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Spin reduction transition in spin-$\frac{3}{2}$ random Heisenberg chains

Gil Refael,[1] Stefan Kehrein,[2] and Daniel S. Fisher[1]
[1]*Department of Physics, Harvard University, Cambridge, Massachusetts 02138*
[2]*Theoretische Physik III, Elektronische Korrelationen und Magnetismus, Universität Augsburg, Augsburg, Germany*
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Random spin-$\frac{3}{2}$ antiferromagnetic Heisenberg chains are investigated using an asymptotically exact renormalization group. Randomness is found to induce a quantum phase transition between two random-singlet phases. In the strong randomness phase the effective spins at low energies are $S_{eff}=\frac{3}{2}$, while in the weak randomness phase the effective spins are $S_{eff}=\frac{1}{2}$. Separating them is a quantum critical point near which there is a nontrivial mixture of spin-$\frac{1}{2}$, spin-1, and spin-$\frac{3}{2}$ effective spins at low temperatures.

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Some of the most dramatic effects of randomness in solids appear in the low-temperature behavior of quantum systems. A (deceptively) simple class of such systems are random quantum spin chains, in particular, Heisenberg antiferromagnetic chains with the Hamiltonian

$$\mathcal{H}=\sum_i J_i \hat{\mathbf{S}}_\mathbf{i}\cdot\hat{\mathbf{S}}_{\mathbf{i}+1}. \tag{1}$$

From a real-space renormalization-group (RG) analysis,[1] it has been shown that the spin-$\frac{1}{2}$ random antiferromagnetic (AFM) chain is strongly dominated by randomness at low temperatures even when the disorder is weak.[2] Its ground state is a *random-singlet* (RS) phase in which pairs of spins—mostly close together but occasionally arbitrarily far apart—form singlets. As the temperature is lowered, some of these singlets form at temperatures of order of the typical exchange and become inactive. But their neighboring spins will interact weakly across them via virtual triplet excitations. At lower temperatures, such further neighbors can form singlets and the process repeats. Concomitantly, the distribution of effective coupling strengths broadens rapidly. Eventually, singlets form on all length scales and the ground state is controlled by an RG fixed point with extremely strong disorder: an *infinite randomness fixed point*.

This low-temperature behavior is in striking contrast to that of the pure spin-$\frac{1}{2}$ AFM chain, in which spin-spin correlations decay as x^{-1} because of long-wavelength low-energy spin-wave (or spinon) modes. In the random-singlet phase, the *average correlations* decay as a power of distance — as x^{-2} — but for a very different reason: A typical pair of widely spaced spins will have only exponentially (in the square root of their separation) small correlations. But a small fraction, those that form a singlet pair, will have correlations of order unity independent of their separation; these rare pairs completely dominate the average correlations as well as the other low-temperature properties of the random system.

Infinite randomness fixed points are ubiquitous in random quantum systems. They probably control phase discrete-symmetry-breaking transitions in *all* random quantum systems — in any dimension[12] — and, in addition to the spin-$\frac{1}{2}$ AFM chain, also control the low-temperature properties of a range of random quantum phases.[15] Because of their ubiquity, further investigation of what types of random quantum phases and transitions can occur should shed light more generally on the combined roles of randomness and quantum fluctuations. The simplest cases to analyze are one dimensional because asymptotically exact RG's can be used to extract much of the universal low-temperature behavior. In this paper, we study random spin-$\frac{3}{2}$ AFM chains and find that they exhibit a novel phenomenon: a quantum transition between two phases with both phases and the transition governed by infinite randomness fixed points.

