Critical Thermodynamics of the Two-Dimensional $\pm J$ Ising Spin Glass

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We compute the exact partition function of $2d$ Ising spin glasses with binary couplings. In these systems, the ground state is highly degenerate and is separated from the first excited state by a gap of size $4J$. Nevertheless, we find that the low temperature specific heat density scales as $\exp(-2J/T)$, corresponding to an "effective" gap of size $2J$; in addition, an associated crossover length scale grows as $\exp(J/T)$. We justify these scalings via the degeneracy of the low lying excitations and by the way low energy domain walls proliferate in this model.

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Spin glasses [1,2] are strongly frustrated materials that have challenged statistical physicists for many years. In particular, there is still no consensus on the nature of these materials' phase diagram, a very basic issue. Surprisingly, open questions remain even in the case of two-dimensional spin glasses. For instance, there is a long-standing dispute [3–5] concerning the $\pm J$ Ising spin glass: it is not clear what kind of singularity arises in its free energy at the critical temperature.

In this Letter we reconsider the nature of these singularities using recently developed methods [6,7] for computing the exact partition function of square lattices with periodic boundary conditions, focusing on the low T scaling properties of the model with binary couplings. We show that although the energy "quantum" of excitation above the ground state is $4J$, such excitations behave as *composite* particles; in fact the specific heat near the critical point scales as if the elementary excitations were of energy $2J$. We justify this picture using properties of excitations and domain walls in this model. Finally, the joint temperature and size dependence shows the presence of a characteristic temperature-dependent length that grows as $\exp(J/T)$, in agreement with hyperscaling.

The model and our measurements—The Hamiltonian of our two-dimensional ($2d$) spin glass is

$$H_J(\{\sigma_i\}) \equiv -\sum_{\langle ij \rangle} J_{ij}\sigma_i\sigma_j, \tag{1}$$

where the sum runs over all nearest neighbor pairs of Ising spins ($\sigma_i = \pm 1$) on a square lattice of volume $V = L \times L$ with periodic boundary conditions. The quenched random couplings J_{ij} take the value $\pm J$ with probability $1/2$. The partition function at inverse temperature $\beta \equiv T^{-1}$ is $Z_J = \sum_{\{\sigma_i\}} e^{-\beta H_J(\{\sigma_i\})}$ and can be written as

$$Z_J(\beta) = e^{2L^2\beta J}, \qquad P_J(X = e^{-2\beta J}). \tag{2}$$

Here $P_J(X)$ is the polynomial whose coefficient of X^p is the number of spin configurations of energy $E = (-2L^2 + 2p)J$. Saul and Kardar [4,5] showed that determining P_J can be reduced to computing determinants which they did using exact arithmetic of arbitrarily large integers. More recently a more powerful approach has been developed [6,7], based on the use of *modular arithmetic* to compute Pfaffians. With this algorithm, one first finds the coefficients modulo a prime number, thereby avoiding costly arbitrary precision arithmetic. Then the computation is repeated for enough different primes to allow the reconstruction of the actual (huge) integer coefficients using the Chinese remainder theorem.

The algorithm proposed and implemented in [6,7] is powerful enough to solve samples with $L \approx 100$; the total CPU time needed to compute Z_J grows approximately as $L^{5.5}$. In our study we have determined Z_J for a large number of disorder samples at different lattice sizes: for instance we have 400 000 samples at $L = 6$, 100 000 at $L = 10$, 10 000 at $L = 30$, 1000 at $L = 40$, and 300 at $L = 50$. The total computation time used is equivalent to about 40 years of a 1.2 GHz Pentium processor. For each sample we derive from Z_J various thermodynamic quantities such as the free energy $F_J(\beta) = -\beta^{-1}\ln Z_J$, the internal energy $U_J(\beta) = \langle H_J \rangle$, and the specific heat dU_J/dT. We also study in detail the number of ground states and of excited states. Note that flipping any spin changes the energy by 0, $\pm 4J$, or $\pm 8J$; the gap between the ground state and the first excited state is thus $4J$.

