Entropic Effects in the Very Low Temperature Regime of Diluted Ising Spin Glasses with Discrete Couplings

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We study link-diluted $\pm J$ Ising spin glass models on the hierarchical lattice and on a three-dimensional lattice close to the percolation threshold. We show that previously computed zero temperature fixed points are unstable with respect to temperature perturbations and do not belong to any critical line in the dilution-temperature plane. We discuss implications of the presence of such spurious unstable fixed points on the use of optimization algorithms, and we show how entropic effects should be taken into account to obtain the right physical behavior and critical points.

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Introduction.—Frustrated systems may have very complex free-energy landscapes at low temperature T which in turn may give rise to very peculiar thermodynamical properties [1–4]. It was recently shown in Ref. [5] for the case of the two-dimensional Edwards-Anderson (EA) model that in such situations $T = 0$ computations as the ones of Ref. [6] may produce misleading results. In Ref. [7] it was shown that there are ways to improve on the results of Ref. [6] using $T = 0$ methods; however, the η exponent is still found to be nonuniversal; this could be due to the entropic effect, which is neglected in Ref. [7]. In this Letter we study entropic effects in the very low temperature regime of disordered models. We consider diluted spin glasses (SG) with discrete coupling distributions at very low temperature and show that previous computations of critical points were incorrect [8,9]. We explain why and we show how to compute the right critical points: considering first order corrections in T allows us to treat the entropic contribution to the free-energy correctly in the limit when T goes to zero. A similar idea has been applied also to models defined on random graphs [10]. Here we find that, on hierarchical as well as 3D lattices, the SG phase persists in a region of higher dilution than calculations done exactly at $T = 0$ would predict. In other words, we find SG ordering induced solely by entropic effects which is a phenomenon somewhat reminiscent of Villain's "order by disorder" [1,11].

We consider two SG models: one defined on the hierarchical lattice [12], where the Migdal-Kadanoff approximation is correct, and the other one on a three-dimensional (3D) lattice. In the former case, we are able to compute the distribution of effective couplings and of the free energies allowing us to determine exactly the location of the critical points and the whole phase diagram. For the 3D case, we have to resort to numerical simulations: using state-of-the-art Monte Carlo (MC) methods for disordered systems, we provide evidence that previously computed critical lines are likely to be incorrect, and by a numerical study of percolation properties we give bounds on the location of the right critical points.

Model.—We consider an Ising SG model defined by the Hamiltonian

$$H(\underline{\sigma}) = \sum_{(i,j)} J_{ij}\sigma_i\sigma_j, \quad (1)$$

with Ising spins $\sigma_i = \pm 1$ and the sum running over all the nearest neighbors pairs on the lattice. The couplings J_{ij} are quenched, independent and identically distributed random variables extracted from the distribution [13]

$$P_0(J) = (1 - p)\delta(J) + \frac{p}{2}[\delta(J - 1) + \delta(J + 1)]. \quad (2)$$

We are interested in the $T = 0$ critical point separating the paramagnetic phase ($p < p_{SG}$) from the SG phase ($p > p_{SG}$). We consider two lattices: the hierarchical lattice and the 3D simple cubic lattice for which the Hamiltonian in Eq. (1) corresponds to the EA model [14].

Hierarchical lattice.—The hierarchical lattice of G generations is obtained by applying the construction shown in the inset of Fig. 1 to all the links of the $G - 1$ generations lattice (the $G = 0$ lattice being a single link connecting two vertices). Such a construction is defined by two parameters: the number b of parallel branches, made of s bonds in series each. The effective dimension of the model is defined by $d = 1 + \ln(b)/\ln(s)$ and it is known that the lower critical dimension for the SG transition is close to $d_\ell \simeq 2.5$ [6,15,16]. Working with $d > d_\ell$ we have $T_{SG} > 0$ for $p = 1$ and a critical line in the (p, T) plane (see Fig. 1). We present results for $b = 3$ and $s = 2$ (i.e., $d = 2.585\ldots$), but we have checked their validity also for other choices of the parameters.