We first review what is known about random spin-1 chains. Pure spin-1 AFM chains behave strikingly differently than spin $\frac{1}{2}$: their ground state is a nondegenerate disordered phase with excitations separated from it by a gap.[3] This Haldane gap provides robustness of spin-1 chains against *weak bounded* randomness.[4,5] But for strong randomness, spin-1 chains will form a random-singlet phase. As is the case in many random quantum systems, there is *not* a transition directly from the gapped phase to the strong randomness phase. Instead, when in some local regions the randomness overcomes the gap, there will be an intervening region in which there are localized gapless excitations but still exponential decay of correlations — a Griffiths-McCoy phase. The system undergoes a quantum transition from this to the random-singlet phase as the randomness is increased further.[4,5]

Pure spin-$\frac{3}{2}$ chains with Heisenberg interactions are gapless and behave very much like their spin-$\frac{1}{2}$ counterparts.[6,7] We will show that *random* spin-$\frac{3}{2}$ chains undergo a phase transition as a function of the randomness between two zero-temperature phases: the strong disorder phase is the spin-$\frac{3}{2}$ analog of the RS phase, with pairs of spins forming singlets [Fig. 1(a)]. Surprisingly, the weak randomness phase is also an RS phase, but of an effectively spin-$\frac{1}{2}$ chain superimposed on a Haldane phase [Fig. 1(b)]. At a critical disorder, there is

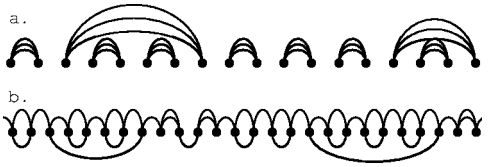

FIG. 1. Each connecting line represents a *spin-half singlet* link. (a) Strong randomness spin-$\frac{3}{2}$ random-singlet phase. (b) Low randomness phase of a spin-$\frac{3}{2}$ chain: valence-bond solid + spin-$\frac{1}{2}$ random singlet.

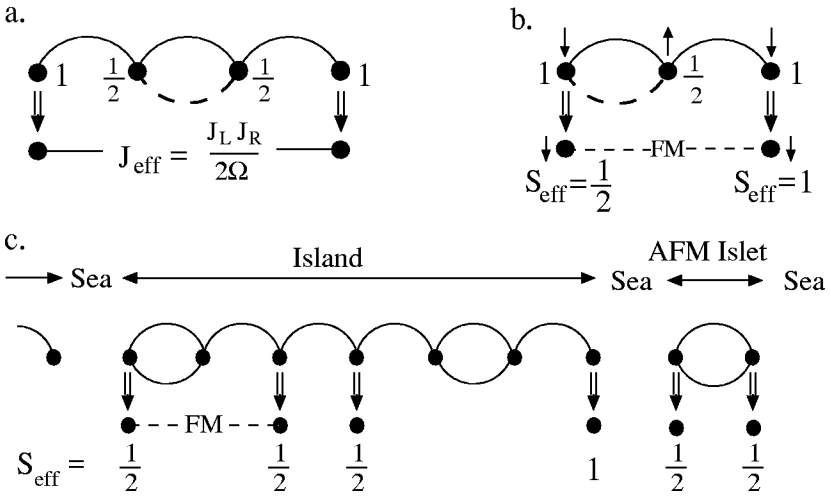

FIG. 2. (a) RG rule for the final decimation of two spin $\frac{3}{2}$'s; these are connected by a dashed line which represents a spin-$\frac{1}{2}$ singlet link being formed. (b) Creation of a FM bond by the formation of a link marked by a dashed line. Small arrows indicate preferred relative orientation of the active spins. (c) Low-energy structure of spin-$\frac{3}{2}$ chain showing a valence-bond solid *island*, composed of effective spin $\frac{1}{2}$'s antiferromagnetically coupled in its interior, with a spin-1 or a spin-$\frac{1}{2}$ pair ferromagnetically coupled at its ends, separated from other islands by AFM *sea* bonds. An AFM *islet*, made of two spin $\frac{3}{2}$'s joined by two links, is also shown. Solid arcs represent already formed links; the effective spin is noted next to each site.

a transition between these phases, with special behavior at the critical point, including a specific combination of spin-$\frac{1}{2}$, spin-1, and spin-$\frac{3}{2}$ character at low temperatures.