Low temperature behavior of c_V—The study of $2d$ Ising spin glasses has a long history. We will only discuss here results about the $\pm J$ model. It is generally agreed that this model is paramagnetic for $T > 0$, spin-glass ordering arising only as $T \to 0$. The critical region thus corresponds to $T \to T_c = 0$. Since there is an energy gap $4J$, the free energy should have a singularity of the form $\exp(-4J/T)$. This is difficult to check, in particular, via Monte Carlo where the free energy is not directly measurable. Instead, it is better to concentrate on the specific

heat density c_V. For that observable, the difference between the models with bimodal ($J_{ij} = \pm J$) and continuous couplings is striking: in the first case c_V goes to zero rapidly as $T \to 0$ while in the second there is a clear linear behavior.

Even though our computations provide us with the free energy, we also prefer to work with c_V. Note that c_V is related to a second derivative of the free energy so the corresponding singularities are directly related. Also, c_V should provide a cleaner signal as irrelevant "constants" such as the ground state energy that fluctuate from sample to sample have been subtracted out. Consider now any given sample. As $T \to 0$, we have the scaling

$$c_V \equiv \frac{\langle [H - \langle H \rangle]^2 \rangle}{L^2 T^2} \approx \frac{16 J^2 e^{S_1 - S_0} e^{-4J/T}}{L^2 T^2}, \qquad (3)$$

where S_0 and S_1 are the logarithms of the degeneracies of the ground state and first excited state energy levels for the given sample. (S_0 and S_1 are microcanonical entropies; we have dropped the index J denoting a sample dependence.) Note that $4J$ appears because it is the energy gap in our system. It thus seems unavoidable that c_V will have an $\exp(-4J/T)$ singularity. Surprisingly, in 1988, Wang and Swendsen [3] postulated that instead

$$c_V \approx T^{-p} \exp(-AJ/T) \qquad (4)$$

with $A = 2$. They performed a Monte Carlo study in which $A \approx 3$ for most of the temperatures they could access, but their effective A drifted and their final prediction was $A = 2$ from an analogy with a one dimensional model (we shall come back to this later). This issue was taken up a few years later by Saul and Kardar [4,5] who claimed $A = 4$; their work is based on exact computations of partition functions and thus does not suffer at low T from the thermalization problems of the Monte Carlo approach. We are aware of no specific heat measurements in this model since. How could A *not* be 4? The subtlety is that we must take $L \to \infty$ at fixed T, and only *after* can we take $T \to 0$; indeed Eq. (4) assumes $L = \infty$ whereas Eq. (3) assumes $T \to 0$ at fixed L.

Using the algorithm in [6,7], together with the availability of cheap and powerful computers, we have extended significantly the study of Saul and Kardar. For the sake of comparison, they had 80 samples at $L = 20$, 22, and 24, and 4 samples at $L = 32$ and $L = 36$. (They also had samples for $L \leq 18$.) We go much beyond that, both in lattice sizes and in the number of samples we consider. In the left part of Fig. 1 we show our first analysis of c_V as follows. Let us set $J = 1$. When $T \to 0$, if naive scaling ($A = 4$) holds, $\ln(T^2 c_V) + 4/T \approx$ const, while $\ln(T^2 c_V) + 4/T \sim [(4 - A)/T]$ if $A \neq A_{\text{naive}}$ and $p = p_{\text{naive}} = 2$. (The c_V resulting from our exact partition function computations has been averaged over disorder samples.) In the plot we see that for any given lattice size, when T becomes small enough there is a saturation toward the naive scaling behavior, i.e., the points go to a constant value. The physically relevant regime is the thermodynamic limit, given by the envelope of these curves; this envelope does appear and seems to be linear in $1/T$. Note that the envelope emerges only on quite large lattices ($L \geq 30$); because of this, the true scaling escaped detection by Saul and Kardar. The straight line in the left part of Fig. 1 is our best linear fit to the $L = 50$ data when $\beta \in [2.5, 5.5]$. It is a very satisfying fit and gives $A = 2.02 \pm 0.03$, close to the integer value $A = 2$.

