Evidence for a genuine ferromagnetic to paramagnetic reentrant phase transition in a Potts spin-glass model

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Many experimental and theoretical efforts have been devoted in the past 20 years to searching for a genuine thermodynamic reentrant phase transition from a ferromagnetic to either a paramagnetic or spin-glass phase in disordered ferromagnets. So far, no real system or theoretical model of a short-range spin-glass system has been shown convincingly to display such a reentrant transition. We present here results from Migdal-Kadanoff real-space renormalization-group calculations that provide strong evidence for ferromagnetic to paramagnetic reentrance in Potts spin glasses on hierarchical lattices. Our results imply that there is no fundamental reason to rule out thermodynamic reentrant phase transitions in all non-mean-field randomly frustrated systems, and may open the possibility that true reentrance might occur in some yet to be discovered real randomly frustrated materials. [S0163-1829(98)06217-1]

I. Introduction. All real materials contain a certain amount of frozen-in random disorder. Often, random disorder leads to randomly competing, or frustrated, interactions.[1] Random frustration is detrimental to the type of order that an otherwise idealized pure material would display for zero disorder. Randomly frustrated systems are ubiquitous in condensed-matter physics. Examples include: magnetic systems,[2] mixed molecular crystals,[3] superconducting Josephson junctions in an applied magnetic field,[4] liquid crystals in porous media,[5] and partially UV polymerized membranes.[6]

One of the main issues at stake in all frustrated systems is how the low-temperature phase of the pure material is affected by weak disorder, and how that state evolves with increasing disorder level. In particular, one of the most intriguing questions is whether a weakly frustrated system can lose upon cooling the long-range ordered phase established at higher temperature and return, or *reenter*, into a thermally disordered phase, or go into a randomly frozen glassy phase. Because of their relative simplicity over other systems, and because of the large number of systems readily available with easily controllable level of disorder, random magnets are ideal systems to study the effects of weak frustration and to investigate the above question. It was originally thought that several weakly frustrated ferromagnets, such as $Eu_xSr_{1-x}S$ and amorphous-$Fe_{1-x}Mn_x$, were displaying a reentrant transition from a ferromagnetically long-range ordered phase to a randomly frozen spin-glass phase upon cooling and for a finite range of disorder, x.[2] However, after 20 years of extensive experimental research, it is now generally believed that a true thermodynamic reentrant phase transition from a long-range ordered ferromagnetic (F) phase to either a spin-glass (SG) or paramagnetic (P) phase does not occur in real magnetic materials.[7–9] Once established at the P-F Curie temperature T_C ferromagnetic order remains down to zero temperature, though with the possibility of a *transverse* spin-freezing transition at $T_\perp$ $(0<T_\perp<T_c)$ in XY and Heisenberg systems, which does not destroy the ferromagnetic order.[7–9] Above a critical disorder level, ferromagnetism occurs only on short length scales, and the system displays, instead, full-blown spin-glass behavior below a glass transition temperature, T_g.[2,7–9]

At the theoretical level, it is also currently believed that reentrance does not occur in *any* random bond spin-glass model.[7–21] This is certainly the case for the infinite range Ising, XY, and Heisenberg models.[2] In two- and three-dimensional Ising and Heisenberg models, high-temperature series expansion,[15,18] Monte Carlo simulations,[2,7,9] and recent defect-wall energy calculations[21] find no reentrant behavior either. Recently, compelling renormalization-group[12,13] and quenched gauge symmetry arguments[16,17] have been put forward for a broad class of spin-glass models, which include the Ising spin glass[2] and the gauge glass model for disordered Josephson-junction arrays and vortex glass in disordered type-II superconductors,[4,19,20,22] and which strongly argue against reentrance. Some of the details of these predictions have been quantitatively tested by high-temperature series expansion,[15,18] while possibly the most detailed checks have been obtained from real-space Migdal-Kadanoff renormalization group (MKRG) calculations of Ising spin-glass models on so-called *hierarchical* lattices.[10–12] Even in the case of the two-dimensional XY model with random Dzyaloshinskii-Moriya couplings, which for a long-time was believed to be a good candidate for reentrant behavior,[9,23] evidence is now rapidly accumulating that reentrance does not occur in that system either.[9,19,20]

