Impurity Driven Phase Transition in the Antiferromagnetic Spin-1 Chain

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(Received 7 August 1996)

We study the random antiferromagnetic spin-1 chain by mapping to a random dimerized spin-1/2 chain with antiferromagnetic and ferromagnetic bonds and applying an asymptotically exact real space renormalization procedure. We find that the chain undergoes an impurity driven second order phase transition from the Haldane phase to the random singlet phase as the bond distribution broadens. In the Haldane phase and near the critical point, there is a Griffiths region in which the excitation gap is filled and the magnetic susceptibility diverges in a nonuniversal manner. The correlation length critical exponent is $\nu \approx 2.3$. [S0031-9007(97)02482-4]

PACS numbers: 75.10.Jm, 75.30.Hx, 75.50.Ee

Recently there has been tremendous interest in the antiferromagnetic (AF) spin-1 chain, inspired by Haldane's famous conjecture [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]. This Letter reports a systematic theoretical study of the effects of bond randomness on the AF spin-1 chain. We map the random antiferromagnetic spin-1 chain to a random dimerized spin-1/2 chain with antiferromagnetic and ferromagnetic bonds and extend the real space renormalization group procedure developed by Ma *et al.* [4] (see also Ref. [10]) and Fisher [5]. In the absence of randomness, the connection between a spin-1 chain and a dimerized spin-1/2 chain was demonstrated by Hida [11] who showed the equivalence of dimer order in terms of spin-1/2 variables and string order in terms of spin-1 variables.

We find that in the presence of bond randomness, two distinct phases in the AF Heisenberg spin-1 chain are separated by a quantum critical point. The nature of these two phases is described below. In the absence of randomness, the Haldane phase ground state has a large overlap with the valence bond solid (VBS) state [12] in which each spin-1 is composed of two symmetrized spin-1/2 objects which form singlets with spin-1/2 objects on neighboring sites. The VBS state resembles the ground state of a dimerized spin-1/2 chain. Both ground states are nondegenerate, have excitation gaps, and have very stable topological structure. Thus we expect the Haldane phase and its topological structure to be *stable* against weak bond randomness [8]. Alternatively, when randomness is strong and the distribution of bond strengths is broad, 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 [4,5,13] 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 extend 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 near the critical point and in the RS phase. Thus we are able to extract *exact* information about the critical point. For example, 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 $2\nu/3 \approx 1.5$.

Consider the Hamiltonian

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

where $\mathbf{S}_i$ are spin-S operators and J_i are random coupling constants (assumed positive unless otherwise specified). When randomness is strong and the width of the distribution of J is very broad (on a logarithmic scale), we can use the decimation renormalization group procedure developed by Ma, Dasgupta, and Hu (MDH) [4] for the special case of $S = 1/2$. We first pick the strongest bond in the system, say, J_2 between spins 2 and 3. Since the bond distribution is broad, bonds J_1 and J_3 will typically 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 $\tilde{J}_{14} = \frac{2}{3}S(S+1)J_1J_3/J_2 + O(1/J_2^2)$. 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 MDH procedure eliminates the strongest bond (and also its two neighbors) in the system, generates a weaker bond between the spins neighboring the decimated ones, and lowers the overall energy scale. Fisher [5] has shown rigorously that as one proceeds with the MDH renormalization the bond distribution broadens and the accuracy of the approximation improves as the energy scale is lowered. It becomes *asymptotically exact* in the long-distance, low-energy limit where the bond distribution flows toward a stable-fixed-point distribution which is energy-scale dependent. Fisher names the phase characterized by this universal bond distribution the random singlet (RS) phase. Thus, in the presence of sufficiently strong bond randomness, a spin-S Heisenberg AF chain will be in the RS phase for integer or half-odd-integer S and irrespective of the size of S.

When there is a finite probability that J_1 and/or J_3 is of similar strength as J_2, the lowest order perturbation is not sufficient. In this case, one must choose the segment of the chain in which all spins are coupled by strong bonds, solve the spectrum of that segment, and keep only the low-energy states. These states are then represented by effective spins which are coupled 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) and is separated from higher-energy states by a gap. In the former case the segment is inert and merely mediates a weak effective AF coupling between the two spins neighboring the segment, while in the latter case the segment is modeled by an effective spin-1/2 at low energy, which is antiferromagnetically coupled to the rest of the chain. The structure of the RG scheme remains the same as the MDH procedure, even if greater care is necessary in the beginning. Thus the RS phase correctly describes the long-distance, low-energy physics of the spin-1/2 chain, even if there is only *weak* randomness [5].

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, two effective *half* spins are 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 $a < 1$ [14]. Thus coupling between the two half spins may be 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 singlet and triplet states formed by the two edge spins are the lowest-energy states of the segment and are separated from higher-energy states by the Haldane gap of order J. This scenario remains correct when there is weak bond randomness. Thus even though the spin chain is composed of spin-1 objects, the *effective* degrees of freedom at low energies are actually half spins. The low-energy physics of a random spin-1 chain may be described by a Hamiltonian with the following structure: the chain consists of half spins *only*; 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. This 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 finite fraction have a much smaller strength J'. In this case the system can 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 [11].

