

Low T scaling in the binary $2d$ spin glass

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Abstract

We investigate $2d$ Ising spin glasses with binary couplings via exact computations of the partition function on lattices with periodic boundary conditions. After introducing the physical issues, we sketch the algorithm to compute the partition function as a polynomial with integer coefficients. This technique is then exploited to obtain the thermodynamic properties of the spin glass. We find an anomalous low temperature scaling of the heat capacity $c_v \sim e^{-2\beta}$ and that hyperscaling holds.

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1. The model

The Ising model (with ferromagnetic interactions $J_{ij}=1$ and its translational symmetry) can be seen as a first approximation of real systems where there are impurities. Considering disordered systems (more specifically, we shall deal with spin glasses) can be seen as a further step that increases the complexity: translational invariance is explicitly broken by the quenched disorder, and frustration appears through the competition of ferromagnetic and anti-ferromagnetic bonds:

$$H \equiv - \sum_{ij} J_{ij} S_i S_j. \quad (1)$$

Here the couplings J_{ij} are chosen from some symmetric distribution, for example a Gaussian distribution, or a bimodal distribution in which case $J_{ij}=\pm 1$; thus, the last case is referred to as the binary coupling case.

The typical approach of theoretical physics is to try to simplify situations that we know to be very complex,

involving for example a huge number of degrees of freedom. One thus introduces models that can describe the macroscopic characteristics of the system without all the microscopic details. Then one wants to know whether one has a phase transition with the correct features, what is the nature of the critical behavior, what are the exponents that govern it. . .

A typical starting point is mean field theory. In the case of spin glasses, mean field theory has been solved [1] and it unveils a very complex structure in phase space (involving at low temperatures T , the so-called Replica Symmetry Breaking, RSB). What happens in finite dimensions remains controversial in spite of many years of work [2]. One expects the upper critical dimension to be 6, and the lower critical dimension to be close to 2.5: in three dimensions, we are very confident that there is a phase transition.

One wants to understand whether a spin glass phase (with a frozen state with no spontaneous magnetization) exists, and what happens as one gets close to the critical temperature T_c . One of the possible approaches to understand these systems is to compute directly what happens at $T=0$ by studying the ground state and excited states of the system.

Following the McMillan renormalization approach [3], the domain wall energy, that is the difference of ground-state

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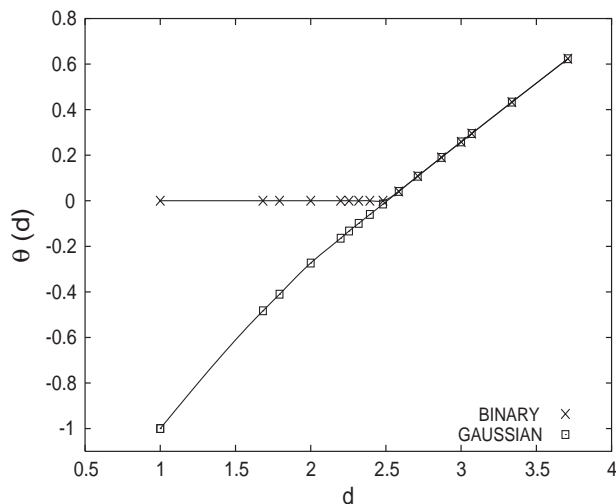


Fig. 1. The exponent θ in a family of Migdal–Kadanoff models defined for continuous dimensions d : note the difference between the Gaussian (\square) and binary (\times) models.

energies with periodic and anti-periodic boundary conditions, corresponds to the effective interaction of block spins at the scale L of the lattice size:

$$\Delta E = E_p - E_a \sim L^\theta, J \sim JL^\theta.$$

A first (slightly naive) classification says that depending on the sign of the exponent θ the system belongs to one of three different classes:

- $\theta > 0$: the interaction becomes stronger at large distance, the thermal fluctuations are irrelevant and the frozen phase exists also at finite temperature;
- $\theta < 0$: the thermal fluctuations destroy the spin glass order at any non-zero temperature;
- $\theta = 0$: marginal behavior: the system is at its lower critical dimension, suggesting that the correlation length grows exponentially.

For the Ising spin glass in $2d$ with a Gaussian distribution of the disorder, the domain-wall exponent is negative ($\theta \approx -0.29$), and the spin glass phase does not survive at non-zero temperature. For the case of the bimodal distribution in $2d$, $\theta = 0$. Following the classification we have given, this suggests that Ising spin glasses with two different realizations of the disorder (different microscopic characteristics) may belong to two different classes; then the microscopic characteristics would influence the critical behavior of the system.

