Permutation-Symmetric Multicritical Points in Random Antiferromagnetic Spin Chains

Kedar Damle[1,2] and David A. Huse[3]

[1]*Physics Department, Harvard University, Cambridge, Massachusetts 02138*
[2]*Department of Physics and Astronomy, Rice University, Houston, Texas 77005*
[3]*Physics Department, Princeton University, Princeton, New Jersey 08544*

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We present a general theory of a class of multicritical points in the phase diagrams of random antiferromagnetic spin chains. We show that low-energy properties of these points are almost completely determined by a permutation symmetry of the effective theory not shared by the microscopic Hamiltonian. One case provides an analytic theory of the quantum critical point in the random spin-3/2 chain, studied in a recent work by Refael, Kehrein, and Fisher.

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Many of the interesting but poorly understood systems of interest to current condensed-matter physics research are quantum many-body systems with both strong quenched randomness and strong interactions. One class of such systems where there are some experimental results [1] and significant theoretical progress has been possible [2–7] is antiferromagnetic Heisenberg spin chains. Much of the physics of these systems is captured by the model Hamiltonian

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

where the operator $\vec{S}_i$ represents a spin S at site i of a linear chain. The nearest-neighbor exchanges J_i are all positive, may be random, and may have an imposed "dimerization" δ:

$$J_i = J[1 + \delta(-1)^i]\exp(R\eta_i), \tag{2}$$

where R measures the strength of the randomness and the η_i are random numbers drawn from a distribution with mean zero, variance one, and all moments finite.

This simple-looking Hamiltonian encodes a variety of low-energy behaviors depending upon the dimerization δ, the randomness R, and the value of the spin S. For example, for $S = 1$, the undimerized chain ($\delta = 0$) has a quantum critical point at some intermediate value of R that separates low-disorder Haldane and high-disorder random singlet (RS) ground states [5,6]; this point is a multicritical point in the R-δ plane at which three phases meet [8]. In recent work, a related transition between low and high-disorder RS states was also seen numerically in undimerized $S = 3/2$ chains [9]. Here we examine these critical points in a larger context, showing that they are but two members of a countably infinite class of random multicritical points. The low-energy statistical properties of these special points exhibit the symmetry of the permutations of N identical objects, S_N, although for $N > 2$ this is *not* a symmetry of the system's bare Hamiltonian.

To proceed, we describe the phases of the spin chain in the valence-bond picture [10] in which each spin S is represented by the fully symmetrized multiplet of $2S$ spin 1/2's. The system's ground state has total spin zero (modulo end effects), so each such spin 1/2 forms a singlet (a *valence bond*) with a spin 1/2 on a neighboring site. Thus, we can classify a ground state by how many such valence bonds are formed across the even links of the lattice: call this number σ. Since each spin S must participate in $2S$ valence bonds, there must be $(2S - \sigma)$ valence bonds across the odd links. We will denote this *valence-bond solid* (VBS) *ground state* as being in the $(\sigma, 2S - \sigma)$ *phase*, or, more compactly, the σ phase. For spin S, there are $(2S + 1)$ such phases, and various phase transitions between them (some phase diagrams are shown in Fig. 1). The VBS ansatz for the ground state assumes that the valence bonds are all between nearest neighbors, which is not precisely correct even at $R = 0$. But there are indeed $2S + 1$ topologically distinct possibilities for the phases to which the real ground state can belong. As suggested by the valence-bond description, these are distinguished by the properties of a chain end: For a chain in the σ phase, if an *even* bond in an infinite

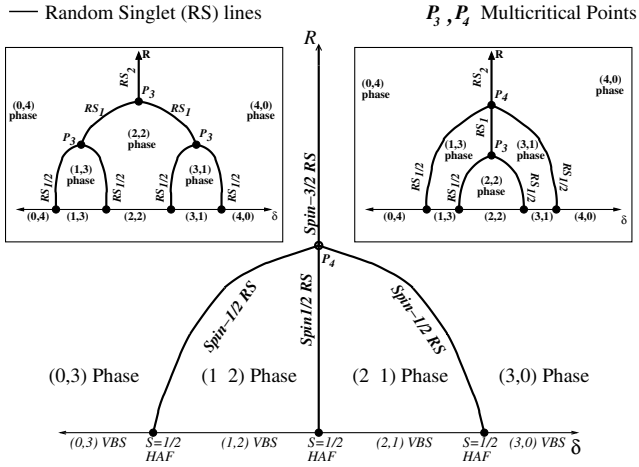

FIG. 1. Schematic phase diagram of $S = 3/2$ chains in the R-δ plane. Inset: Possible phase diagrams for $S = 2$ chains.

chain is removed, the two resulting semi-infinite chains have ground states that contain free spin ($\sigma/2$)'s localized near their ends.