A model defined on the hierarchical lattice can be solved exactly by recursive decimation: starting from a lattice of G generations and summing over the spins introduced in the last generation one can easily obtain a lattice of $G - 1$ generations with renormalized couplings. At each step of

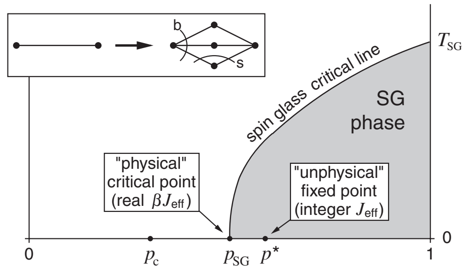

FIG. 1. Phase diagram of the diluted $\pm J$ spin glass in the temperature versus bond-density plane, where p_c denotes the geometric percolation threshold, p_{SG} the percolation threshold for spin glass order, and p^* the percolation threshold for spin glass order determined at $T = 0$. Inset: Elementary step for the construction of hierarchical lattice with $b = 3$ and $s = 2$.

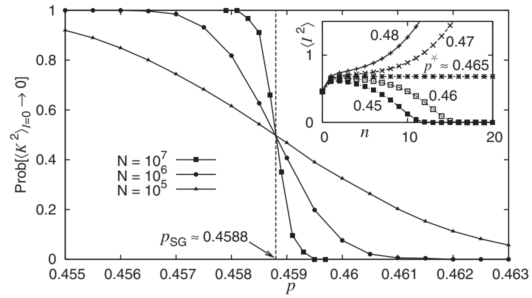

FIG. 2. The probability that the variance of the renormalized "entropic" couplings K goes to zero as a function of bond density p, for different sizes N of the population evolved numerically. The inset shows the behavior of the variance of the renormalized "energetic" couplings I, obtained analytically in the $N \to \infty$ limit.

this renormalization procedure the couplings undergo two elementary transformations: (i) each s-tuple of couplings in series produces an effective coupling $\tilde{J}$ and (ii) each b-tuple of effective couplings in parallel linking the same pair of variables is summed together, giving the renormalized coupling. In the $T \to 0$ limit, one renormalization step can be written as

$$\tilde{J}^{(n)} \stackrel{d}{=} \text{sgn}(J_1^{(n)} \times \cdots \times J_s^{(n)}) \min(|J_1^{(n)}|, \ldots, |J_s^{(n)}|), \quad (3)$$

$$J^{(n+1)} \stackrel{d}{=} \tilde{J}_1^{(n)} + \cdots + \tilde{J}_b^{(n)}, \quad (4)$$

where equalities hold in distribution sense and the index (n) stays for the number of renormalization steps. Applying these functional recursion equations, the initial distribution P_0 of couplings flows to the fixed point one P_∞. The critical density of links p^* is defined such that P^*_∞ is nontrivial, i.e., different from the paramagnetic one, $\delta(J)$, and the SG one, $[\delta(J - \infty) + \delta(J + \infty)]/2$.

In Ref. [8] Bray and Feng computed the distribution P^*_∞ under the assumption that the renormalized couplings remain integer, which is indeed a possible solution to Eqs. (3) and (4). Actually in Ref. [8] only three values for the couplings $(0, \pm 1)$ were considered; the extension to a symmetric distribution involving all the integer values between $-M$ and M is straightforward, and leads in the limit of large M to $p^* \simeq 0.465$. In the inset of Fig. 2 we show the variance of $J^{(n)}$ as a function of n for various values of p. This critical point p^* has been considered up to now the boundary between the paramagnetic and the SG phases. Nevertheless, we find that in the plane (p, T) the point $(p^*, 0)$ does not belong to *any* critical line; i.e., it is an isolated point (see Fig. 1), and for this reason it is irrelevant for the thermodynamics at any positive T. Even at $T = 0$ it does not correspond to the border between two different phases, i.e., $p^* \neq p_{SG}$.