We study this model using an extended MDH procedure, which properly accounts for strong ferromagnetic bonds. At any stage of RG, the energy scale Ω is set by the strongest *antiferromagnetic* bond in the system. We separate the odd bonds into two groups: group A consists of all AF bonds and those F bonds that are weaker than Ω, while group B consists of F bonds that are stronger than Ω. The extended MDH 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 and the MDH procedure is followed. If i is even and both neighbors belong to group A we again follow the MDH 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 so these spins drop out at low energy and mediate an effective AF coupling between spins $i-2$ and $i+3$. The extended MDH procedure keeps the original structure of the system; i.e., even bonds are AF and odd bonds are F or AF.

The flow equations for the distributions of bonds in the extended MDH procedure are

$$-\frac{dP_e(J,\Omega)}{d\Omega} = [P_0(\Omega,\Omega) + N^2(\Omega)P_e(\Omega,\Omega)]\int_0^\Omega dJ_1 P_e(J_1,\Omega)\int_0^\Omega dJ_2 P_e(J_2,\Omega)\delta\left(J - \frac{J_1J_2}{\Omega}\right) + \{P_e(\Omega,\Omega)[1 - N^2(\Omega)] - P_0(\Omega,\Omega)\}P_e(J) - \delta(\Omega - J)P_e(\Omega,\Omega), \quad (2)$$

$$-\frac{dP_0(J,\Omega)}{d\Omega} = P_e(\Omega,\Omega)\int_{-\Omega}^\Omega dJ_1 P_0(J_1,\Omega)\int_{-\Omega}^\Omega dJ_2 P_0(J_2,\Omega)\delta\left(J - \frac{J_1J_2}{\Omega}\right) - \delta(\Omega - J)P_0(\Omega,\Omega) + 2P_e(\Omega,\Omega)N(\Omega)P_0(-J,\Omega) + \{P_0(\Omega,\Omega) - P_e(\Omega,\Omega)[1 - N^2(\Omega)]\}P_0(J), \quad (3)$$

$$-\frac{dN(\Omega)}{d\Omega} = \{P_0(\Omega,\Omega) - P_e(\Omega,\Omega)[1 - N^2(\Omega)]\}N(\Omega) + P_0(-\Omega,\Omega). \quad (4)$$

Here $P_e(J,\Omega)$ is the normalized probability distribution of even bonds with $\Omega > J > 0$, $P_0(J,\Omega)$ is the probability distribution of odd bonds with $\Omega > J > -\Omega$, and $N(\Omega)$ is the fraction of odd bonds that are strongly ferromagnetic $J < -\Omega$. $P_0(J,\Omega)$ and $N(\Omega)$ are related by the normalization condition $\int_{-\Omega}^{\Omega} dJ P_0(J,\Omega) + N(\Omega) = 1$. Since the bond distribution becomes very broad in the low-energy limit, we neglected factors of order 1 in the strength of generated bonds, which become irrelevant in the asymptotic limit [5]. We also assume that ferromagnetic bonds stronger than Ω are *much* stronger than Ω, 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 unpaired spins at scale Ω satisfies

$$-\frac{d\rho(\Omega)}{d\Omega} = -\{P_e(\Omega,\Omega)[1 + N^2(\Omega)] + P_0(\Omega,\Omega)\} \times \rho(\Omega). \quad (5)$$

These spins are essentially free at temperatures higher than Ω. All thermodynamic quantities can be determined from $\rho(\Omega)$ [5,15,16].

Using the combined distributions

$$Q_+(J,\Omega) = \frac{1}{1 - N(\Omega)}[P_0(J,\Omega) + P_0(-J,\Omega)], \qquad P_-(J,\Omega) = P_0(J,\Omega) - P_0(-J,\Omega), \quad (6)$$

the fixed point solutions to the flow equations are power laws in J with $P_e(x) = Pe^{-Px}$ and $Q_+(x) = Qe^{-Qx}$, where $P_- = 0$ and a Jacobi transformation has been made to the variable $x = \ln(\Omega/J)$ [15,16]. The variables P, Q, N, and ρ obey

$$\frac{dP}{d\Gamma} = -N^2P^2 - \frac{(1 - N)}{2}QP, \qquad \frac{dQ}{d\Gamma} = -(1 - N)QP, \qquad \frac{dN}{d\Gamma} = (1 - N^2)\left(\frac{Q}{2} - NP\right), \qquad \frac{d\rho}{d\Gamma} = -\left[(1 + N^2)P + \frac{1 - N}{2}Q\right]\rho, \quad (7)$$

where $\Gamma = \ln(\Omega_i/\Omega)$ (Ω_i is the initial cutoff of AF bonds). Two classes of stable fixed points correspond 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). The solution at the critical point is ($P = Q = 2\Gamma^{-1}$, $N = \frac{1}{2}$, $\rho \propto \Gamma^{-3}$). In the following we describe the physical nature of these phases.