This conclusion should hold if $\theta = 0$ is really a complete signal of being at the lower critical dimension for the system. But is that true? If we look for example at a class of Migdal–Kadanoff approximations, for the case of the bimodal distribution, θ is equal to zero for all dimensions below or equal to the lower critical dimension (see Fig. 1); so, in this case, the fact that $\theta = 0$ does not imply that one is at a lower critical dimension [4].

2. The heat capacity of the $\pm J$ spin glass

The best way to check what happens in our two dimensional spin glass is to look at the scaling of the correlation length close to the critical temperature. When $\theta < 0$, the McMillan scaling picture shows that $\xi(T) \sim T^{1/\theta}$ as $T \rightarrow 0$. The thermal exponent ν is thus given by $\nu = -1/\theta$. This conclusion is fine (and is confirmed [11]) for the Ising spin glass with Gaussian couplings ($\theta \approx -0.29$). But in the case of the $\pm J$ spin glass, $\theta = 0$, and so the expectation there is that ξ diverges faster than any inverse power of T as $T \rightarrow 0$. A likely behavior is that the correlation length grows exponentially in $1/T$.

Unfortunately looking directly at the correlation length can be cumbersome. Using Monte Carlo simulations, it is possible to get all the information about configurations and energies, but the problem is equilibration at very low T (since $T_c = 0$). A different possible approach is the calculation of the whole partition function: in this way, we can escape the problem of equilibration, but we do not have any information about the microscopic configurations of the elementary variables, and we have to rely on the measurement of some other thermodynamic quantity.

When calculating the partition function, we determine the degeneracy of all energy levels of the system: from that it is very easy to extract the heat capacity c_v or other observables like the entropy. From these data we shall perform extrapolations to get the behavior in the thermodynamic limit.

The 1988 work by Wang and Swendsen [5] gives some information about the low T scaling of the heat capacity. Using an optimized Monte Carlo, they concluded that the scaling of c_v is “anomalous”, in the sense that c_v scales for low T as $e^{-2\beta J}$, even though the energy gap is $4J$. Indeed, in standard systems, if $\Delta E = E_1 - E_0$ is the lowest excitation energy (the gap), c_v goes as $e^{-\beta \Delta E}$.

A possible explanation of this anomalous scaling may be found by looking at the case of the one-dimensional (pure) Ising model. The pure Ising model has a marginal behavior in $1d$, its lower critical dimension. For the finite size system with **periodic boundary conditions** at fixed volume and very low T , c_v goes as $e^{-4\beta J}$, since the minimum energy excitation is $4J$ (see Fig. 2).

In Fig. 2 the lower line is for spins $S_i = -1$, while the upper line is for spins $S_i = +1$. Starting from the ground state, if we want to flip spins and make a minimum energy excitation, because of the periodic boundary conditions, this minimum energy excitation has always an energy cost equal to $4J$ ($2J$ on the left, when the lower line jumps to the upper, and $2J$ on the right when the upper line jumps to the lower).

If we look to the $1d$ pure Ising model with free boundary conditions, the minimal energy excitation is $2J$, and



Fig. 2. A kink–antikink pair excitation when using periodic boundary conditions.



Fig. 3. A single kink excitation when using free boundary conditions.

$c_v \sim e^{-2\beta J}$ (see Fig. 3). Because the boundary conditions are free, the minimum excitation costs only $2J$ (when the lower line jumps to the upper).

An exact computation of c_v for the $1d$ Ising model is easy, and it gives that in the thermodynamic limit $c_v \sim e^{-2\beta J}$. Why does the minimum excitation with free boundaries survive in the thermodynamic limit? The main point is that the $4J$ excitations are not elementary: their number grows as V^2 , and they are composite, made by assembling elementary excitations of energy $2J$, whose number grows linearly with the system's volume.

Five years after the Wang and Swendsen work, Saul and Kardar [6] reexamined the problem by calculating the partition function using the Kac–Ward formula. Making the comparison with the fully frustrated model, where the exact solution gives $c_v \sim \beta^3 e^{-4\beta J}$, they concluded that the scaling of the heat capacity is governed by the energy gap, $c_v \sim \beta^\rho e^{-4\beta J}$, but with $\rho \neq 0$. We will see later that it is not appropriate to make this analogy between the fully frustrated model (that does not contain disorder) and a spin glass model.