To make progress, we first review the RG Ref. 1 analysis of random spin-$\frac{1}{2}$ AFM chains. This proceeds by gradually reducing the energy scale, Ω. First, the pair of spins with the strongest coupling, $J_{max}=\Omega_I$ — the initial energy scale, forms a singlet [Fig. 2(a)], and is decimated. Virtual triplet excitations cause the two sites neighboring the singlet to weakly interact with the effective coupling:

$$J_{eff} \approx \alpha \frac{J_l J_r}{J_{max}}, \tag{2}$$

where J_l, J_r are, respectively, the bonds to the left and right of the decimated pair and $\alpha=\frac{1}{2}$. By repeating this procedure, we gradually reduce the energy scale, Ω, and the number of active spins in the chain. In the limit of low energy, the random-singlet phase emerges and singlets form on all length scales. That this occurs for arbitrarily weak randomness, as it does,[8] cannot be convincingly shown by this RG as it is initially approximate when the distribution of J's is not broad. But its qualitative validity for weak randomness is suggested, since J_{eff} is always less than $J_{l,r}$ due to the prefactor $\frac{1}{2}$ in Eq. (2). The multiplicative structure of Eq. (2) suggests that the distribution of J's broadens without bound. This means that the perturbative result (2) becomes *exact* at late stages of the RG,[2] and the universal low-energy properties of the system can be found exactly.

The wide distribution of J's allows one to associate the renormalized energy scale Ω with the temperature T. Bonds stronger than T become frozen, and the remaining spins act as though they are free since almost all of their couplings are much weaker than T at low temperatures.

The RG flow is simply parametrized in terms of

$$\Gamma = \ln\frac{\Omega_I}{\Omega}, \quad \beta_i = \ln\frac{\Omega}{J_i}. \tag{3}$$

As the RG evolves, Ω is reduced, and Γ increases. At low energies the coupling distributions become scale-invariant functions of β/Γ; as $\Gamma\to\infty$ at the fixed point, the distributions become infinitely broad. The density of active spins decays as

$$\rho \sim \frac{1}{\Gamma^{1/\psi}} \tag{4}$$

with $\psi=\frac{1}{2}$ a universal exponent characterizing the random-singlet phase.[2] As ψ relates the *logarithm* of energy scales to length scales $(1/\rho)$, it replaces the exponent z which parametrizes power-law energy-length scaling at conventional quantum critical points.

The strong randomness phase of the spin-$\frac{3}{2}$ chain can be understood similarly. Combining strongly interacting neighbors into a singlet yields Eq. (2) with $\alpha=\frac{5}{2}$. Strong randomness in the J's will guarantee that despite the large prefactor $(\frac{5}{2})$ the new coupling will almost always obey $J_{eff}<J_{l,r}$, yielding flow towards the random-singlet phase. In Fig. 1(a), this is indicated by varying length *triple links* representing singlets of spin $\frac{3}{2}$.

When the randomness is weak, the RG for spin $\frac{3}{2}$ fails to reduce the energy scale, suggesting that strong randomness behavior might not be obtained. To proceed, we generalize the method of Monthus, Golinelli, and Jolicoeur.[4] Instead of fully decimating strongly coupled pairs of spins, we only *partially* decimate them, eliminating their highest-energy subspace. Thus, when a spin pair, $\mathbf{S}_L$, $\mathbf{S}_R$, is renormalized, its totally ferromagnetic (maximum spin) combination is eliminated. This corresponds to breaking each spin into spin-$\frac{1}{2}$ parts — a spin-$\frac{3}{2}$ consists of three spin-$\frac{1}{2}$'s symmetrized —