In order to prove that the fixed point $(p^*, 0)$ is isolated as in Fig. 1, we study coupling renormalization at infinitesimal T. We start from the positive T rule for decimating $s = 2$ bonds in series (for $s > 2$ the same transformation must be applied more than once)

$$\tanh(\beta\tilde{J}) = \tanh(\beta J_1)\tanh(\beta J_2), \quad (5)$$

with $\beta = 1/T$. Similarly to [17], for very low T, we rewrite $J = TK$ in case J is vanishing for $T \to 0$, and $J = \text{sgn}(I)(|I| - TK)$ if $\lim_{T\to 0} J = I \neq 0$. The choice in the sign is dictated by the fact that thermal fluctuations decrease the coupling intensity. We have checked that higher order corrections in temperature are unnecessary in the $T \to 0$ limit. Plugging these new variables in Eq. (5) we find that in the $T \to 0$ limit the "energetic" component, I, gets renormalized following Eq. (3), while the "entropic" component, K, follows

$$\tilde{K} = K_1 \quad \text{if } |I_1| < |I_2| \quad (6)$$

$$\tanh(\tilde{K}) = \tanh(K_1)\tanh(K_2) \quad \text{if } I_1 = I_2 = 0 \quad (7)$$

$$\exp(2\tilde{K}) = \exp(2K_1)\exp(2K_2) \quad \text{if } I_1 = I_2 \neq 0. \quad (8)$$

Before renormalization, the original couplings are T-independent and distributed according to P_0; thus, we start with $I \in \{0, \pm 1\}$ and $K = 0$. The recursive equation for I is the one already studied above and gives a coupling flowing to 0 for $p < p^*$ (see inset of Fig. 2). Nevertheless, even if $I = 0$ for all the renormalized couplings, the entropic correction may be non-null, thus giving a nonzero correlation of the order of $\tanh(\beta J) = \tanh(K) \neq 0$, even in the $T \to 0$ limit. Please note that if the temperature was set to zero at the beginning of the calculation such a nonzero correlation would not be found.

Under renormalization the variance of entropic couplings goes to zero or diverges, depending on the value of p. In the main panel of Fig. 2 we show the probability that $\langle K^2\rangle_{I=0}$ flows to zero, where N is the size of the population used for simulating the decimation procedure. It clearly shows the existence of a critical value $p_{SG} \simeq 0.4588$ such that for $p < p_{SG}$ correlations decay to zero at large distances, while for $p > p_{SG}$ there are long-range correlations (of SG type, since $\langle K\rangle = 0$).

On hierarchical lattices, the inequality $p_{SG} < p^*$ holds in general, and implies that for $T = 0$ and $p \in (p_{SG}, p^*)$ the long-range order is induced solely by entropic effects. That is the two ground states obtained by fixing the outermost spins of the hierarchical lattice in a parallel or antiparallel way have exactly the same energy, but very different entropies; long-range correlations from the ground state with the largest entropy will dominate ensemble averaged correlations. Such long-range correlations arise because when summing two parallel effective bonds such that $\tilde{I}_1 + \tilde{I}_2 = 0$ it may be that $\tilde{K}_1 + \tilde{K}_2 \neq 0$; i.e., there is no perfect cancellation and an effective coupling of intensity $\mathcal{O}(T)$ persists. In the $T \to 0$ limit these couplings induce nonzero correlations, which may eventually increase under renormalization (as for $p > p_{SG}$). It is worth noticing that this mechanism for generating $\mathcal{O}(T)$ couplings may work perfectly well also when applying a decimation procedure on regular lattices [9].

A similar argument also tells us that on the very first steps of decimation, when K takes few and discrete values (for large n, K becomes dense on $\mathbb{R}$), exact cancellations, both in I and K, take place. If the original model had a bond density slightly larger than the percolating density p_c (for $b = 3$ and $s = 2$, $p_c = 0.389\,391\dots$) these exact cancellations would produce a renormalized lattice which is below the percolating point, preventing any long-range correlation from arising. So also the inequality $p_c < p_{SG}$ must hold in general for any frustrated model with discrete couplings on the hierarchical lattice.

