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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, the associated 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 since 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, 4, 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 work 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 known properties of domain walls in this model. Finally, our finite size scaling analysis 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

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

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 $1/2$ as first proposed in [8]. 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

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

Here $P_J(X)$ is the polynomial whose coefficient of X^p is the number of spin configurations of energy $E = -2L^2 + 2pJ$. It was shown by Saul and Kardar [4, 5] 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 400000 samples at $L = 6$, 100000 at $L = 10$, 10000 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 the works most relevant for our study, namely those focusing on the thermodynamics of the $\pm J$ model. It is generally agreed that this model is paramagnetic for $T > 0$, spin glass ordering arising only as $T \rightarrow 0$. The critical region thus corresponds to $T \rightarrow T_c = 0$. 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 [9, 10]: in the first case c_V goes to zero rapidly as $T \rightarrow 0$ 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 $T \rightarrow 0$, we have the scaling

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

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; furthermore to lighten the expressions, 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, Wang and Swendsen [3] postulated in 1988 that instead

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

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 $L \rightarrow \infty$ at fixed T , and only after can we take $T \rightarrow 0$; indeed Eq. (4) assumes $L = \infty$ whereas Eq. (3) assumes $T \rightarrow 0$ 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 Fig. 1 we show our first analysis of c_V as follows. When $T \rightarrow 0$, if naive scaling ($A = 4$) holds, $\ln(T^2 c_V) + 4/T \approx \text{const}$, while $\ln(T^2 c_V) + 4/T \sim \frac{4-A}{T}$ if $A \neq A_{\text{naive}}$ and $p = p_{\text{naive}} = 2$. (The c_V resulting from our exact partition function computations has

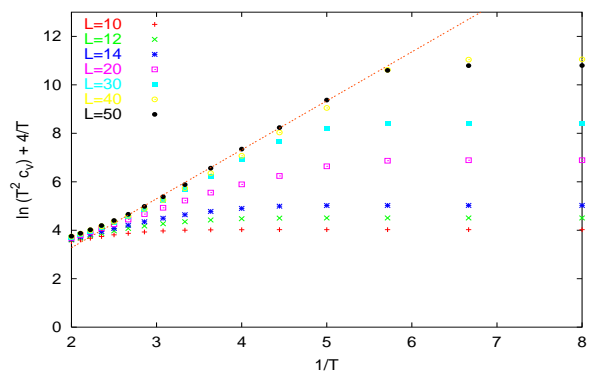


FIG. 1: $\ln(T^2 c_V) + 4/T$ versus $1/T$.

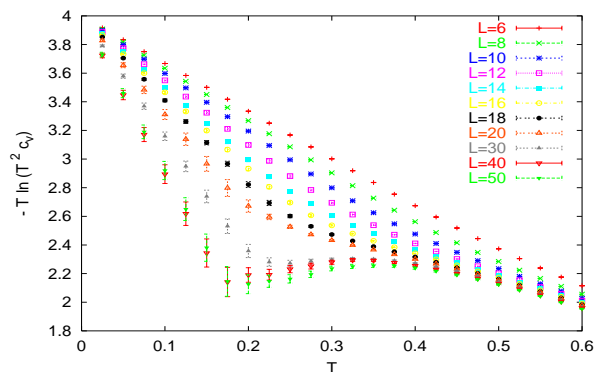


FIG. 2: $-T \ln(T^2 c_V)$ versus T .

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. With our statistics and lattice volumes we are not able to detect any signs of logarithmic corrections in Fig. 1, suggesting that $p = p_{\text{naive}} = 2$ indeed holds. The straight line 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 $A = 2$.

We can also present the data in a slightly different fashion. In Fig. 2 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 (non-thermodynamic 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

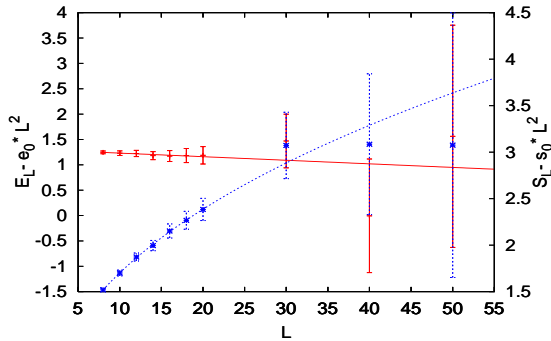


FIG. 3: Finite size corrections to the energy (left) and entropy (right) density in the ground state as a function of L .

value $A \approx 2$ emerges. One should notice that this is the same region where in 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 thus there is no scaling.

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 [11] suggest that the mean ground state energy density has power corrections in $1/L$:

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

Data and fits are shown in Fig. 3; 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 [11] is that $\Theta^{(e)} = \theta_{DW}$, the exponent associated with domain wall energies. Following the work of Hartmann and Young [12], 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 [11].

We have performed a similar study for the mean ground state entropy density $s_0(L)$. The data and resulting fit are displayed in Fig. 3, leading to $s_0^* = 0.0714(2)$ which compares well with the recent work of [13] 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 an interesting and subtle organization of the ground states.