with each contributing one spin-$\frac{1}{2}$ to form a *spin-half singlet link*, leaving a pair of spins with $S'_{L,R}=S_{L,R}-\frac{1}{2}$ and modified couplings between them as well as between each one and its other neighbor. In the ground state, every site must have three links joining it to others, e.g., as in Fig. 1. When a link forms between two spin $\frac{1}{2}$'s [Fig. 2(a)], both spins disappear and the J_{eff} between the remaining neighboring spins is given by Eq. (2). As can be seen in Fig. 2(b), whenever only *one* of an antiferromagnetically coupled pair is spin $\frac{1}{2}$, it will be decimated, and its partner will form a *ferromagnetic effective bond* across it. Such ferromagnetic (FM) bonds can themselves be decimated forming, e.g., a spin $\frac{3}{2}$ from a spin-1 and spin-$\frac{1}{2}$ pair; however, no spins greater than $\frac{3}{2}$ can form. We thus see that as the energy scale is lowered, the *distribution of effective spins* changes. In the strong randomness phase at low energies, virtually all the active (undecimated) spins have $S_{eff}=\frac{3}{2}$. But this will not be the case when the randomness is weak.

For a spin-1 chain with a narrow distribution of exchanges, i.e., weak randomness, all of the bonds between spin-1's would rapidly be partially decimated. The resulting (approximate) state which has one link connecting each site with each of its neighbors is the *valence-bond solid* picture of the Haldane phase.[9] The scale Ω_∞ at which the last spin is eliminated is the gap. For stronger randomness, some double links will form and the gap will disappear. But not until a critical randomness is reached does the continuous line of links break into finite segments; it is this that distinguishes the topological order of the Haldane phase from the random-singlet phase.[4,5]

The phases of a spin-$\frac{3}{2}$ chain can be understood in a related way. With weak randomness, decimation induces singlet links between most neighboring pairs, creating *islands* of valence-bond solids. Inside the islands, the active degrees of freedom are spin $\frac{1}{2}$'s left over from the decimations with spin 1's at the ends of islands [Fig. 2(c)]. The islands grow until the entire chain consists of one island with only spin $\frac{1}{2}$'s remaining. At lower energies, these spin $\frac{1}{2}$'s form spin-$\frac{1}{2}$ random singlets: the ground state is thus a spin-$\frac{1}{2}$ random-singlet phase superimposed on a (spin-1-like) valence-bond solid; see Fig. 1(b).

Generally, the low-energy structure of a spin-$\frac{3}{2}$ chain will consist of valence-bond islands separated by AFM ''sea'' bonds with no links yet formed across them. Each island consists of a number — possibly zero — of antifermagnetically coupled active spin $\frac{1}{2}$'s in the interior with each end being either spin 1 or two ferromagnetically coupled spin $\frac{1}{2}$'s as in Fig. 2(c). The exceptions to this are *islets* consisting of a single AFM bond between two spin-$\frac{1}{2}$ ends; these arise from a pair of spin-$\frac{3}{2}$ sites connected by two links [Fig. 2(c)]. There can also be original undecimated spin $\frac{3}{2}$'s.

It is convenient to describe all this in terms of a purely *spin-$\frac{1}{2}$ effective model* with a spin 1 represented as a pair of spin-$\frac{1}{2}$ sites with a FM interaction stronger then the energy scale, Ω, and a spin $\frac{3}{2}$ by an island of three sites with two strong FM bonds. This has the advantage that coupling distributions and bond types remain *independent* if they are so initially; thus the number, n, of internal spin $\frac{1}{2}$'s in an island is distributed *exponentially* with density $\propto B^n$. There are four coupling distributions: AFM sea bonds, FM edge bonds, AFM intraisland bonds, and (AFM) islet bonds. The other parameters are B and q, the fraction of active spins that are in islets. The RG flows always broaden without bound the distributions of weak ($<\Omega$) bonds,[10] justifying the claim that the RG is asymptotically exact. In the strong randomness limit, $B\to 0$, $q\to 0$, so that all islands are three spin $\frac{1}{2}$'s strongly ferromagnetically coupled internally and weakly antiferromagnetically coupled between them equivalent to spin $\frac{3}{2}$'s. In contrast, for weak randomness at low energies, $B\to 1$ and $q\to 0$, so that an infinite island forms and the system becomes equivalent to a random spin-$\frac{1}{2}$ chain; this then forms a spin-$\frac{1}{2}$ RS phase. Separating these two zero-temperature phases is a novel critical point with nontrivial B and q. Both phases and the critical point are controlled by infinite randomness fixed points.