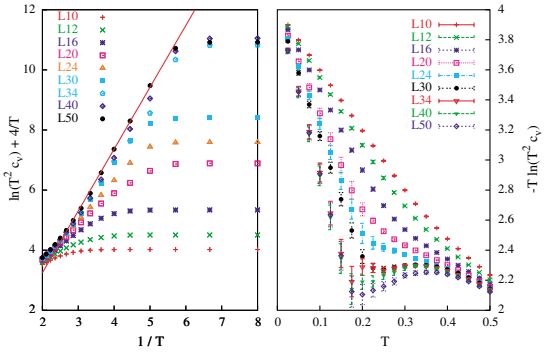

FIG. 1 (color online). On the left: $\ln(T^2 c_V) + 4/T$ versus $1/T$. On the right: $-T \ln(T^2 c_V)$ versus T.

We can also present the data in a slightly different fashion. In the right part of Fig. 1 we plot $-T \ln(T^2 c_V)$ versus T. Here the coefficient A is given by the intercept of the envelope's extrapolation to $T = 0$, the left axis of the picture. We can distinguish three regions. The first region is for very low T values. Here the naive (nonthermodynamic scaling) with $A = A_{\text{naive}} = 4$ is very clear. This region, where the intercept at $T = 0$ is 4, shrinks to zero with increasing lattice size. In a second region we have the physical scaling; for the large lattice sizes we have, the value $A \approx 2$ emerges. Notice that this is the same region where in the left part of Fig. 1 the $L = 50$ data lie on a straight line. The third and last region corresponds to "high" T ($T \gtrsim 0.4$) where one is far from the critical point and no scaling is apparent.

Our conclusion here is that thanks to the larger sizes available to us and to a technique that does not suffer from low temperature critical slowing down, the thermodynamic scaling of c_V is now finally clarified.

Ground state properties—Our computations also give the ground state energies and degeneracies. Theoretical arguments [8] suggest that the mean ground state energy density e_0 has power corrections in $1/L$:

$$e_0(L) = e_0^* + aL^{-2+\Theta^{(e)}}. \qquad (5)$$

We have $e_0^* = -1.4017(3)$ which agrees well with previous work. We also find $\Theta^{(e)} = -0.08(7)$; note that the prediction in [8] is that $\Theta^{(e)} = \theta_{DW}$, the exponent associated with domain wall energies. Following the work of

Hartmann and Young [9], there is general agreement that $\theta_{DW} = 0$ in the $2d \pm J$ model. Thus our estimate for $\Theta^{(e)}$ is in excellent agreement with the conjecture in [8].

We have performed a similar study for the mean ground state entropy density $s_0(L)$. We find $s_0^* = 0.0714(2)$ which compares well with the recent work of [10] in which $s_0^* = 0.0709(4)$. The fit also gives $\Theta^{(s)} = 0.42(2)$, though if we take into account systematic effects we cannot rule out $\Theta^{(s)} = 1/2$. We believe that this large value, unrelated to θ_{DW}, denotes the presence of a subtle organization of the ground states.

Anomalous density of excitations—The microcanonical entropy $S(E)$ of an energy level E is defined as the logarithm of the number of spin configurations having exactly that energy. Clearly, $S(E)$ is obtained from the knowledge of P_J as computed in Eq. (2). Of major interest is $S_1 - S_0$, the increase of entropy when going from the ground state energy E_0 to the lowest excitation energy. In the pure ferromagnetic model, the lowest excitation corresponds to taking the ground state (all spins parallel) and flipping a single spin. This gives $S_1 - S_0 = \ln(V)$. One says that the excitations are "elementary," and the system at low temperature is accurately described as a gas of independent excitations.

The situation changes dramatically when a large enough fraction of J_{ij} is negative, taking the system from a ferromagnetic to a spin-glass phase. In such a phase, the large V law of $S_1 - S_0$ is modified. This is illustrated in Fig. 2 where we plot our numerical estimate of $\overline{S_1 - S_0}$ as a function of $\ln(V)$. The dotted line is $\ln(V)$ while the dash-dotted one is $2\ln(V)$. We see that the true scaling behavior emerges only for large lattices and that the large V behavior is compatible with a $2\ln(V)$ growth. How can one interpret this anomalous growth? Imagine classifying all excitations in terms of the size of the cluster of spins flipped when comparing to a given ground state configuration. (Naturally, one may ignore all clusters of zero excitation energy, and it is enough to focus on connected clusters.) Just as in the ferromagnetic case, some of the excitations correspond to single spin flips;

