Finite size scaling in Villain’s fully frustrated model and singular effects of plaquette disorder

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Abstract

The ground state and low $T$ behavior of two-dimensional spin systems with discrete binary couplings are subtle but can be analyzed using exact computations of finite volume partition functions. We first apply this approach to Villain’s fully frustrated model, unveiling an unexpected finite size scaling law. Then we show that the introduction of even a small amount of disorder on the plaquettes dramatically changes the scaling laws associated with the $T = 0$ critical point.

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Two-dimensional frustrated systems typically have a high ground-state degeneracy: this can lead to unusual physical properties \[1\]. In the absence of disorder, the zero-temperature spin states can often be mapped \[2\] to Baxter type or solid on solid models, leading to a relatively good understanding of the low temperature regime. Unfortunately, the incorporation of disorder renders analytic approaches powerless and one must resort to numerical treatment. In the limit of very strong disorder, one expects to have a spin glass, at least at zero temperature. It has recently been shown that the critical behavior of two-dimensional spin glasses with binary quenched random couplings is rather subtle, being very different from the naïve low temperature expansion \[3, 4, 5, 6\]. In this work, we focus on the change of critical behavior of the 2\textit{d} fully frustrated model (FFM) when one adds disorder. In the FFM each elementary plaquette of the lattice is frustrated, and the couplings between the spins are all of the same magnitude. At \(T = 0\) (the model’s critical point), the FFM exhibits a power-law decay of spin-spin correlation functions. Furthermore, for \(T > 0\), the correlation length diverges exponentially in \(1/T\). Suppose now we allow some plaquettes to be unfrustrated; does this reduction in the frustration leave the critical properties invariant, or is it instead a strong perturbation? Using exact partition functions on finite lattices, we shall show that even small amounts of disorder dramatically change the thermodynamic singularities of the model.

\textit{Villain’s Fully Frustrated model} — We consider a two dimensional square lattice with Ising spins on the sites and binary couplings \(J_{ij}\) on the bonds; without loss of generality, we set \(|J_{ij}| = J = 1\). The Hamiltonian is

\[
H(\{\sigma_i\}) \equiv - \sum_{(ij)} J_{ij} \sigma_i \sigma_j ,
\]

where the sum runs over all pairs of nearest neighbor sites and boundary conditions are periodic. We shall consider both \(L \times L\) lattices and the strip geometry \((L \times \infty)\). In the FFM the product of the four couplings on each elementary plaquette is \(-1\): there are many different ways to do this and most of them are gauge equivalent. More precisely, for a fully frustrated lattice with periodic boundary conditions, there are four equivalence classes, corresponding to whether the product of the \(J\) along a loop winding around a direction of the lattice is \(+1\) or \(-1\). Following Villain \[7\], we choose the periodic implementation where all \(J\)s are set to 1 except on the vertical bonds where lines of couplings alternate between \(+1\) and \(-1\) values. Villain applied the transfer matrix formalism to extract the free energy.
density in the infinite volume limit:

$$-\beta f_{\infty}(\beta) = \ln(2 \cosh(\beta J)) + \frac{1}{16\pi^2} \int_0^{2\pi} dh \int_0^{2\pi} dk \ln[(1 + z^2)^2 - 2z^2(\cos 2h + \cos 2k)] .$$

Here $z = \tanh(\beta J)$, $\beta \equiv T^{-1}$ is the inverse temperature, and $f_{\infty}$ is the free energy per site in the infinite volume limit.

The free energy turns out to be analytic everywhere except at $T = 0$. The $T = 0$ entropy density of the system (normalized to the number of sites), $s_0$, is finite: $s_0 = C/\pi$, where $C$ is the Catalan number. The ground state energy density $e_0$ is $-J$ (one quarter of the links are unsatisfied), and the low $T$ expansion of Eq. (2) to leading order is

$$\beta f_{\infty}(\beta) \simeq \beta e_0 - s_0 + c_1 \beta e^{-4\beta J} .$$

This makes clear the non-analyticity of the free energy at the critical point $T = 0$: a well behaved low temperature expansion of $\beta f_{\infty}$ would give a series in $y = \exp(-4\beta J)$ while in expression (3) a factor $\beta$ (i.e., a factor $\ln(y)$) multiplies the leading contribution $y = e^{-4\beta J}$.