To verify the above claims and quantitatively study the critical point, we implemented the full RG numerically. Initially, $\mathcal{H}$ (1) is all spin $\frac{3}{2}$ with the J's uniformly distributed in (J_{min}, J_{max}) and we define $\delta\equiv \mathrm{var}(\ln J)$. We studied 100 realizations of length 5×10^6, measuring the evolution with an energy scale of the active spin density ρ, the effective spin distribution, and the coupling distributions.

For $\delta>\delta_c$ the chain flows to the $S_{eff}=\frac{3}{2}$ random-singlet phase, while for $\delta<\delta_c$ it flows to the $S_{eff}=\frac{1}{2}$ random-singlet phase. The density ρ in both random-singlet phases obeys Eq. (4), as expected, with $\psi=\frac{1}{2}$.

The critical point is at $\delta_c=0.22\pm 0.01$. The corresponding fixed point is very different from the stable fixed points. The fractions of active spins are (± 0.02)

$$p_{1/2}=0.54, \quad p_1=0.33, \quad p_{3/2}=0.13. \tag{5}$$

The appearance of spin-1 excitations may be surprising: in pure spin-$\frac{3}{2}$ chains, they do *not* appear at the ends because of the gapless nature of the bulk. At the critical point, the active spin density, ρ, decays with a larger power of Γ than in either phase:

$$\frac{1}{\psi}=\frac{1}{\psi_c}=3.85\pm 0.15. \tag{6}$$

This implies that the dynamics is *faster* at the critical point than in the adjacent phases. At infinite randomness fixed points, ψ also controls the decay of *typical* correlations:[11,12]

$$\ln(|\langle \mathbf{S}_i\cdot\mathbf{S}_j\rangle|)\approx -C_{ij}|i-j|^{\psi} \tag{7}$$

with the random coefficient C_{ij} having a universal distribution. The *average* correlations will, however, decay as $1/|i-j|^2$ at the critical point as in both phases.

Deviations from the critical point, $\delta-\delta_c$, are relevant perturbations and grow as $\Gamma^{1/\nu\psi_c}$ as the energy scale is reduced, with ν the correlation length exponent. We find

$$\frac{1}{\nu\psi_c}=1.2\pm 0.1 \Rightarrow \nu=3.2\pm 0.3. \tag{8}$$

Many physical quantities are dominated by the almost decoupled active spins that remain at scale $\Omega=T$ correspond-