Summing up, it appears that the case against reentrance in *randomly* frustrated systems and non-mean-field theoretical models[24] is at this time simply overwhelming.[25] In fact, the evidence is sufficiently strong that it could be interpreted as an indication that some profound, though yet unknown, reason(s) formally forbid reentrance in *all* spin glasses, *even* those which do not exhibit a quenched gauge invariance.[11,12,16,17] This is not impossible given that our understanding of the nature of the ground state(s) and of the low-lying excitations in glassy systems is still limited. In this paper we present a counterexample to this common belief, what we believe is the first strong evidence for a reentrant transition in a simple *non-mean-field* spin glass model where thermal fluctuations and the question of lower-critical spatial dimension play a key role.[24] Specifically, we consider the three-state ferromagnetic Potts model with a concentration x of random antiferromagnetic bonds on hierarchical lattices. We investigate the thermodynamic behavior of this model using the MKRG scheme, which is an exact method for hierarchical lattices.[26] We present results which show that this model exhibit ferromagnetic to paramagnetic reentrance for a finite concentration range of antiferromagnetic bonds. Reentrance is made possible by the fact that the system prefers to lower its free energy through short-range antiferromagnetic (AF) correlations rather than to preserve long-range ferromagnetic order. Since the lower critical dimension for antiferromagnetic long-range order for the $Q=3$ Potts model on hierarchical lattices is 4,[27] the system can be reentrant in two and three dimensions. It is interesting to note that the MKRG method has in the past been used as one of the key methods in establishing the absence of reentrance in Ising,[10–12,14] XY,[9] and possibly also in Dzyaloshinskii-Moriya XY spin glasses.[9,19,20,23]

II. Model and method. The Hamiltonian for the Q-state Potts model is

$$H=-\sum_{\langle i,j\rangle} J_{ij}\delta_{\sigma_i,\sigma_j}, \tag{1}$$

where $J_{ij}>0$ for ferromagnetic couplings and $J_{ij}<0$ for antiferromagnetic ones. $\delta_{\sigma_i,\sigma_j}$ is the Kronecker delta: the spin, σ_i at lattice site i can take Q states, $Q=0,1,2,\ldots Q-1$. The bond energy between two spins is $-J_{ij}$ if the two spins are in the same state $\sigma_i=\sigma_j$, and zero otherwise. The familiar Ising model is equivalent to a $Q=2$ state Potts model with a shift of total energy of the system, and a rescaling of the exchange coupling J_{ij} by a factor 2. Although ''less popular'' than the Ising model, the three-state Potts model is also important in modeling real condensed-matter systems. For example, the two-dimensional antiferromagnetic three-state Potts model on the frustrated *kagomé* lattice captures some of the essentials of the low-temperature thermodynamics of the Heisenberg antiferromagnet on that lattice.[28] Also, it has been suggested that the orientational freezing in molecular glasses, such as N_2-Ar and KBr-KCN, can be partially described by a three-dimensional three-state Potts spin-glass model.[3]

Here we consider the situation where the bonds J_{ij} in Eq. (1) are distributed randomly, and given by a quenched biased bimodal probability distribution, $\mathcal{P}(J_{ij})$:

$$\mathcal{P}(J_{ij})=x\,\delta(J_{ij}-J)+(1-x)\,\delta(J_{ij}+J). \tag{2}$$

A bond between sites i and j has a probability x to be ferromagnetic and of strength J, and a probability $1-x$ of being AF and of strength $-J$. We study the thermodynamic properties of this system on hierarchical lattices using the MKRG scheme.[9–12,14,19,29,30] One considers a sequence of b J_{ij} bonds in series, each we label $J^{(k)}$ $(k=1,2,\ldots b)$, where $(b-1)$ spins are summed over (we have dropped the subscript ij). The above Hamiltonian preserves its invariant form (apart from a spin-independent term) under the decimation of the $(b-1)$ spins. This results in a new effective coupling $J_{ij}(l+1)$, at the RG decimation step

$$\exp\{\beta J^{(n)}(l+1)\} = 1+\frac{Q}{\Pi_{k=1}^{k=b}(1+Q/\{\exp(\beta J^{(k)}(l))-1\})-1} \tag{3}$$

and $\beta=1/k_{\mathrm{B}}T$. In dimension d, $b^{(d-1)}$ such parallel paths of b bonds in a series, each with its end-to-end coupling $J^n(l+1)$, are then added together to give *one* new coupling

$$J_{ij}(l+1)=\sum_{n=1}^{n=b^{(d-1)}} J^{(n)}(l+1). \tag{4}$$

In practice, the procedure is implemented by first creating a large pool of N $(N\approx10^6)$ bare couplings, $J_{ij}(l=0)$, distributed according to Eq. (2). Then, b couplings are randomly picked out of that pool combined to create a serial coupling $J^n(l+1)$ as given by Eq. (3). Then, $b^{(d-1)}$ such couplings $J^n(l+1)$ are added together to give one new coupling $J_{ij}(l+1)$. The procedure is repeated N times to repopulate a new pool of N couplings $J_{ij}(l+1)$ at RG step $(l+1)$.