Anomalous density of excitations — The partition function Z_J also gives the number of configurations of energy $4J$ above the ground state level. Of main interest is the excess entropy $S_1 - S_0 \equiv S(E_0 + 4J) - S(E_0)$ of this level where E_0 is the ground state energy. In Fig. 4 we plot $S_1 - S_0$ vs $\ln(V)$ where $V = L^2$. The dotted line is $\ln(V)$ while the dash-dotted one is $2\ln(V)$. We

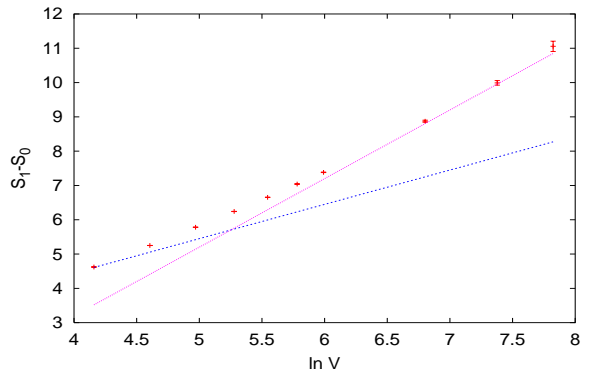


FIG. 4: $S(E_0 + 4J) - S(E_0)$ versus $\ln(V)$ and the functions $\ln(V)$ and $2\ln(V)$.

see that the true scaling behavior emerges only for large lattices. How can one interpret the $2\ln(V)$ scaling? In the $2d$ ferromagnetic Ising model, the lowest excitation corresponds to taking the ground state (all spins parallel) and flipping a single spin. This leads to $S_1 - S_0 = \ln(V)$. One says that the excitation is “elementary”, and the system is described quite accurately as a gas of independent excitations at low temperature. In the case of our spin glass, we naturally also have nearly independent spin flips among the excitations. However, since we have $S_1 - S_0 \approx 2\ln(V)$, we are forced to conclude that single spin flips are irrelevant: necessarily large scale excitations *dominate* the set of excitations of energy $4J$.

Following Wang and Swendsen, we consider an analogy with the $1d + J$ Ising model. In that system, when using periodic boundary conditions, the lowest excitation is composite, corresponding to a kink pair of 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.*, the same law as we find in our $2d$ system. One can then conjecture that the “physically relevant” gap in our $2d$ model is $2J$ rather than $4J$; this then leads one to guess that $A = 2$ exactly.

It is not clear what we learn from this “analogy”; in particular, one does not see why it should apply to the $2d$ and not to the $3d$ model. We propose here a possible mechanism for the anomalous scaling of $S_1 - S_0$ as follows. The starting point is the fact that zero energy domain walls arise in an important fraction if not the majority of the disorder samples in the $2d \pm J$ model [12]. (This phenomenon does not arise in $3d$.) A single domain wall does *not* provide an excitation for our system because of the periodic boundary conditions: we need instead two domain walls; one will be of zero energy, the other of energy $4J$. These form the analogs of the (composite) kink pairs in the $1d$ system. For symmetry reasons, let us consider first the case where L is odd. Then the lowest domain wall energy (using periodic boundary conditions)

is $2J$ instead of 0. Having two domain walls gives an excitation energy $4J$; we conjecture that each such domain wall has an excess entropy of $\ln(L^2) = \ln(V)$: we expect one $\ln(L)$ term to come from the possible mean transverse positions of the interface, and another from the degeneracy at a given position. The total excess entropy compared to that of the ground state would thus be $2\ln(V)$ which is the desired result. This argument can be extended to L even. One of the domain walls will have zero energy, the other an energy $4J$. 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 $\ln(L)$ to the excess entropy and the second $3\ln(L)$, leading again to the desired $2\ln(V)$ result. Such a conjecture is both elegant and completely consistent with our findings.

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

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

Here $\Lambda(T)$ is a temperature dependent length that determines the cross-over 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 towards a constant. (Note that 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), so necessarily $\mathcal{F}(x) \approx x^2$ as $x \rightarrow 0$ to get the correct L dependence. (Recall that we found $S_1 - S_0 \sim 2\ln(V)$.) This leads immediately to

$$\Lambda(T) \sim \exp(-\beta J) \quad (7)$$

up to a multiplicative factor that may include powers of T . This scaling form is confirmed when analyzing the c_V data in Fig. 1 as follows. To each L associate the temperature $T^*(L)$ where the horizontal asymptote crosses the envelope (the slanted line). The value $T^*(L)$ gives the temperature at which $L = \Lambda(T)$; from this we obtain $\Lambda(T)$ values whose scaling is compatible with Eq. (7).

Summary and discussion — We have focused on the critical thermodynamics of the $2d$ Ising spin glass with binary couplings. Our main conclusion is that the specific heat density scales as $c_V \sim \exp(-AJ\beta)$, where A turns out to be very close to 2. 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 $L \geq 30$ and

to understand the finite size effects. The work of Saul and Kardar [4, 5] incorrectly concluded that $A = 4$ most certainly because they used too small lattice sizes. We also found that the degeneracy of the first excited level grew 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, and that these excitations are composite, justifying 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 that the length scale $\Lambda(T)$ controlling finite size effects for c_V scaled as $\exp(J/T)$. This is exactly as expected from hyperscaling arguments which assume that the singular part of the free energy density goes as Λ^{-d} in dimension d ; taking $d = 2$ and an exponential singularity for Λ gives $c_V \sim \Lambda^{-2}$ up to power corrections in T . Finally, a study of the $T = 0$ physics allowed us to validate the conjecture $\Theta^{(\epsilon)} = \theta_{DW}$ proposed in [11]. We hope that this work will stimulate further studies, for instance to test the conjectures we put forward concerning the role of domain walls.

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