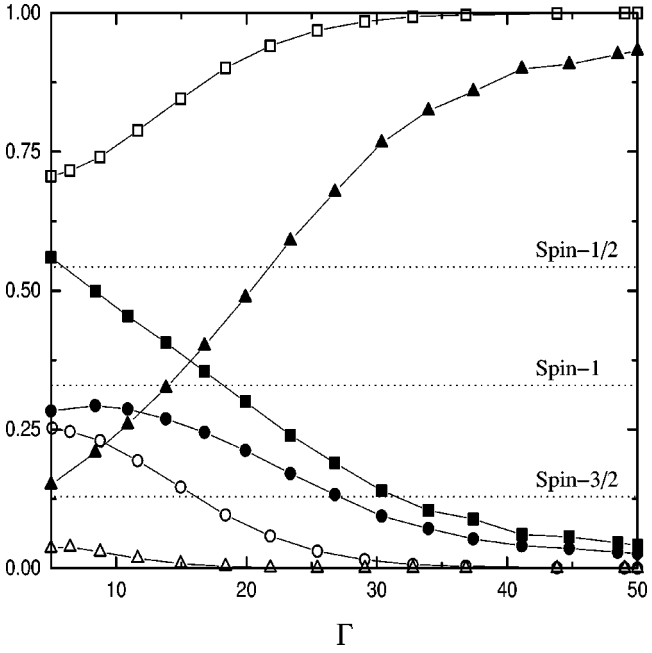

FIG. 3. Evolution of the effective spin fractions as a function of Γ. squares are spin 1/2, circles spin 1, and triangles spin 3/2. Filled symbols mark high randomness: $\delta=0.44$; empty symbols mark low randomness: $\delta=0.04$. The three horizontal lines mark the value of the fractions at the fixed point, $\delta=0.22$.

ing to $\Gamma_T=\ln(\Omega_I/T)$. The magnetization density at temperature T and applied field $H\sim T$ is the sum of that of the three kinds of spins with weights, $\{p_{S(\Gamma_T,\delta)}\}$ (see, e.g., Fig. 3). The linear susceptibility obeys a universal scaling form: $\chi(\delta,T)\approx\rho_{\Gamma_T}/T\sim\Gamma_T^{-1/\psi_c}\mathcal{N}((\delta-\delta_c)\Gamma_T^{1/\psi_c\nu})/T$. For $x\to 0$, $\mathcal{N}(x)$ approaches a nonzero constant, yielding $\chi(T)\approx 1/T\ln^{1/\psi_c}T$ for $|\delta-\delta_c|<|\ln T|^{-1/\psi_c\nu}$. For large x, $\mathcal{N}(x)\sim|x|^{(1-2\psi_c)\nu}$ leading to $\chi(\delta,T)\approx X(\delta)/T\ln^2 T$ in *both* random-singlet phases. Near the critical point, $X(\delta)$ vanishes as $X(\delta)\sim|\delta-\delta_c|^{(1-2\psi_c)\nu}$ for $|\delta-\delta_c|>|\ln T|^{-1/\psi_c\nu}$. Unfortunately, this dip in the susceptibility would be hard to observe because of the low temperatures needed. But because of the $\ln T$ in scaling functions, a wide regime of the low-temperature phase diagram will be governed by the *critical* fixed point with the spin mixture described approximately by the universal fractions in Eq. (5).

Spatiotemporal correlations can be investigated by neutron scattering. The magnetic structure factor, $\mathcal{S}(q,\omega)$, will be dominated at low frequencies by excitations of spins that are paired together with an energy scale ω. At fixed ω, $\mathcal{S}(q,\omega)$ will show a peak at $q\sim\rho_{\Gamma(\omega)}$, the typical spacing between such spin pairs.[13] At the critical point, we also expect some strong ferromagnetic correlations between widely separated pairs on the same sublattice. These may give rise to an interesting dependence on δ of the peak in $\mathcal{S}(q,\omega)$ near the zone boundary.

The dynamics of nominally pure spin-$\frac{3}{2}$ Heisenberg chains were recently studied experimentally in $CsVCl_3$ and $CsVBr_3$, cf. Itoh *et al.*[14] If mixtures of these or other pairs of compounds can be made with random AFM exchange, it should be possible to investigate some of the phenomena discussed here. Additional complications that would have to be investigated include the effects of random anisotropy. For spin-$\frac{1}{2}$ random chains, there is considerable robustness of the random-singlet-like phases unless Ising anisotropy dominates.[2] But for higher spin, this needs exploring. Another intriguing possibility is three-leg spin ladder compounds,[16] if ones can be found with combinations of ferro- and antiferromagnetic interactions. More generally, the model studied here shows how regimes with complicated mixtures of effective spins can arise at low temperatures from seemingly simple Hamiltonians.

The spin-$\frac{3}{2}$ AFM chain appears to be the first example of a system in which two phases and the transition between them are all governed by infinite randomness fixed points. How much of this behavior persists in other contexts, in particular with lower symmetry or in higher dimensions, is a subject for future investigations.

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