The nature of the magnetic phase at a given temperature T and concentration x of antiferromagnetic bonds is determined by monitoring the l dependence of the average value $\overline{J(l)}$ and the width $\Delta J(l)$ of the distribution of N bonds $J_{ij}(l)$. As $l\rightarrow\infty$, $\overline{J}$ and ΔJ evolve in the various phases as

$$\lim_{l\to\infty}\overline{J}\rightarrow0,\quad \lim_{l\to\infty}\Delta J\rightarrow0:\quad \text{paramagnetic}, \tag{5}$$

$$\lim_{l\to\infty}\overline{J}\rightarrow+\infty,\quad \lim_{l\to\infty}\frac{\Delta J}{\overline{J}}\rightarrow0:\quad \text{ferromagnetic}, \tag{6}$$

$$\lim_{l\to\infty}\overline{J}\rightarrow-\infty,\quad \lim_{l\to\infty}\frac{\Delta J}{\overline{J}}\rightarrow0\quad \text{antiferromagnetic}, \tag{7}$$

$$\lim_{l\to\infty}\Delta J\rightarrow\infty,\quad \lim_{l\to\infty}\frac{\overline{J}}{\Delta J}\rightarrow0:\quad \text{spin glass}. \tag{8}$$

To allow for the existence of an antiferromagnetic phase, we must work with odd values of b, as even values of b ''frustrate'' the antiferromagnetic phases and map an initial startup antiferromagnetically biased $\mathcal{P}(J_{ij})$ into a ferromagnetic phase already at iteration step 1. Here we focus on hierarchical lattices with $b=3$.

III. Results. The temperature vs concentration of antiferromagnetic bonds phase diagram for the three-dimensional $d=3$ case (with $b=3$) is shown in Fig. 1. The phases have been determined according to the criteria given above. Firstly, there is no AF or SG phase at nonzero temperature in this system in the whole range $0\leqslant x\leqslant1$. The most remarkable feature of this phase diagram is the existence of a reentrant ferromagnetic to paramagnetic phase transition for the range $x\in[0.765,0.855]$. The value of 0.855 obtained by extrapolating these nonzero temperature results agrees with the

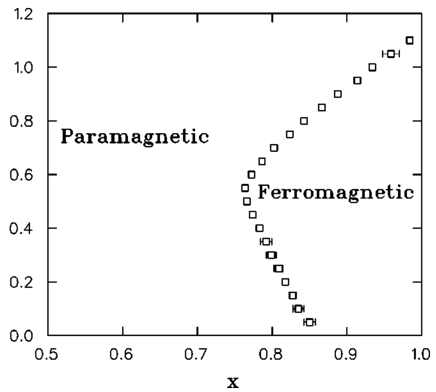

FIG. 1. Temperature T concentration x of antiferromagnetic bonds phase diagram for the $Q=3$ state Potts spin glass on a $d=3$, $b=3$ hierarchical lattices. Ferromagnetic to paramagnetic reentrance occurs in the range $0.765<x<0.855$. There is no spin-glass or antiferromagnetic phase in this model at nonzero temperature.

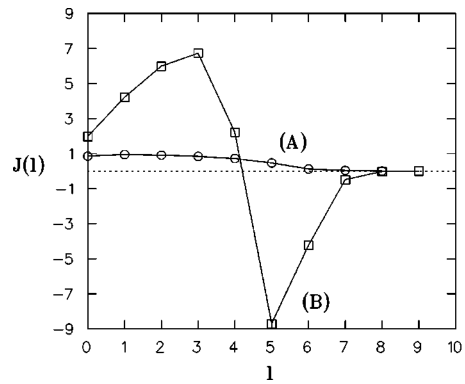

FIG. 2. Iteration number l dependence of the average coupling $\overline{J}(l)$ slightly in the paramagnetic phase close to the upper (curve A, $x=0.80$, $T=0.70$) and lower reentrant (curve B, $x=0.80$, $T=0.30$) P-F phase boundary.

one obtained by iterating the MKRG equations above at zero temperature exactly.[29] Similar results were obtained for $d=2$.