The phase diagrams in the R-δ plane are simple for zero or small R: At $R = 0$, all the phases (with $\sigma = 0, 1, \ldots 2S$) can be accessed by sweeping δ from -1 to $+1$, passing a succession of $2S$ critical points [11]; for integer S, the (S, S) phase that occurs around $\delta = 0$ is the familiar Haldane phase [12], while for half-integer S, the critical point between $\sigma = S \pm (1/2)$ occurs at $\delta = 0$. At $R = 0$, the low-energy properties of critical points separating phases $(\sigma, 2S - \sigma)$ and $(\sigma + 1, 2S - \sigma - 1)$ arise from *residual spin-1/2's* obtained by first forming σ valence bonds across the even links and $2S - \sigma - 1$ valence bonds across the odd links. This leaves one unpaired spin $1/2$ per site, and these spins behave as a (critical) spin-$1/2$ chain. Now, since the phases are gapped at $R = 0$, they survive for small R as well. Likewise, the critical points must extend to critical lines at $R \neq 0$, with the same low-energy properties as the random-exchange spin-$1/2$ chain [2,3]: Along these lines, the chain is in the spin-$1/2$ random singlet ($\mathrm{RS}_{1/2}$) state. In this critical state, the *residual spin 1/2* at any given site "pairs" into a singlet with one at some other site not necessarily close to it, with the randomness determining the pairing; this produces a glass of single valence bonds with specific statistical properties at low energies [3].

The behavior in the opposite limit of strong randomness is also readily understood. Because of the broad distribution of exchanges at large enough R, a spin-S version (RS_S) of the random singlet state obtains for $\delta = 0$. This is a glass of $2S$-fold valence bonds with the same statistical properties as the single valence bonds in the $\mathrm{RS}_{1/2}$ state. Turning on $\delta \neq 0$ in this regime drives the system into either the $(2S, 0)$ or the $(0, 2S)$ phase, so the RS_S state is a critical line at $\delta = 0$ separating these two phases. Given this picture of the phase diagram in the two limiting cases, one is immediately led to the interesting possibility that all the $\mathrm{RS}_{1/2}$ critical lines meet the RS_S line at a single point at intermediate R and $\delta = 0$, producing a multicritical point at which all $2S + 1$ distinct phases of the spin-S chain meet. Indeed, a general theory of such multicritical points $\mathcal{P}_N$ at which N distinct phases meet forms the focus of the present Letter.

We begin by addressing the question of *existence:* Recent work [8] shows that the $\delta = 0$ transition from the gapless Haldane (1,1) phase to a RS_1 state in $S = 1$ chains studied earlier [5,6] is such a multicritical point (with $N = 3$), where all three phases of the system meet. In the recent RG study of the $S = 3/2$ case with $\delta = 0$, a single quantum phase transition between a $\mathrm{RS}_{1/2}$ state for small R and a $\mathrm{RS}_{3/2}$ state for large R was observed numerically [9]. Our discussion above shows that this transition is actually a multicritical point (with $N = 4$), at which all four distinct phases of a $S = 3/2$ chain meet. For $S = 2$ or higher spin, the $N = 2S + 1$ multicritical point is not generically present when one only varies R and δ, to locate it requires tuning other parameters. For $S = 2$, in particular, the possible topologies of the R-δ phase diagram are shown in Fig. 1.

Such multicritical points represent points at which the local ground state of the chain can be in any one of N possible phases. Thus, we develop a theory for the low-energy physics of these points in terms of the domain structure of the chain. We begin with a low-energy picture of the chain as being made up of a sequence of domains, each belonging to one of the N possible phases of a spin-S chain ($N \equiv 2S + 1$). Neighboring domains are separated by *domain walls*. These domain walls each carry spin: The magnitude of the spin on a wall is given by the number of unpaired spin $1/2$'s due to the difference of σ across the wall. For two adjacent domains D_1 and D_2, with σ_1 and σ_2, as in Fig. 2, the spin on the domain wall separating them has magnitude $S_{12} = |\sigma_1 - \sigma_2|/2$.