Taking the second derivative with respect to $T$ gives the leading behavior of the specific heat density:

$$c_V(\beta) \simeq 16 c_1 J^2 \beta^3 e^{-4\beta J} .$$

In the present case of the FFM, Eq. (2) tells us everything about the temperature scaling of thermodynamic quantities. But it is also possible to obtain the free energy in a finite volume: we shall use this to extract both the correlation length and the finite size scaling.

The FFM in a finite volume or on a strip — Computing the partition function of the FFM in a finite volume is not difficult. For a finite lattice with periodic boundary conditions, the partition function associated to the Hamiltonian of Eq. (1) can be expressed as the sum of four Pfaffians, each multiplied by a plus or minus sign: because of these signs, there are large cancellations when combining the contributions of the four Pfaffians. Thus it is necessary to compute each Pfaffian to very high precision; we have done so with the “Mathematica” program that allows for arbitrary precision computations. Basically, in this approach, the double integral of Eq. (2) becomes a sum over a discrete set of momenta, where the support of this set is different for the four Pfaffians. We have also considered a strip geometry, where the vertical direction (where couplings are ±1) is infinite and the
other has a width $L$. In this case we have to compute mixed sums and integrals from which we obtain the free-energy density of the FFM in the strip geometry (typically we get 15 or more significant digits). We now focus on how the thermodynamic limit is reached with increasing $L$.

The correlation length — The diverging correlation length of a physical system approaching criticality can be defined in different ways: for example one can use the exponential decay of spin-spin correlations or the exponential convergence of the free energy density with increasing lattice size. Since in our approach we do not have access to the spin-spin correlation functions, we use the second definition. Consider the strip geometry associated with a lattice of infinite length in one direction and of width $L$ in the other (with periodic boundary conditions): the correlation length $\xi$ can be defined via the relation
\[
(f_L - f_\infty) \sim e^{-L/\xi},
\]
where the exponential can have a prefactor that depends smoothly on $L$, for example via a power law.

In Fig. (1) we show $\ln(f_\infty - f_L)$ as a function of $L$ (points) and the best fits to the form $a(T) - m(T)L - c(T)\ln(L)$ (continuous lines), for five temperatures ($T \in [0.4, 0.6]$). $m(T) \equiv 1/\xi(T)$ is the inverse correlation length. The quality of the fits is excellent, and we find that $c(T)$ depends only weakly on $T$ and is close to 1.5. Because of that, it is appropriate to parametrize the $L$ dependence via the correlation length $\xi$ through the relation
\[
f_L - f_\infty = A(T) \frac{e^{-L/\xi}}{L^{1.5}},
\]
where $A(T)$ is a smooth function of $T$. From this we can extract $\xi$ when $L$ is large; since our numerical values of $f_L - f_\infty$ loose precision beyond $L = 200$, and getting higher precision would have demanded a very large computational effort, we have been able to extract $\xi$ by curve fitting only for $T \geq 0.4$. In the inset of Fig. (1) we plot $\ln(\xi)$ as a function of $1/T$, and find a straight line with slope very close to 2. Similarly, the prefactor of the exponential is very close to $\frac{1}{2}$ and we conjecture that this is in fact the exact value (note that this prefactor has not been estimated previously). We thus conclude that
\[
\xi(T) \simeq e^{2J/2}/2 .
\]
This scaling form applies as $T \to 0$, but it holds to good accuracy even when $\xi$ is not so large: for example at $T = 1$ where $\xi \approx 4$ the value given by (6) is only 10% off from the actual measured $\xi$. In the standard hyperscaling framework, the singular part of $\beta f_\infty$ is
given by $\xi^{-d}$ for a d-dimensional model (up to constants and possible logarithmic terms in $\xi$). Using Eq. (6), we then expect the singular part of $f_\infty$ to go as $\exp(-4\beta J)$, which is what was found from Eq. (3): in the FFM, hyperscaling holds.

**Finite size scaling** — We have discussed the $1 \ll \xi \ll L$ region. It is also of interest to consider the regime where $L \ll \xi$: only by controlling this region we can reach a full understanding of the finite size scaling of the system.