Regarding the issue of the universality, we checked that starting from any point on the critical line extending from $(p_{SG}, 0)$ to $(1, T_{SG})$, see Fig. 1, the same fixed point coupling distribution is obtained; note that, at a positive temperature, couplings J/T gets renormalized exactly by Eq. (7). This fixed point distribution has nothing to do with the integer-valued one obtained from $(p^*, 0)$.

3D simple cubic lattice.—The phase diagram shown in Fig. 1 is exact for the SG model defined by Eq. (1) with coupling distribution from Eq. (2) on the hierarchical lattice (or equivalently in the Migdal-Kadanoff approximation). We present now evidence that the main qualitative features of that phase diagram are preserved when a 3D lattice is considered. With this in mind, we show by MC simulations and by percolation arguments that (i) a SG transition takes place at finite temperature for $p < p^*$, thus implying $p_{SG} < p^*$, and that (ii) there exists a percolating phase with no long-range order, thus implying $p_c < p_{SG}$ with $p_c = 0.248\,812\,6(5)$ [18].

The MC technique we use to simulate the 3D link-diluted $\pm J$ EA model close to the percolation threshold is a combination of the replica cluster update moves [19] embedded in parallel tempering [20] as described in Ref. [21] in alternation with standard Swendsen-Wang [22] cluster updates on each of the replicas. The additional Swendsen-Wang updates are very efficient close to percolation and speed up the simulation considerably [23]. This is an important issue because close to percolation we encounter noticeable finite-size effects, and therefore relatively large lattices have to be simulated to see a good signal for a SG transition below p^*. We use the value $p^* = 0.272(1)$ determined by Boettcher [9] from the behavior of the domain-wall defect energies of the ground states using an optimization algorithm [24].

To check for the presence of a SG transition we measure the second-moment correlation length $\xi(L, T)$ on a lattice of size L defined as [25]

$$\xi(L,T) = \frac{1}{2\sin(|\mathbf{k}_{\min}|/2)}\left[\frac{\chi_{SG}(\mathbf{0})}{\chi_{SG}(\mathbf{k}_{\min})} - 1\right]^{1/2}, \quad (9)$$

where the wave-vector-dependent SG susceptibility is

$$\chi_{SG}(\mathbf{k}) = \frac{1}{L^3}\sum_{\mathbf{x}}\sum_{\mathbf{r}} e^{i\mathbf{k}\mathbf{r}}\overline{\langle q_{\mathbf{x}} q_{\mathbf{x}+\mathbf{r}}\rangle}, \quad (10)$$

and $\mathbf{k}_{\min} = (0, 0, 2\pi/L)$ is the smallest nonzero wave vector allowed by periodic boundary conditions. We denote thermal averages by $\langle\cdot\rangle$ and disorder averages by $\bar{\cdot}$.

In Fig. 3 we display the behavior of $\xi(L, T)/L$ for four different values of p. In the upper left-hand panel we show the result below the percolation threshold ($p = 0.24 < p_c$) for which there is no SG transition as can be seen from the absence of a crossing of $\xi(L, T)/L$ for different lattice sizes. The upper right-hand panel shows the situation for $p_c < p = 0.2625 < p^*$ where again the curves do not cross and therefore there is no sign for a SG transition. For $p = 0.268$, slightly below p^*, we find—amongst noticeable finite-size effects—that the $\xi(L, T)/L$ for different lattice sizes do cross indicating the presence of a SG transition. The crossing point is moving slightly towards a smaller effective T_c as L is increased, but this is also the case for $p = 0.2725 \sim p^*$ and larger values of p. The fact