As observed and discussed in other papers,[9–12,14,19,29,30] the MKRG scheme is difficult to implement for spin-glass models at low temperatures (as $T\rightarrow 0+$). The reason for this is as follows. The occurrence of a ferromagnetic phase is monitored by the criterion $[\overline{J}\rightarrow+\infty, \Delta J/\overline{J}\rightarrow 0]$. In practice the ferromagnetic phase is detected when numerical overflow occurs as $l\rightarrow\infty$ on the ferromagnetic side of the P$-$F boundary. In a spin-glass model, where the distribution of $\exp\{\beta J_{ij}(l)\}$ is broad at low temperature in the ferromagnetic phase close to either the P-F or F-SG boundary, one encounters overflow at iteration step $l_{\max}$ way before $\overline{J}(l)$ has increased by several order of magnitude compared to $\overline{J}(l=0)$. In previous MKRG studies of spin glasses[9–12,14,19] the F-P or the F-SG phase boundary did not give any ''peculiar'' reentrant boundary, and the *extrapolated* finite-temperature F-P or F-SG boundary down to $T=0$ agreed with explicit MKRG calculations at $T=0$. Consequently, there has been until now no incentive to push the limit of the numerics in MKRG calculations of spin glasses as $T\rightarrow 0+$. However, in our case here, with this reentrant behavior, one could be concerned that the lower reentrant portion of the phase boundary is a numerical artifact. Specifically, it would *a priori* seem possible that the flow between 0.765 and 0.855 seems to indicate a paramagnetic phase according to the criterion given above for $1\leqslant l\leqslant l_{\max}$, but actually, be found to ''reverse itself'' for a value $l>l_{\text{rev}}$ with $l_{\text{rev}}>l_{\max}$, *if* numerical overflow bounds allowed it to be seen, and such that the asymptotic large length scale behavior for $0.765<x<0.855$ was ferromagnetic in the limit $l\rightarrow\infty$. In such a scenario, the reentrant region would result from a combination of short length scale physics added to a finite limit to overflow bounds imposed by the computer used for the calculations.

To address this issue, we parametrized each of the $\exp\{\beta J_{ij}(l)\}$ ''coupling terms'' via a two-component vector $\exp\{\beta J_{ij}(l)\}=\{M_{ij}(l),E_{ij}(l)\}$, where $M_{ij}(l)$ and $E_{ij}(l)$ are the mantissa and the exponent, in base 10, of $\exp\{\beta J_{ij}(l)\}$. The MKRG computer code was then rewritten in terms of direct algebraic mantissa operations and exponent shifting operations. With this improved version of the MKRG computer code, the upper limit for overflow for double-precision calculations on a 32-bit machine moves from 10^{308} to $\approx 10^{(10^{308})}$; a tremendous improvement. With this modification, the MKRG iterations become for all practical purposes devoid of overflow limitations. Our results with this version of the MKRG scheme gave an identical phase boundary to the one obtained using straightforward conventional double-precision calculations on a 32-bit machine. The results in Fig. 1 for $T/J\leqslant 0.25$ were actually obtained with the ''improved'' version of the MKRG scheme. We are therefore confident that the reentrant phase transition displayed by the $Q=3$ bimodal Potts spin-glass model on the $b=3$ hierarchical lattice in $d=2$ and $d=3$ is a genuine one, and not an artifact due to limitation imposed by numerical overflow at low temperatures.

The reentrance found here implies that the long-range ferromagnetic phase has higher entropy than the low-temperature paramagnetic phase. How can we understand this? A first hint can be obtained by considering the behavior of the flow of $\overline{J}(l)$ close to the upper and lower (reentrant) F-P boundary (see Fig. 2). We see that $J(l)$ approaches $J(l\rightarrow\infty)\rightarrow 0+$ *monotonously* as $l\rightarrow\infty$ close to the upper P-F boundary (curve A). However, $J(l)$ swings negative for intermediate length scale (curve B) for all temperatures below the lower (reentrant) P-F boundary before eventually approaching the trivial paramagnetic fixed point $J(l\rightarrow\infty)=0$. In other words, the system establishes short-range antiferromagnetic correlations in the reentrant portion of the phase diagram for $T<0.60$ and $0.755<x<0.855$.

