Permutation-Symmetric Multicritical Points in Random Antiferromagnetic Spin Chains.

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(July 9, 2002)

The low-energy properties of a system at a critical point may have additional symmetries not present in the microscopic Hamiltonian. This letter presents the theory of a class of multicritical points that provide an interesting example of this in the phase diagrams of random antiferromagnetic spin chains. One case provides an analytic theory of the quantum critical point in the random spin-3/2 chain, studied in recent work by Refael, Kehrein and Fisher [cond-mat/0111295].

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 [2–5] is antiferromagnetic Heisenberg spin chains. Much of the physics of these systems is captured by the model Hamiltonian

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

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” \( \delta \):

\[ J_i = J[1 + \delta(-1)^i] \exp(R \eta_i), \]

where \( R \) measures the strength of the randomness and the \( \eta_i \) 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 \( \delta \), 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 [3]; this point is a multicritical point in the \( R-\delta \) plane at which three phases meet [3]. In recent work, a related transition between low and high disorder RS states was also seen numerically in undimerized \( S = 3/2 \) chains [4]. 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 \( \sigma \). 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 \( \sigma \) 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 \( \sigma \) phase, if an even bond in an infinite 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 \( R-\delta \) 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 \( \delta \) 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 \( \sigma \) 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 [13]: Along these lines, the chain is in the Spin-1/2 Random Singlet (RS\(_{1/2} \)) state. In this critical state, the
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The behavior in the opposite limit of strong-randomness is also readily understood. Due to the broad distribution of exchanges at large R, the value of S is not crucial, and a spin-S version (RS_S) of the random singlet state obtains for δ = 0; at low energies, such a state is a glass of 2S-fold valence-bonds with the same statistical properties as the RS_{1/2} state. When δ is non-zero and (say) positive, the valence-bonds in the RS state will have their left end-point more often on an even site than on an odd site, and the resulting state is in the (2S, 0) phase. Thus, turning on δ in this regime drives the system into either the (2S, 0) or (0, 2S) phase, and the RS state is the critical line 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 RS_{1/2} critical lines meet the RS_S line at a single point at intermediate R and δ = 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 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 [3] shows that the δ = 0 transition from the gapless Haldane (1,1) phase to a RS_1 state in S = 1 chains studied earlier [3] 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 δ = 0, a single quantum phase transition between a RS_{1/2} state for small R and a RS_{3/2} state for large R was observed numerically [3]. 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 [3].

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 dominans, each belonging to one of the N possible phases of a spin-S chain (N = 2S + 1). Neighbouring 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 [3], the spin on the domain wall separating them has magnitude \( σ = |σ_1 − σ_2|/2 \).

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 \( P_σ(β|σ) \) for the corresponding log-couplings \( β = \ln(Ω(J)/|J|) \geq 0 \), where Ω is the cutoff energy (the strongest exchange), and \( Γ = \ln(Ω_0/Ω) \) 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 [3], 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 \( J_2 S_{12} S_{23} \). 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 \( ≡ |σ_1 − σ_3|/2 \). For this to be true, J_2 must be antiferromagnetic (positive) if \( σ_1 − σ_3 \) and \( σ_3 − σ_2 \) are of the same sign, and ferromagnetic (negative) otherwise.
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 configurations) $Z_L \equiv \text{Tr}(W^L)$ 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 $\ldots \mu_0 \mu_1 \mu_2 \ldots$, to occur in the spatial sequence of domain-types is now given by modifying the expression for $Z$ by introducing appropriate projection operators $\Pi_{\sigma \sigma'} \equiv \delta_{\sigma \sigma'} \delta_{\mu \mu}$ at the corresponding places in the product of $W$‘s, yielding the expression $\text{Tr}(\ldots W_{\mu_0} W_{\mu_1} W_{\mu_2} W_{\ldots})$. Thus, the probability of the $k^{th}$ domain being type $\mu$ is $\rho_\mu$, that of the $k^{th}$ domain being type $\mu$ and the $(k+1)^{th}$ being type $\nu$ is $\sqrt{\rho_\mu \rho_\nu} V_{\mu \nu}$, etc. (for $L \to \infty$).

Given the broad probability distributions $P_\sigma$ of the log-couplings $\beta$ in our domain model, we can analyze the low energy properties using a strong-disorder RG approach that eliminates, at each step, all excited states of the strongest-coupled pair of remaining domain-wall spins [1]. For our domain-wall model, the RG action is rather simple, and in this strongly random limit does not generate any correlations between domains beyond those given by the nearest-neighbor transfer matrix $W$: Consider Fig 1, and let $J_2$ be the strongest bond. 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. A little book-keeping yields the RG flow equations corresponding to this procedure:

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

$$\frac{\partial P_\sigma}{\partial \beta} \equiv \frac{\partial P}{\partial \beta} + P_\sigma \rho_\sigma (\beta \Gamma) + V_{\sigma \sigma'} (P_\sigma \otimes P_\sigma - P_\sigma),$$

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

where $V_{\alpha \beta} \equiv \sum_{\mu} W_{\alpha \mu} P_\mu^0 W_{\mu \beta}$, $P_\mu \equiv P_\mu (0 | \Gamma)$, $P_\sigma \otimes P_\sigma \equiv \sum_{\mu} \rho_{\mu} V_{\mu \sigma} \rho \cdot P^0 = \sum_{\nu} \rho_{\nu} V_{\nu \sigma} \rho \cdot P^0 = \text{the sums run over the labels of the } N \text{ domain types.}$

Moreover, the flow of $W$ also induces a change in $\rho$: $\frac{d\rho_\sigma}{d\Gamma} = \rho_\sigma (P_\sigma^0 + V_{\sigma \sigma'} - \rho \cdot P^0 - Y).$