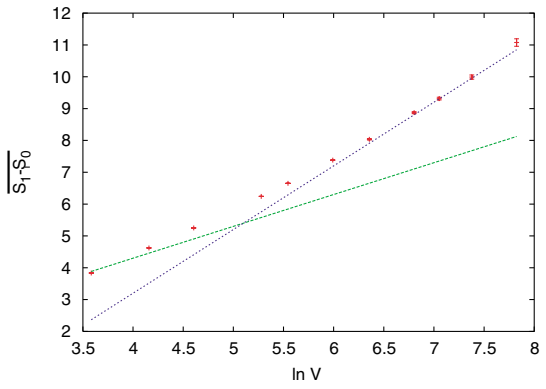

FIG. 2 (color online). $\overline{S(E_0 + 4J) - S(E_0)}$ versus $\ln(V)$ and the functions $\ln(V)$ and $2\ln(V)$.

there are $O(V)$ such objects. For any bounded-size cluster, the number of objects is $O(V)$, leading to $S_1 - S_0 \approx \ln(V)$. Since one has instead $\overline{S_1 - S_0} \approx 2\ln(V)$, finite-size clusters are irrelevant: necessarily large scale excitations *dominate* the set of excitations of lowest energy.

It is important to understand the nature of these large scale excitations, but unfortunately our computational approach does not give us configurations, it merely counts their number. There are other ways to gain insight into this problem. To begin, we consider as in [3] an analogy with the $1d$ pure Ising model. In that system, when using periodic boundary conditions, the lowest excitation is composite, corresponding to a pair of kinks with a total energy $4J$; however the "true" elementary excitations are *single* kinks, necessarily absent when using periodic boundary conditions. It is easy to see that for this $1d$ model the quantity $S_1 - S_0$ grows as $2\ln(V)$, i.e., as in our $2d$ system.

How may objects of energy $2J$ appear in our $2d$ lattices with periodic boundary conditions for which the gap is $4J$? To answer this question, consider in a ground state configuration any connected cluster of spins and associate to its surface the corresponding closed path $\mathcal{P}$ on the dual lattice [11]. (The cluster's surface is the set of edges connecting the cluster to its complement.) When flipping the cluster, the change in the configuration's energy comes only from those bonds crossing $\mathcal{P}$; in fact, for each such bond that is satisfied ($J_{ij}S_iS_j = 1$), the energy increases by $2J$, and otherwise it is decreased by $2J$. It is easy to see that all clusters lead to $\mathcal{P}$ with an even number of bonds, and thus excitation energies are quantized in units of $4J$. However, there are closed paths that are *not* associated with clusters: an example is a path that winds around one of the directions of the lattice. Such topologically nontrivial paths are called domain walls; when comparing periodic and antiperiodic boundary conditions, the set of bonds in the ground state that are changed from satisfied to unsatisfied or vice versa form exactly such a path. When L is odd, domain walls have energies $\pm 2J$, $\pm 6J, \ldots$ and the quantum $2J$ appears. Of course, to have a physical excitation, one needs to introduce domain walls in *pairs*; then the flipped cluster of spins is topologically a strip with a surface in two pieces, one for each domain wall, while its energy is a multiple of $4J$. Note that this is exactly what happened in the one dimensional case, the domain walls there being simply kinks which also arise in pairs.

To justify the anomalous scaling of $S_1 - S_0$, we appeal to the fact realized a few years ago by Hartmann and Young [9] that low energy domain walls proliferate in the $\pm J$ spin glass. Let δS be the typical entropy of a single domain wall; if we focus on those excitations of energy $4J$ associated with two domain walls of energy $2J$, we have an excess entropy $\Delta S = 2\delta S$. Our data thus suggest $\delta S = \ln(L^2)$; this law can be interpreted by saying that δS is the sum of a $\ln(L)$ term coming from the L possible mean