Interestingly, for the Potts model, a ground state with antiferromagnetic correlations in presence of random ferromagnetic bonds has *lower* entropy than a ferromagnetic state with random antiferromagnetic bonds. Consider three spins, σ_1, σ_2, and σ_3 with ferromagnetic bonds J_{12} and J_{23}. If one of the bonds is, instead, antiferromagnetic, σ_2 becomes an idle and entropy-carrying spin with zero effective average exchange field at $T=0$ from ferromagnetically aligned σ_1 and σ_3. However, for σ_1 and σ_3 antiferromagnetically aligned via the other $b^{(d-2)}$ bonds, σ_2 is in a unique (nonidle) state for a ferromagnetic J_{12} bond and an antiferromagnetic J_{23} bond. Consequently, antiferromagnetically correlated triplets of spins $(\sigma_1,\sigma_2,\sigma_3)$ carry lower entropy in presence of random ferromagnetic bonds than a ferromagnetic state with random antiferromagnetic bonds. The antiferromagnetic state also has *lower energy*, $(E=-J)$, as compared to the ferromagnetic configuration $(E=0)$. Naively, in order to minimize the free energy, $F=E-TS$, this observation suggests that, upon cooling, local antiferromagnetic correlations should become more and more favorable since entropy is less important at low temperatures. This makes plausible that the system, at low temperatures, prefers to form ferromagnetic domains that are antiferromagnetically aligned (e.g., on intermediate length scales, as found in Fig. 2) rather than to keep the long-range ferromagnetic order established at higher temperatures. However, and this is an important point, true long-range antiferromagnetic order cannot occur since it is known that the lower critical dimension for antiferromagnetic order on the $b=3$ hierarchical lattice is four $(d=4)$.[27] Thus, for a certain concentration range of random AF bonds, reentrant behavior from a ferromagnetic phase to a paramagnetic phase with local antiferromagnetic correlations can occur. In $d=4$ (Fig. 3), the F→P reentrance disappears and gives rise, instead, as expected from the previous argument, to an F→AF transition upon cooling, where here ''AF'' refers to the Berker-Kadanoff phase characterized by a nontrivial *attractive* fixed point at nonzero temperature.[27]

IV. Conclusion. In conclusion, we have shown that the $Q=3$ Potts spin-glass model on two- and three-dimensional hierarchical lattices undergoes a ferromagnetic to paramagnetic reentrance upon cooling. This reentrance is due to (1) the combination of antiferromagnetically correlated spins at low temperatures in the phase ''rich'' in ferromagnetic bonds carrying less entropy than ferromagnetically correlated spins and (2) the fact that the lower critical dimension for antiferromagnetic order for the $Q=3$ Potts antiferromagnet on hierarchical lattices is four, while the lower critical dimension

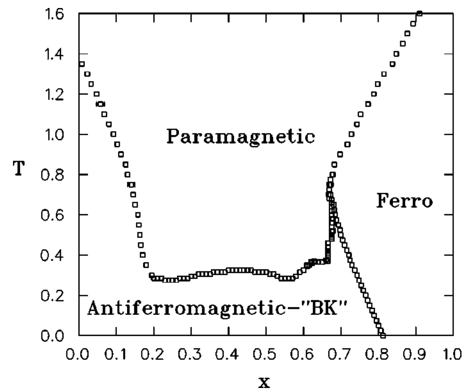

FIG. 3. Temperature T concentration x of antiferromagnetic bonds phase diagram for the $Q=3$ state Potts spin glass on a $d=4$, $b=3$ hierarchical lattice. The antiferromagnetic−''BK'' phase refers to the antiferromagnetically ordered phase characterized by a fixed point at finite coupling $\overline{J}(l=\infty)=-10.946\,61$ (Ref. 30).

for ferromagnetic order for the $Q=3$ Potts ferromagnet is one. Consequently, reentrance occurs at $T>0$ in two- and three-dimensional such lattices. The results presented here demonstrate that there is no *fundamental* reason forbidding a thermodynamic reentrant phase transition in *all* randomly frustrated systems. Our results open the possibility that reentrance might occur in some yet to be discovered real randomly frustrated systems with Euclidean lattices.[31] We hope that our results will stimulate further studies in that direction.

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