We turn now to a fixed point analysis of these RG equations. The multicritical point $P_N$ is controlled by a fixed point with $S_N$ statistical symmetry corresponding to freely interchanging between the $N$ phases that meet at this point. This fixed point has $W_{\mu \nu} = 1/(N-1) \vee \mu \neq \nu$, $P_\mu (\beta \Gamma) = (N-1) e^{-(N-1)\beta \Gamma} / \Gamma \forall \mu$, and $P_\mu = 1/N \forall \mu$. Also, the number of domains decreases with the cutoff as $L(\Gamma) = L(0)/\Gamma^{1/\psi}$, 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 $p_\sigma$ 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 $1/\psi_4 = 4$, $p_{1/2} = 1/3$ and $p_{3/2} = 1/6$: the numerical estimates of $\psi_N$ are in reasonable agreement with these results. [The low-temperature specific heat and susceptibility at the critical point are completely determined by $\psi$ and $p_\sigma$.]

To get information on off-critical scaling properties, we need to analyze small perturbations about this $P_N$ fixed point. Fortunately, the $S_N$ symmetry imposes enough structure on the linearized flows to allow a full calculation of all RG eigenvalues $\lambda$ which govern the $\Gamma^\lambda$ growth or decay of the corresponding eigen-perturbations: There are only $N-1$ relevant eigenvectors, all having eigenvalue $\lambda_N^\infty = (\sqrt{4N+1} - 1)/2$. 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. [In contrast, usual (non-random) multicritical points in Landau theory or in two-dimensions do not generically have $S_N$ low-energy symmetry. For example, at the critical fixed point of the two-dimensional three-state Potts model, there are four relevant modes, two of which produce flows to generic tricritical points that do not have the $S_3$ symmetry of the Potts model.] The relevant eigenvectors can be chosen to correspond to perturbations which make only one of the $N$ phases fall out of favour, 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 $\Gamma$), 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 other ‘infinitely’ irrelevant perturbations, i.e., decaying exponentially with $\Gamma$—these are not considered here.]

In the $S = 3/2$, $N = 4$ case, we thus predict a relevant eigenvalue of $\lambda_4^\infty = (\sqrt{17} - 1)/2$, and a correlation length exponent $\nu = 1/\lambda_4^\infty \approx 2.56$ (note that the numerical estimate of $\psi$ differs significantly from this prediction, probably due to slow transients or finite-size effects). Deviations from $P_4$ in the $R-\delta$ 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 $P_4$. The slope of two of the four phase boundaries is fixed by noting that any phase boundary between phases related by the $\delta \rightarrow -\delta$ 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. To fix their slopes, consider one of them, say the $(2,1)$ to $(3,0)$ phase boundary: These two phases are degenerate here, but the other two have higher energy. A positive $\delta$ lowers the energy of both phases (since they have more singlets on the even bonds than on the odd bonds), with the energy of the $(3,0)$ phase lowered more than that of the $(2,1)$ phase. Decreasing $R$, on the other hand, lowers the energy of the $(2,1)$ phase relative to the $(3,0)$ phase. Thus, these two phases will remain degenerate if $R$ is decreased with increasing $\delta$, and this phase boundary must leave $P_4$ with a negative slope (see Fig. 1).

The above RG equations also admit fixed points of lower symmetry $S_M$ (with $M < N$) at which domains of $M$ phases each occur with equal probability, and other domain-types do not occur at low energy. These fixed points govern loci of multicritical points $P_{S_M}$ at which $M$ of the phases meet. Two examples of such loci are the $RS_{3/2}$ and $RS_{5/2}$ lines in the $R-\delta$ phase diagram of $S = 3/2$ chains (these have $M = 2$). Other examples (with $M = 3$) include the points $P_3$ in the $R-\delta$ phase diagram (see Fig. 1) of $S = 2$ chains—these have the same exponents as the point $P_3$ of $S = 1$ chains. In addition to these lower-order multicritical points, the RG equations also admit ‘Griffiths’ fixed points, which describe the continuously varying power-law singularities within the individual phases $S_M$.

Turning to $S > 3/2$, it is now clear that the generic phase diagram in the $R-\delta$ plane for $S = 2$ will look like one of the two insets shown in Fig. 1, with the putative $S_5$ symmetric point $P_5$ splitting into lower-order multicritical points as shown. All five phases of the $S = 2$ chain will only meet at $P_5$ upon fine-tuning some additional parameter in the model (such as nearest-neighbor interactions more general than simply the exchange $S_i \cdot S_{i+1}$). Similar considerations also rule out the generic occurrence of such maximally symmetric multicritical points in the $R-\delta$ plane for all $S > 2$.

Finally, we note that the basic structure of the domain-wall model used here can also be motivated from a more microscopic argument with $S_1$ as the starting point. Consider treating $S_1$ for arbitrary $S$ with a generalization of the approximate extended Ma-Dasgupta-Hu 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 anti-ferromagnetic; the RG rules for signs and magnitudes of couplings are as in Ref [6,9].] Assign the formal domain label $\sigma = 0 (\sigma = 2S)$ to every even (odd) bond of the unrenormalized Hamiltonian $H$. Eqn (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 $H$ 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 $J_2S_{12} \cdot S_{23}$ 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 $\sigma_2$ 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 $J_{13}$ 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 couplings that remain after the next step. Although this RG procedure is approximate, it is expected to be qualitatively accurate for low-energy properties [6,9], and the formal device above thus provides an alternative route to our domain model.

We acknowledge useful discussions with I. Affleck, D. S. Fisher and G. Refael, and the support of NSF-DMR grants 9981283, 9714725, & 9976621 (KD), and 9802468 (DAH).

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