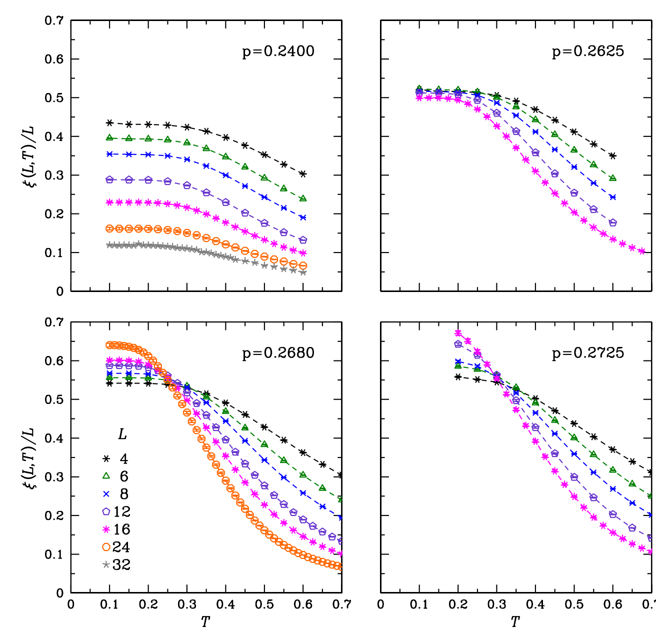

FIG. 3 (color online). $\xi(L, T)/L$ as a function of temperature for several system sizes L and different bond densities p.

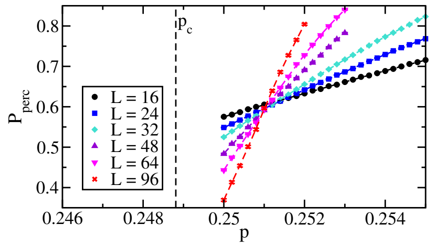

FIG. 4 (color online). Percolation probability in a 3D $\pm J$ diluted spin glass model, reduced with $T = 0^+$ rules.

that the crossing happens at a value of $\xi(L, T_c)/L \approx 0.6$, with a tendency to increase for larger L, is an important evidence for a SG transition since this value is a renormalization group invariant quantity and was found to lie between 0.60 and 0.65 in different recent studies of the 3D SG transition [21,26,27].

To show that indeed $p_c < p_{SG}$ holds in 3D, we apply to the Hamiltonian in Eq. (1) the reduction rules for weakly connected lattice sites (i.e., with degree 1 or 2) as described in Ref. [9]. Instead of applying these rules exactly at $T = 0$ we again keep terms of order T for the resulting effective couplings leading to a more connected remaining graph than the same procedure at $T = 0$ would produce. We apply the reduction rules recursively until the graph cannot be reduced any further. At this point we determine whether there exists at least one path, along which the remaining effective couplings are nonzero, that connects the $z = 0$ and $z = L$ plane of the 3D lattice with periodic boundary conditions in the x and y and open boundary conditions in the z direction. The presence of such a path is a necessary, but not a sufficient, condition for a SG phase. In Fig. 4 we show the probability that such a path exists as a function of p for different sizes L. It clearly shows that exact cancellations also in 3D lead to $p_c < p_{SG}$.

Discussion.—An important comment is in order: optimization methods that compute ground state energies as in Ref. [9] are typically sensible to the "unphysical" isolated critical point at p^* rather than to the "physical" critical point at p_{SG}. To detect the right critical point these optimization methods should be modified to include entropic effects. In Ref. [28] an attempt in that direction was made, leading to a change in physical observables. The decimation method used in Ref. [9] can be easily extended to consider first order corrections in temperature, thus leading to a more connected lattice after decimation.

However, even if a correct procedure is employed, taking into account entropic effects, the presence of the spurious fixed point at p^* may lead to very strong crossover effects. For example, for $p \in (p_{SG}, p^*)$, as long as energetic couplings are present, they dominate the behavior of any observable; the right physical behavior, given by entropic couplings, can be measured only at length scales where energetic couplings have disappeared, and these scales may be extremely large. In the $b = 3$ and $s = 2$ hierarchical lattice such a length scale is always larger than $s^{15} = 32\,768$, roughly. Increasing the dimensionality we find that p_{SG} and p^* get closer, thus making the crossover length even larger. This argument suggests that any numerical method at zero temperature is plagued by the unphysical fixed point up to unreachable length scales.

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