Our approach [7] is based on the exact computation of the partition function for finite lattices, using the algorithm based on the work of [8] and [9].

3. The algorithm

Our model can be represented by a weighted graph where the sites of the model play role of nodes and the interactions J_{ij} between spins the role of weights w_{ij} of the edges of the graph. Then all the states of an Ising spin glass are equivalent to all possible cuts of the graph $G(V, E)$ (V is set of all sites, and E is set of all edges). A cut C is a partition of V into two parts V_1 (spins equal to $+1$) and V_2 (spins equal to -1):

$$H(\sigma) = -\sum_{\{i,j\} \in E} J_{ij} \sigma_i \sigma_j = \sum_{\{i,j\} \in C} J_{ij} - \sum_{\{i,j\} \in E/C} J_{ij} = 2w(C) - W, \quad (2)$$

where $W \equiv \sum_{\{i,j\} \in E} J_{ij}$, and $w(C) \equiv \sum_{\{i,j\} \in C} J_{ij}$. For any partition of V we can define the *generating function of cuts*

$$C(G, x) = \sum_{\text{cut } C} x^{w(C)} = \sum_k c_k x^k.$$

We can connect this to the partition function of the model by the low-temperature series:

$$\begin{aligned} Z &= \sum_{\sigma} e^{-\beta H(\sigma)} = 2 \sum_{\text{cut } C} e^{\beta(2w(C)-W)} = 2e^{\beta W} \sum_{\text{cut } C} e^{-2\beta w(C)} \\ &= 2e^{\beta W} C(G, e^{2\beta}). \end{aligned}$$

Consider now the high-temperature expansion which gives the partition function as a power series (with only even powers) of $\tanh(\beta J_{ij})$

$$Z = 2^V \prod_{\{i,j\} \in E} \cosh(\beta J_{ij}) \sum_{U \subset E} \prod_{\{i,j\} \in U} \tanh(\beta J_{ij}). \quad (3)$$

Given this series (in $\tanh(\beta J_{ij})$), it is not difficult to construct the low-temperature series in $e^{-\beta J_{ij}}$, which is more convenient for most computational purposes. Indeed there is a “1-1” mapping between weighted subgraphs associated with these two expansions. In graph theoretical terms this Expression (3) for the partition function is in fact a generating function for the *Eulerian subgraphs*, $\varepsilon(G, x)$. An *Eulerian subgraph* is a set of edges U such that each vertex of V is incident to an even number of edges from U (the even powers of $\tanh(\beta J_{ij})$ in the expansion).

To compute $\varepsilon(G, x)$ one relies on a mapping [10] to the problem of *perfect matching*, which consists in determining a set of edges P such that each vertex of V is incident to exactly one edge from P . This requires modifying the graph G by splitting the vertices; the problem is then translated to the generating function of all *perfect matchings* of the modified graph G_s of larger size [10].

Our model is defined on a $2d$ lattice with periodic boundary conditions: the underlying topological object is a torus (i.e., a manifold of genus $g=1$): a graph G of genus g has 4^g *relevant orientations* such that a suitable linear combination of the corresponding Pfaffians is equal to the generating function of perfect matchings of G_s . A *Pfaffian* is an object (similar to a determinant) which can be defined for a given graph G_s given an orientation of each of its edges. If we put an appropriate orientation on G_s , we define the matrix A whose elements are

- $a_{ij} = x^{w_{ij}}$, if (i, j) is a directed edge;
- $a_{ij} = -x^{w_{ij}}$, if (j, i) is a directed edge;
- $a_{ij} = 0$, otherwise.

To define the Pfaffian, first consider all possible partitions of the index set $\{1, 2, \dots, 2n\}$ into two pairs $i_1 < j_1, i_2 < j_2, \dots, i_n < j_n$ (here $2n$ is the number of nodes of G_s). This partitioning corresponds to assigning which is the starting node and which is the ending node for every link: this assignment is given by the orientation of the graph that we have discussed before. Then each term contributing to the Pfaffian is a product of matrix elements weighted by the sign of the permutation of the nodes $(i_1, j_1, i_2, j_2, \dots, i_n, j_n)$:

$$P_f(A) = \sum_P \text{sgn}(P) a_{i_1 j_1} a_{i_2 j_2} \dots a_{i_n j_n}.$$

In practice, the Pfaffian for this type of graph can be computed efficiently. For our $2d$ model with periodic boundary conditions, we need to evaluate 4 Pfaffians, then taking a suitable linear combinations of the four Pfaffians gives the generating function of perfect matchings of the modified graph G_s .