The low-energy properties of our chain are now controlled by the effective exchange couplings between neighboring domain-wall spins. In the absence of neighboring domain walls, each domain-wall spin represents a zero-energy multiplet, with the spin localized near the wall. Neighboring domain-wall spins thus interact with an effective exchange J that falls off rapidly with the domain length, and is consequently broadly distributed in magnitude (it can be of either sign). We allow each type of domain, σ, to have its own probability distribution for the length of the domain and thus the exchange across the domain. We thus have N probability distributions $P_\sigma(\beta|\Gamma)$ for the corresponding log couplings $\beta \equiv \ln(\Omega/|J|) \geq 0$, where Ω is the cutoff energy (the strongest exchange), and $\Gamma \equiv \ln(\Omega_0/\Omega)$ with Ω_0 a bare cutoff.

The signs of the exchanges J_i in the domain picture are dictated by the domain sequence. Consider the configuration in Fig. 2, assuming that J_2 is the strongest of the three exchanges shown. At energy below $|J_2|$ but above $|J_1|$ and $|J_3|$, it should be possible to describe the system by replacing S_{12} and S_{23} with a single effective spin S_{13} whose value is determined by the ground-state multiplet of the two-spin Hamiltonian $J_2 \vec{S}_{12} \cdot \vec{S}_{23}$. Consistency requires that this must be the same as eliminating D_2 and having a direct domain wall between D_1 and D_3 carrying spin $S_{13} \equiv |\sigma_1 - \sigma_3|/2$. For this to be true, J_2 must be antiferromagnetic (positive) if $\sigma_1 - \sigma_2$ and $\sigma_3 - \sigma_2$ are of the same sign, and ferromagnetic (negative) otherwise.

This basic structure of the low-energy theory can also be obtained from a more microscopic argument with (1)

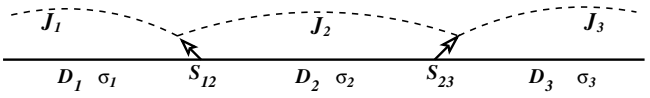

FIG. 2. A configuration of three adjacent domains.

as the starting point. Consider treating (1) for arbitrary S with a generalization of the approximate *extended Ma-Dasgupta-Hu* (MDH) renormalization group (RG) approach [6,9]. [For general S, the procedure eliminates *all excited states* of the most strongly coupled pair of spins if this coupling is ferromagnetic, while taking care to eliminate only the highest excited state if it is antiferromagnetic; the RG rules for signs and magnitudes of couplings are as in Refs. [6,9].] Assign the formal domain label $\sigma = 0$ ($\sigma = 2S$) to every even (odd) bond of the unrenormalized Hamiltonian (1). Equation (1) with this labeling is consistent with the rules for domain-wall spins and signs of couplings in our domain wall model; we can therefore formally think of each J of (1) as straddling a domain of the corresponding type. Now, if the renormalized Hamiltonian and choice of labels at a given stage of the RG is consistent with this domain interpretation, it is possible to relabel the couplings after each RG step to preserve this property: Let $J_2 S_{12} \cdot S_{23}$ in Fig. 2 be the term with the largest gap between lowest and highest energy states. If $J_2 > 0$, and neither S_{12} nor S_{23} are spin $1/2$, change σ_2 to $\sigma_2 + (\sigma_1 - \sigma_2)/|\sigma_1 - \sigma_2|$ after the next RG step (which reduces both S_{12} and S_{23} by $1/2$). If $J_2 > 0$ and $S_{12} = S_{23} = 1/2$, attach the common label of J_1 and J_3 to the new coupling $\tilde{J}_{13}$ that reaches across them after the next step (which puts them into a singlet state). In all other cases, there is no need to relabel any of the renormalized couplings.

Although this RG procedure is not exact, it is expected to be accurate for low-energy properties [5,6,9]; the formal device above thus provides an alternative route to our domain model. Moreover, the present argument rules out any biquadratic and other higher order interactions between domain-wall spins so long as one starts with the Hamiltonian of (1). What about a small higher order interaction added to the original Hamiltonian? Such a perturbation will certainly not grow during the extended MDH RG iterations, and the resulting low-energy model will again have a consistent interpretation in terms of domain-wall spins, since small higher order terms will not affect the spin of the ground-state multiplet or the ordering of excited states for any pair of domain-wall spins — the dominant effect of such a term will be to modify the relative probabilities with which different domain sequences occur in the low-energy effective model. Conversely, Hamiltonians with very large higher order interaction terms may be in a different universality class, not necessarily described by the present results.

