diverges as a power law with a nonuniversal exponent \( \chi \sim T^{-(1-P_0)} \). The flow equations are only valid when the disorder is broad, and so can not describe the crossover from gapped to gapless behavior within the Haldane phase as the randomness is increased.

To determine critical exponents we consider small perturbations near the unstable fixed point:

\[
\begin{align*}
P &= \frac{2}{\Gamma}(1 + \delta_P \Gamma^\lambda) \\
Q &= \frac{2}{\Gamma}(1 + \delta_Q \Gamma^\lambda) \\
N &= \frac{1}{2}(1 + \delta_N \Gamma^\lambda)
\end{align*}
\]

and expand the flow equations to linear order in \( \delta \). There are two irrelevant perturbations \( (\lambda = -1, \lambda = \frac{-1+\sqrt{13}}{2}) \) and one relevant perturbation \( (\lambda_+ = \frac{-1+\sqrt{13}}{2}) \). For relevant flows, if
\( \delta_n > 0 \), the odd bonds are stronger than the even bonds, the density of spin-1’s is increasing, and the system flows to the random singlet fixed point. If \( \delta_n < 0 \) the even bonds are stronger than the odd bonds, the density of spin-1’s is decreasing, and the system flows to the random Haldane phase. The crossover from critical to Haldane behavior occurs at the energy scale where \( \delta \Gamma^\lambda \approx 1 \). The energy scale at which this occurs is \( \Gamma_0 = \delta^{- \frac{3}{\lambda_+}} \). The density of spins at this scale is \( \rho_0 = \Gamma_0^{-3} \), so the correlation length is \( \xi \approx \rho_0^{-1} = \delta^{-\nu} \) where \( \nu = \frac{3}{\lambda_+} \approx 2.3 \).

Following the same analysis as in Ref. [8], the string-topological order parameter defined as

\[
T = \lim_{j-i \to \infty} \langle \Psi_0 \left| S_i^z \exp \left[ i\pi \sum_{i<k<j} S_k^z \right] S_j^z \right| \Psi_0 \rangle, \tag{9}
\]

scales as \( T \propto (-\delta_n)^{2\nu} \), in the Haldane phase near the critical point. Just like the RS fixed point for the spin-1/2 chain [3], the bond distributions become infinitely broad on a logarithmic scale. Thus our scheme becomes asymptotically exact at the critical point, and the critical exponents we find here are exact.

Before closing we briefly discuss relations between the present work and some existing papers. Our model is related, but different from that studied by Westerberg et al. [7]. In their model, ferromagnetic bonds may appear in both even and odd bonds, and spins of arbitrarily large size appear at low energy. The special topological structure of our model prevents this from happening in the present system. Boechat et al. [16] also anticipated the existence of a random singlet phase for strong randomness. As in our previous work [4], they also find spontaneously dimerized chains are unstable against weak randomness. They did not, however, address the weak randomness regime of the spin-1 chain, and the phase transition that we discuss here. The correlation length exponent \( \nu \approx 2.3 \) we find here is extremely close to that of the delocalization transition in integer quantum Hall systems. Lee [17] showed that the integer quantum Hall transition may be mapped onto the dimerization transition in the pure SU(0) spin chain. It is unclear at this stage, whether this is merely a coincidence, or there exists a fundamental physical reason, that these two apparently different transitions have the same critical exponent.
To summarize, in this letter we determined the critical properties of the randomness driven phase transition of the spin-1 chain. For weak randomness, the spin-1 chain is in the Haldane phase and the ground state resembles the valence bond solid state. The ground state has topological order, spin-spin correlations decays exponentially and there is a gap to the excited states. For broader distributions the gap is filled in and the correlation length increases but the topological order persists. Eventually the critical point is reached and the correlation length diverges. The correlation length exponent is $\nu = \frac{6}{\sqrt{13} - 1} \approx 2.3$. Beyond the critical point the topological order is zero, the disorder averaged spin-spin correlations decay algebraically, and the ground state resembles the random singlet state.

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REFERENCES

[1] F. D. M. Haldane, Phys. Lett. 93A, 464 (1983); Phys. Rev. Lett. 50, 1153 (1983).

[2] K. Rommelse and M. den Nijs, Phys. Rev. Lett 59, 2578 (1987); S. M. Girvin and D. P. Arovas, Phys. Scr. T27, 156 (1988).

[3] J. P. Renard, M. Verdaguer, L. P. Regnault, W. A. C. Erklens, J. Rossat-Mignod, W. G. Stirling, Europhys. Lett., 3, 945 (1987); J. P. Renard, L. P. Regnault, M. Verdaguer, J. Phys. C, 8, 1425 (1988).

[4] S. K. Ma, C. Dasgupta and C-K Hu, Phys. Rev. Lett. 43, 1434 (1979); C. Dasgupta and S. K. Ma, Phys. Rev. B 22, 1305 (1979).

[5] D. S. Fisher, Phys. Rev. B 50, 3799 (1994).

[6] D. S. Fisher, Phys. Rev. B 51, 6411 (1995).

[7] E. Westerberg, A. Furusaki, M. Sigrist, and P. A. Lee, Phys. Rev. Lett. 75, 4032 (1995); A. Furusaki et al., Phys. Rev. Lett. 73, 2622 (1994).

[8] R. A. Hyman, Kun Yang, R. N. Bhatt, and S. M. Girvin, Phys. Rev. Lett. 76, 839 (1996).

[9] Kun Yang, R. A. Hyman, R. N. Bhatt, and S. M. Girvin, J. Appl. Phys. 79, 5096 (1996).

[10] R. N. Bhatt and P. A. Lee, Phys. Rev. Lett. 48, 344 (1982); R. N. Bhatt, Phys. Scr. T14, 7 (1986).

[11] I. Affleck, T. Kennedy, E. H. Lieb and H. Tasaki, Phys. Rev. Lett., 59, 799 (1987)

[12] M. Hagiwara, K. Katsumata, Ian Affleck, B.I. Halperin, and J.P Renard, Phys. Rev. Lett. 65, 3181 (1990).

[13] K. Hida, Phys. Rev. B 45, 2207 (1992).

[14] R.A. Hyman, Random Antiferromagnetic Spin Chains, Ph.D. dissertation, Indiana Uni-
versity (1996).

[15] R.A. Hyman, unpublished.

[16] Beatriz Boechat, Andreia Saguia, and Mucio A. Continentino, preprint cond-mat/9602013.

[17] Dung-Hai Lee, Phys. Rev. B 50, 10788 (1994).