In any implementation of the algorithm, a big problem is the precision needed during the calculations. To approach the thermodynamic limit, we need large lattices (at least $L \sim 50$), that means that the number of relevant states is very large (2^{L^2}): calculations with such large numbers can easily run into troubles because of numerical precision.

In the present implementation of the algorithm, to avoid the precision problem, all the calculations are made modulo some prime number. The following results guarantee that we can eventually reconstruct the full partition function without ambiguities.

A first theorem: let $P(x)$ be a polynomial of degree n with integer coefficients, $GF[m]$ a finite field of size $m > n$ and x_0, x_1, \dots, x_n distinct elements of $GF[m]$. Then there exists a unique polynomial $Q(x)$ of degree n over $GF[m]$ such that

$$Q(x_i) = P(x_i) \pmod{m}, \quad i = 1, \dots, n.$$

Moreover, the coefficients of $Q(x)$ are equal to the coefficients of $P(x) \pmod{m}$.

A second theorem: Let p_1, p_2, \dots, p_k be k different prime numbers. Then for any a_1, a_2, \dots, a_k , $0 \leq a_i < p_i$, there is exactly one x , $0 \leq x < \prod_{i=1}^k p_i$, such that

$$x \pmod{p_i} = a_i, \quad i = 1, \dots, k.$$

After repeating the calculation of the coefficients of $C(G, e^{2\beta})$ for a large enough number of primes (so that $\prod_{i=1}^k p_i > 2^V$), we can reconstruct the complete partition function. The computations for different prime numbers are independent (making parallelization trivial): for every prime number, we get the partition function as a polynomial modulo the prime number. Then using the Chinese Remainder Theorem (CRT), we can reconstruct the full polynomial:

- we take k prime numbers p_1, p_2, \dots, p_k so that $\prod_{i=1}^k p_i > 2^V$, in such a way to satisfy the requirements of the Chinese Remainder Theorem (since the coefficients of our polynomial can not be bigger than 2^V);
- for all our prime numbers p_i we determine the polynomial partition function modulo p_i . We then “compose” the partial coefficients and find the complete polynomial;
- we choose $m+1$ distinct points x_0, x_1, \dots, x_m , where m is the maximum possible degree of the generating function; for any of the points x_i , we calculate the 4^s Pfaffians, and we obtain the value of the generating function of perfect matchings at the points x_i (we know the connection between generating functions of perfect matchings and the partition function of our system);
- all operations are performed modulo p_i : now using the results for the generating function at all the points x_i we make an interpolation (still in $GF[p_i]$);
- we repeat the procedure for all chosen p_i . When finished, we apply the CRT and we get the complete partition function of our system.

4. Results

4.1. Scaling of c_v

The previous algorithm, which output is the list of all energy levels and their degeneracies for the given disordered sample (the J_{ij}), allows one to easily determine any physical quantity that can be calculated from the partition function. We are interested in the behavior of the heat capacity C_v

$$C_v = \frac{d}{dT} \langle E \rangle,$$

$$C_v = \frac{\langle E^2 \rangle - \langle E \rangle^2}{T^2}.$$

If V is the total number of sites, we have $C_v = c_v V$. The scaling of heat capacity is connected to the scaling of the energy–energy correlation length, and, through the hyper-scaling relation, to the exponent of the spin–spin correlation length.

The subtle differences in the behavior of heat capacity for different lattice sizes can be seen on the upcoming figures. Consider the expected form for c_v at low T :

$$c_v = T^{-2} e^{-\frac{A}{T}} (1 + aT + bT^2).$$

Then we have

$$-T \log(c_v T^2) = A - T \log(1 + aT),$$

leading us to focus on the function

$$-T \log(c_v T^2) = A - aT^2.$$

With the choice of the y axis as the function $-T \log(c_v T^2)$, we see that in the thermodynamic limit, the curves should touch the y axis at the point A which gives the true (thermodynamic) scaling exponent for c_v , with quadratic corrections in T .

In Fig. 4 we can distinguish three different regions in T .

First, on the right, the region with high T ($T > 0.5$) is not relevant for the scaling close to the critical point ($T_c = 0$).