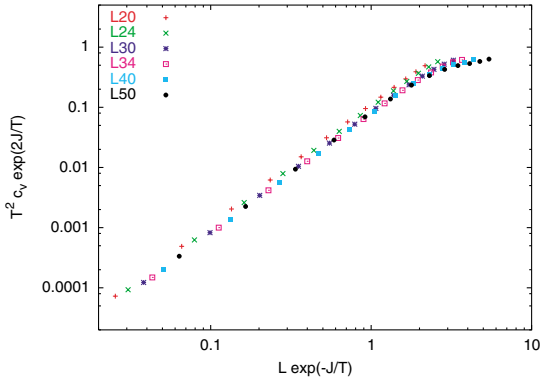

FIG. 3 (color online). Data collapse plot of the finite size scaling function $\mathcal{F}[L/\Lambda(T)]$ with $\Lambda(T) = \exp(J/T)$ and $J = 1$.

transverse positions of the domain wall and of an additional $\ln(L)$ term coming from the degeneracy (proliferation) at a given position. To extend this reasoning to the case of L even, we first remark that the domain walls there have energies $0, 4J, \ldots$. To have a "strip" excitation, we need one domain wall of energy $4J$ and one of 0 energy. Undoubtedly, the entropy of these domain walls increases with their energy; a simple pattern is obtained if we conjecture that the excess entropy increases by $\ln(L)$ every time the energy increases by the quantum $2J$. If this is so, the first domain wall will contribute $3\ln(L)$ to the excess entropy and the second $\ln(L)$, leading again to the desired $2\ln(V)$ result. Such a conjecture is quite elegant and should be amenable to testing using a recent Monte Carlo method [12].

Finite-size scaling—Given the result for $S_1 - S_0$, we go back to Eq. (3) to understand the finite-size scaling of c_V. When $T \to 0$ and $L \to \infty$ simultaneously, standard arguments lead to

$$T^2 c_V(L,T) e^{2\beta J} \approx \mathcal{F}[L/\Lambda(T)]. \tag{6}$$

Here $\Lambda(T)$ is a temperature-dependent length that determines the crossover between the thermodynamic scaling of c_V (going as $\exp[-2\beta J]$ when $L = \infty$) and the "naive" scaling as in Eq. (3). $\mathcal{F}$ is a finite-size scaling function; when its argument is large, $L \gg \Lambda(T)$, we recover the thermodynamic limit and thus necessarily $\mathcal{F}$ must tend toward a constant. (Since c_V is intensive, the L dependence must drop out.) On the contrary, when $L \ll \Lambda(T)$, we recover the behavior of Eq. (3) where c_V goes as $\exp(-4\beta J)$ *but* diverges as $L \to \infty$. Interestingly, in this regime c_V is not self-averaging and so one should apply finite-size scaling for the whole probability distribution of c_V. Just as before where we computed $\overline{S_1 - S_0}$ and not $\log[\overline{\exp(S_1 - S_0)}]$, we focus on the typical behavior and so we consider the median rather than the average of c_V (this distinction is relevant only in the very low T, unphysical region, while it is irrelevant in our scaling region for T, say, close to 0.3). When using this data we have a very reasonable data collapse, consistent with Eq. (6) as shown in Fig. 3. We find that this median scales as $L^2 \exp(-2\beta J)$ at low T and thus $\mathcal{F}(x) \approx x^2$ as $x \to 0$. This then gives

$$\Lambda(T) \sim \exp(\beta J). \tag{7}$$

Summary and discussion—We have investigated the critical thermodynamics of the $2d$ Ising spin glass with binary couplings. Our main conclusion is that the specific heat density scales as $c_V \sim \exp(-2J\beta)$. This scaling is "anomalous" in the sense that it does not follow from the size of the energy gap (which is $4J$). To find this scaling law, it is necessary to go to rather large systems, $L \geq 30$. We also found that the typical degeneracy of the first excited level grows about L^4 times faster than that of the ground state level. We believe this high degeneracy has its roots in the proliferation of domain walls, two domain walls enabling one to define a composite excitation. Such a picture justifies the analogy with kink pairs proposed many years ago by Wang and Swendsen [3]: each domain wall may indeed play the role of a kink, albeit with an additional entropy contribution. Finally, using finite-size scaling, we found a crossover length scale $\Lambda(T)$ that grows as $\exp(J/T)$; this divergence is exactly as expected from hyperscaling arguments.

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