To proceed further, we need to specify the probabilities with which different domain sequences occur. We do this within a nearest-neighbor transfer matrix formalism. Thus we have a symmetric, purely off-diagonal $N \times N$ transfer matrix $W_{\sigma\sigma'}$ which gives the relative weights for the two types of domains $\sigma \neq \sigma'$ to be present and adjacent to each other. We normalize W to make its largest eigenvalue $+1$ (we denote the components of the corresponding normalized eigenvector as $\sqrt{\rho_\sigma}$). This guarantees that the "partition function" (sum over all possible domain configuratins) $Z_L \equiv \mathrm{Tr}(W^L)$ for a sequence of L domains with periodic boundary conditions tends to unity as $L \to \infty$. The unconditional probability for a given segment, say $\ldots \mu_a \mu_b \mu_c \ldots$, to occur in the spatial sequence of domain types is now given by modifying the expression for Z by introducing appropriate projection operators $\Pi^{\mu}_{\sigma\sigma'} \equiv \delta_{\sigma\sigma'}\delta_{\sigma\mu}$ at the corresponding places in the product of W's, yielding the expression $\mathrm{Tr}(\ldots W \Pi^{\mu_a} W \Pi^{\mu_b} W \Pi^{\mu_c} W \ldots)$. Thus, the probability of the kth domain being type μ is ρ_μ, that of the kth domain being type μ *and* the $(k+1)$th being type ν is $\sqrt{\rho_\mu \rho_\nu} W_{\mu\nu}$, etc. (for $L \to \infty$).

Given the broad probability distributions P_σ of the log couplings β in our domain model, we can analyze the low-energy properties using a *strong-disorder RG* approach [5] that eliminates, at each step, *all* excited states of the strongest-coupled pair of remaining domain-wall spins (this procedure is expected [3,5] to yield asymptotically exact results for low-energy properties). For our domain-wall model, the strong-disorder RG action is rather simple, and does not generate any correlations between domains beyond those given by the nearest-neighbor transfer matrix W: Let J_2 of Fig. 2 be the strongest bond in the chain. At each step, this RG "integrates out" the domain (in this case D_2) straddled by the strongest coupling: If $\sigma_1 \neq \sigma_3$, D_2 is eliminated, a direct domain wall between D_1 and D_3 is formed, and the signs, but *not* the magnitudes, of J_1 and J_3 are altered (if necessary) to conform to the requirements of the sign rule for this new configuration. If $\sigma_1 = \sigma_3$, D_2 is eliminated and D_1 and D_3 are merged together into one domain. This merged domain is straddled by a renormalized coupling of magnitude $|J_{13}| = |J_1 J_3 / J_2|$ and sign determined by our sign rule. [These RG rules remain unaffected in the strong-disorder limit if a small additional higher order interaction between domain-wall spins is also present.] A little bookkeeping yields the RG flow equations corresponding to this procedure:

$$\frac{dW_{\sigma\sigma'}}{d\Gamma} = V_{\sigma\sigma'} - \frac{W_{\sigma\sigma'}}{2}[P^0_\sigma + P^0_{\sigma'} - V_{\sigma\sigma} - V_{\sigma'\sigma'}],$$

$$\frac{\partial P_\sigma}{\partial \Gamma} = \frac{\partial P}{\partial \beta} + P^0_\sigma P_\sigma(\beta|\Gamma) + V_{\sigma\sigma}(P_\sigma \otimes P_\sigma - P_\sigma), \quad (3)$$

$$\frac{dL}{d\Gamma} = -L[\rho \cdot P^0 + Y],$$

where $V_{\alpha\beta} \equiv \sum_\mu W_{\alpha\mu} P^0_\mu W_{\mu\beta}$, $P^0_\mu \equiv P_\mu(0|\Gamma)$, $P_\sigma \otimes P_\sigma \equiv \iint d\beta_1 d\beta_2 P_\sigma(\beta_1|\Gamma) P_\sigma(\beta_2|\Gamma) \delta(\beta - \beta_1 - \beta_2)$, $Y = \sum_\nu \rho_\nu V_{\nu\nu}$, $\rho \cdot P^0 = \sum_\mu \rho_\mu P^0_\mu$ and the sums run over the labels of the N domain types. Moreover, the flow of W also induces a change in ρ:

$$\frac{d\rho_\sigma}{d\Gamma} = -\rho_\sigma(P^0_\sigma + V_{\sigma\sigma} - \rho \cdot P^0 - Y). \quad (4)$$