In the random singlet phase, the odd bonds are F bonds much stronger than the AF even bonds. The spin-1/2's are ferromagnetically combined into spin-1's, which are coupled 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 takes the universal form in the low temperature limit: $\chi \sim [T\ln^2 T]^{-1}$. 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 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 do 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:

$$P = \frac{2}{\Gamma}(1 + \delta_p\Gamma^\lambda), \qquad Q = \frac{2}{\Gamma}(1 + \delta_q\Gamma^\lambda), \qquad N = \frac{1}{2}(1 + \delta_n\Gamma^\lambda), \quad (8)$$

and expand the flow equations to linear order in the δ's. 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 $\delta_n > 0$, odd bonds are stronger than even bonds, the density of spin-1's increases, and the system flows to the random singlet fixed point. If $\delta_n < 0$ even bonds are stronger than odd bonds, the density of spin-1's decreases, and the system flows to the random Haldane fixed point. 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 $\Gamma_0 = \delta^{-\frac{1}{\lambda_+}}$. 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 $\nu = \frac{3}{\lambda_+} \approx 2.3$. The string-topological order parameter [2],

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

measures the square of the density of active spins. Active spins are spins that have not yet formed singlets plus those spins that have formed singlets but are not enveloped by other singlets. Following the method outlined by Fisher [5] for calculating the flow of distributions with auxiliary variables, we find that the average number of active spins per bond scales like Γ^ϕ, where $\phi = 2$. In the Haldane phase near the critical point the topological order scales as $T \propto (-\delta_n)^{2\nu/3(3-\phi)} = (-\delta_n)^{2\nu/3}$ [16,17]. At the critical point the topological order decays with the distance as $r^{-2/3}$ [16].

Like the RS fixed point for the spin-1/2 chain [5], the bond distributions become infinitely broad on a logarithmic scale. Thus our approach is asymptotically exact at the critical point; the critical exponents are also exact.

Westerberg *et al.* [7] studied the random spin-1/2 chain with antiferromagnetic and ferromagnetic bonds in which both even and odd bonds may be ferromagnetic, and as a result spins of arbitrarily large size appear at low energy. In our model of the spin-1 chain, only odd bonds may be ferromagnetic. Boechat *et al.* [13] anticipated the existence of a spin-1 random singlet phase for strong randomness. As in our previous work [9], they find *spontaneously* dimerized chains are unstable against *weak* randomness. They did not address the phase transition that we discuss here. The correlation length exponent $\nu \approx 2.3$ is extremely close to that of the delocalization transition in integer quantum Hall (IQH) systems. Lee [18] showed that the IQH transition may be mapped onto the dimerization transition in the pure SU(0) spin chain. It is unclear whether this is a coincidence or if 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 decay exponentially, and there is an excitation gap. For broader distributions the gap is filled, topological order persists, and the spin-spin correlations decay exponentially with correlation length exponent $\nu = \frac{6}{\sqrt{13}-1} \approx 2.3$. Beyond the critical point there is no topological order, the disorder-averaged spin-spin correlations decay algebraically, and the ground state resembles the random singlet state.

R. A. H. and K. Y. were supported by NSF DMR-9416906, DMR-9531115, and DMR-9400362. The authors are grateful to Patrik Henelious for sharing his unpublished data. We also thank S. M. Girvin, R. N. Bhatt, and D. S. Fisher for valuable discussions.

[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, and W. G. Stirling, Europhys. Lett. **3**, 945 (1987); J. P. Renard, L. P. Regnault, and 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 (1980).
[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**, 4302 (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] K. Hida, Phys. Rev. B **45**, 2207 (1992).
[12] I. Affleck, T. Kennedy, E. H. Lieb, and H. Tasaki, Phys. Rev. Lett. **59**, 799 (1987).
[13] B. Boechat, A. Saguia, and M. A. Continentino, Solid State Commun. **98**, 411 (1996); M. A. Continentino, J. C. Fernandes, R. B. Guimarães, B. Boechat, H. A. Borges, J. V. Valarelli, A. Hannapel, and A. Lacerda, Philos. Mag. **B73**, 601 (1996).
[14] M. Hagiwara, K. Katsumata, Ian Affleck, B. I. Halperin, and J. P. Renard, Phys. Rev. Lett. **65**, 3181 (1990).
[15] R. A. Hyman, Ph.D. dissertation, Indiana University (1996).
[16] R. A. Hyman (unpublished).
[17] In Ref. [8], we calculated the topological order of a random dimer chain neglecting the contribution from spins in exposed singlets. With these spins included the topological order scales like $T \propto (-\delta)^\alpha$ with $\alpha = 3 - \sqrt{5}$ in agreement with a similar calculation for the random transverse field Ising chain [6].
[18] Dung-Hai Lee, Phys. Rev. B **50**, 10 788 (1994).