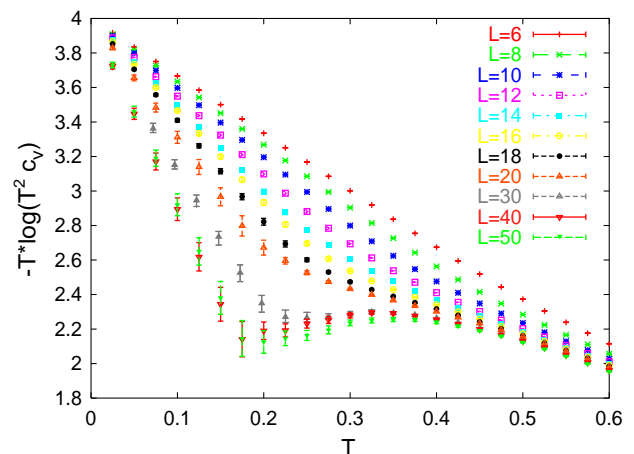


Fig. 4. $T \log(T^2 c_v)$ versus T .

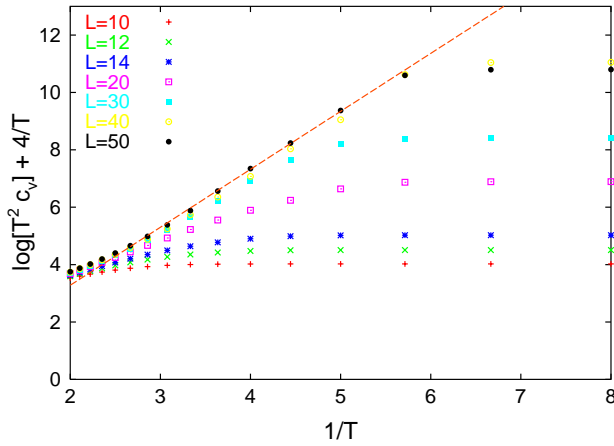


Fig. 5. $\log(T^2 c_v) + 4/T$ versus $1/T$. The straight line is for our best fit to the $L=50$ data (see the text for details).

On the left, the region has too low T ($T < 0.2$): the system is away from the thermodynamic limit (the system size is too small compared with the correlation length at these temperatures); the scaling of c_v for $T < 0.2$, $c_v \sim \beta^2 e^{-4/T}$, is not physically relevant, it is not the scaling that appears in the macroscopic system.

In the intermediate region ($0.2 < T < 0.5$), we start to reach the thermodynamic limit with our accessible lattice sizes: we see an envelope curve which seems to be a quadratic function in T . From the graphic in this range of T , it is obvious that the true thermodynamic exponent is very different from 4. If Saul and Kardar missed this point, it is mainly because they were limited to small lattices and to lower statistics.

From Fig. 5 we can guess what the thermodynamic scaling exponent is. Consider the expected form

$$c_v \sim \beta^2 e^{-A\beta}.$$

Then,

$$\log(\beta^{-2} c_v) \sim -A\beta,$$

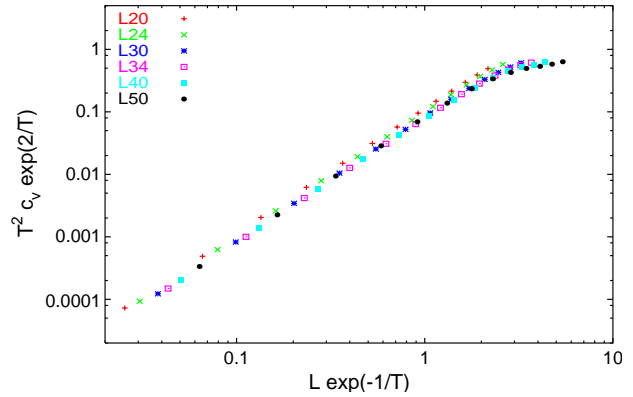


Fig. 7. Finite size scaling plot for c_v .

leading us to plot

$$y(T) \equiv \log(\beta^{-2} c_v) + 4\beta = (4 - A)\beta.$$

The points from the intermediate T region ($0.2 < T < 0.5$) should lie on the same line with a slope equal to $4 - A$, where A is the true scaling exponent; we also expect that the points from the too low T region will saturate (leading to horizontal data points). This is confirmed in Fig. 5.

The fit of the points for $\beta \in [2.5, 5.5]$ gives for the scaling exponent $A = 2.02 \pm 0.03$.