The multicritical point $\mathcal{P}_N$ is controlled by a fixed point of these equations with S_N statistical symmetry corresponding to freely interchanging between the N phases that meet at this point. This fixed point has $W_{\mu\nu} = 1/(N-1)\ \forall\ \mu \neq \nu$, $P_\mu(\beta|\Gamma) = (N-1)e^{-(N-1)\beta/\Gamma}/\Gamma\ \forall\ \mu$, and $\rho_\mu = 1/N\ \forall\ \mu$. Also, the number of domains decreases with the cutoff as $L(\Gamma) = L(0)/\Gamma^{1/\psi_N}$, with the exponent $\psi_N \equiv 1/N$. Thus, all N domain types are equally likely at this fixed point, with any two types of domains equally likely to be adjacent to each other. The fractions p_s of the domain walls in the low-energy effective Hamiltonian that have spin S follow simply from this. In the $S = 3/2$, $N = 4$ case, we predict $1/\psi_4 = 4$, $p_{1/2} = 1/2$, $p_1 = 1/3$, and $p_{3/2} = 1/6$; the numerical estimates of [9] are in reasonable agreement with these results. (The low-temperature specific heat and susceptibility at the critical point are completely determined [3,5,6,9] by ψ and p_s.)

To get information on off-critical scaling properties, we need to analyze small perturbations about this $\mathcal{P}_N$ fixed point. Fortunately, the S_N symmetry imposes enough structure on the linearized flows to allow a full calculation of all RG eigenvalues λ which govern the Γ^λ growth or decay of the corresponding eigenperturbations: There are only $N-1$ relevant eigenvectors, all having eigenvalue $\lambda_N^+ \equiv (\sqrt{4N+1} - 1)/2$. Since one has to tune $N-1$ "knobs" in general to get N phases to all be "degenerate," this coincides with the minimal possible number of relevant directions at a N-fold multicritical point; thus, this S_N fixed point governs *all* such strongly random N-fold multicritical points of (1) and its generalizations that include small additional biquadratic and higher order couplings. [In contrast, usual (nonrandom) N-fold multicritical points in Landau theory or in two dimensions do not generically have S_N low-energy symmetry for $N > 2$ [13].] The relevant eigenvectors can be chosen to correspond to perturbations which make only one of the N phases fall out of favor, thus reducing the symmetry from S_N to S_{N-1}. In addition we have one irrelevant eigenvector with eigenvalue -1 (representing an additive shift in Γ), for $N > 2$ there are $N-1$ irrelevant eigenvectors with eigenvalue $-(\sqrt{4N+1} + 1)/2$, and for $N > 3$ there are $N(N-3)/2$ irrelevant eigenvectors with eigenvalue $-N$. (We also expect [3] other "infinitely" irrelevant perturbations, i.e., decaying exponentially with Γ; these are not considered here.)

In the $S = 3/2$, $N = 4$ case, we thus predict a relevant eigenvalue of $\lambda_4^+ = (\sqrt{17} - 1)/2$, and a correlation length exponent $\nu \equiv 1/\lambda_4^+\psi_4 \cong 2.56$ (note that the numerical estimate of [9] differs significantly from this prediction, probably due to slow transients or finite-size effects). Deviations from $\mathcal{P}_4$ in the R-δ plane contain linear combinations of the three relevant perturbations. The fact that the RG eigenvalues are all the same means that the phase boundaries come in linearly at $\mathcal{P}_4$. The slope of two of the four phase boundaries is fixed by noting that any phase boundary between phases related by the $\delta \to -\delta$ symmetry of the problem (corresponding to an interchange of even and odd sites) must lie on the R axis. The same symmetry forces the the remaining two to be reflections of one another about the R axis. Moreover, thinking in terms of the relative energies of different VBS states makes it clear that both these phase boundaries must leave $\mathcal{P}_4$ sloping downwards (see Fig. 1).

Finally, it is now clear that the generic phase diagram in the R-δ plane for $S = 2$ will look like one of the two insets shown in Fig. 1, with the putative S_5 symmetric point $\mathcal{P}_5$ splitting into lower-order multicritical points as shown. Such lower-order points are described by fixed points of the RG with a lower symmetry S_M (with $M < N \equiv 2S + 1$) at which domains of M phases each occur with equal probability and other domain types do not occur at low energies [14]. All five phases of the $S = 2$ chain will only meet at $\mathcal{P}_5$ upon fine tuning some additional parameter in the model (such as nearest-neighbor interactions more general than simply the exchange $\vec{S}_i \cdot \vec{S}_{i+1}$). Similar considerations also rule out the generic occurrence of such maximally symmetric multicritical points in the R-δ plane for all $S > 2$.

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