An explanation of this “anomalous” scaling is given with next figure. Recall that for any given sample the algorithm gives us the number of configurations at each energy level. Let us thus consider the entropy S_0 of the ground state and S_1 that of the first excited state. In standard systems, $S_1 - S_0$ goes as $a + b \log V$ with $b = 1$ (V is the system’s volume). From the data displayed we find that at large enough sizes one has $b \approx 2$ (dashed line). Thus, in the 2d Ising spin glass with bimodal couplings, the minimum energy excitations ($\Delta E = 4J$) are not elementary:

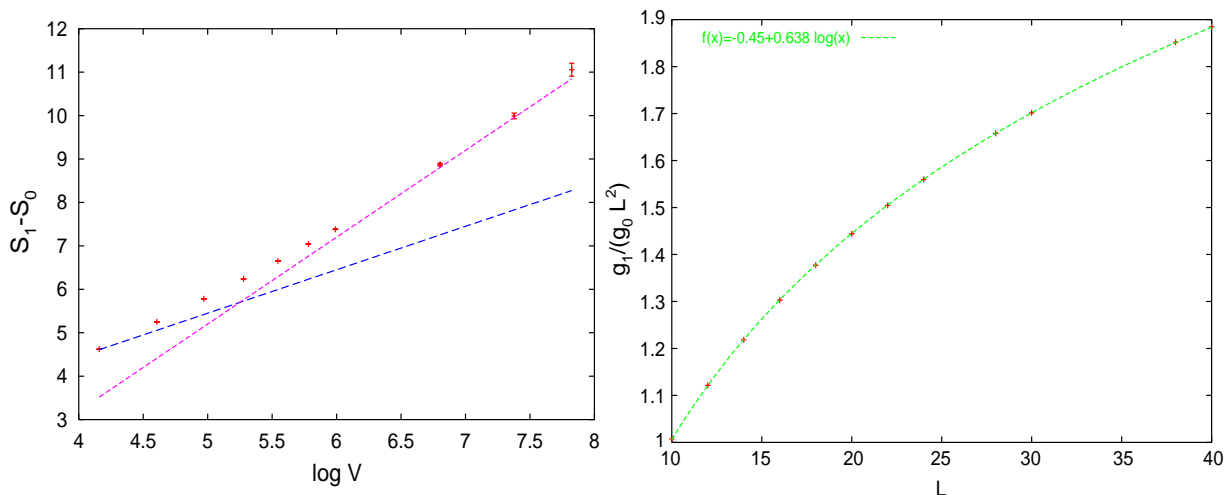


Fig. 6. Left: $S_1 - S_0$ for the bimodal Ising spin glass in 2d. Right: $g(E_0 + 4J)/g(E_0)L^2$ for fully frustrated model versus L (where $g(E_0 + 4J)$ is the degeneracy of first excited state and $g(E_0)$ that of the ground state).

in the thermodynamic limit, their typical degeneracy goes as V^2 rather than as V .

When we perform the same analysis on the fully frustrated model that Saul and Kardar had considered, we find that $S_1 - S_0 \approx a + \log V + \log(\log V)$. This deviation from the standard form (without the $\log(\log V)$) is too weak to change the $\exp(-\beta\Delta E)$ naive scaling obtained from the gap.

4.2. FSS and divergence of the correlation length

We are not able to extract directly the correlation length as we do not have spin configurations, only their number as a function of energy; nevertheless, we can get some information through the *finite size scaling* (FSS) of the heat capacity.

From the low-temperature expansion, we know that c_v , in the range of $T < 0.2$ where we have “naïve” scaling, goes as

$$c_v \sim \frac{e^{(S_1 - S_0)}}{L^2} \beta^2 e^{-4\beta}.$$

In Fig. 6 we see that in fact

$$e^{(S_1 - S_0)} \sim L^4.$$

Then, for very low T , the typical c_v scales as

$$c_v \sim L^2 \beta^2 e^{-4\beta}. \quad (4)$$

On the other hand, in the physically relevant region of T ($0.2 < T < 0.5$), we saw (Fig. 5) that c_v goes as $c_v \sim \beta^2 e^{-2\beta}$. Finite size scaling should connect these two regions through the FSS formula (Fig. 7)

$$c_v \sim \beta^2 e^{-2\beta} \Phi\left(\frac{L}{\xi}\right),$$

where $\Phi(x)$ has property

$$\Phi(x) = \text{constant}, \text{ if } x \gg 1,$$

$$\Phi(x) = x^2, \text{ if } x \ll 1. \quad (5)$$

Replacing the functional form (5) of $\Phi(x)$ into (4) we get that the correlation length scales as $\xi \sim e^\beta$. This is in agreement with hyperscaling.

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