As a start, we notice that good data collapse is obtained as $T \to 0$ when we multiply $(f_L - f_\infty)$ by the factor $\beta L^2$, i.e., we find

$$\beta L^2(f_L - f_\infty) \simeq W(L/\xi),$$

where $W(L/\xi)$ is an adimensional function of the ratio $L/\xi$. When $x = L/\xi \to \infty$ we recover the previous analysis and $W(x) \approx \sqrt{x} \exp(-x)$. In the opposite limit, $x = L/\xi \to 0$, the function $W$ goes to a constant [13]. Using the relations (3), (5) and (7), we find

$$f_L \simeq e_0 - \frac{s_0}{\beta} + c_1 e^{-4\beta J} + \frac{W}{\beta L^2}.$$  

Dividing and multiplying the last term by $\xi^2$ and substituting $2\beta$ by $\ln(\xi)$ (cf. Eq. (8)) we obtain

$$f_L \simeq e_0 - \frac{s_0}{\beta} + c_1 e^{-4\beta J} \left(1 + \tilde{W} \left(\frac{L}{\xi}\right) / \ln(\xi)\right)$$

where $\tilde{W}$ is a scaling function simply related to $W$. The important point is that in Eq. (8) the adimensional scaling function $\tilde{W}(L/\xi)$ is divided by a factor $\beta \sim \ln(\xi)$, so one has an *anomalous* finite size scaling law.
The function $\tilde{W}$ satisfies

$$
\tilde{W}(x) = \begin{cases}
  x^{-2} & \text{when } x \to 0 , \\
  \text{constant} & \text{when } x \to \infty .
\end{cases}
$$

We show all of our data for $\beta((f_L(\beta) - e_0 + \frac{s_0}{\beta})e^{4\beta J}/c_1 - 1)$ versus $L/\xi$ in Fig. (2). Here $10 \leq L \leq 180$ and $0 < T \leq 1.0$. $c_1$ has been determined with a best fit to $f_\infty$ and has the value $c_1 = -1.273$. The data collapse is excellent and since it involves a correction to $f_L$, one can conclude that finite size effects are under very good control.

To complete our study of the FFM without disorder, we consider finally the low temperature expansion of $f_L(\beta)$:

$$
f_L(\beta) \simeq e_0 - \frac{s_0}{\beta} - \frac{1}{\beta L^2 g_0} \exp(-4\beta J) ,
$$

where $g_0$ and $g_1$ are the respectively the degeneracy of the ground state and of the first excited state. We determine $g_0$ and $g_1$, finding that to very good accuracy

$$
g_1/g_0 \simeq AL^2 + BL^2 \ln(L) ,
$$

with $A = -0.44$ and $B = 0.63$. It is possible to show that the scalings (10) and (8) are mutually compatible.

Adding disorder / diluting frustration in the FFM — At this point the large $L$ and $\xi$ behavior of the FFM is well understood. Now we move on to see what happens when frustration is partly removed. We do this by unfrustrating a small fraction of the plaquettes, choosing these at random. The set of couplings $J_{ij}$ entering the Hamiltonian (1) is now such that on a fraction $p_1$ of the plaquettes their product is equal to 1. We shall refer refer to this as the Plaquette Disorder (PD) ensemble. Does this modification to the Hamiltonian change the scaling laws of the FFM? Interestingly, the change is in fact dramatic, as we now reveal.

The computational tool — The presence of plaquette quenched disorder breaks the translation invariance of the Hamiltonian; because of this, the transfer matrix cannot be diagonalized by going to Fourier space. Instead, we rely on the explicit computation of Pfaffians; this can be done for any set of $J_{ij}$. A very effective approach for computing such Pfaffians, based on modular arithmetic, has been proposed and implemented in [12]. One evaluates the partition function in a (large) finite volume via its low temperature series:

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

(11)
exactly of a given energy. The algorithm \cite{12} determines these integers
analyzing the system even for very low temperatures.

\[ \beta = \frac{c_1}{L} \]

\( \text{FIG. 2: } \beta((f_L(\beta) - e_0 + \frac{J^2}{4})_c/L^2 - 1) \text{ versus } L/\xi. \) Here \( c_1 = -1.273. \) Inset: \(-T \ln(T^2 c_V) \) vs. \( T \) showing the convergence to \( A = 4 \) (cf. section with disorder).

where \( P_J(x) \) is a polynomial whose integer coefficients are the number of spin configurations of a given energy. The algorithm \cite{12} determines these integers exactly, allowing one to analyze the system even for very low temperatures.

In our implementation \cite{5, 12} the CPU time to compute \( Z_J \) grows approximately as \( L^{5.5} \). We have mainly studied the model with an unfrustrated fraction of plaquettes \( p_1 = 1/8 \), by determining \( Z_J \) on lattices with sizes ranging from \( L = 24 \) (2000 samples) up to \( L = 56 \) (200 samples). We have also analyzed the case of \( p_1 = 1/4 \) on lattices with \( L = 32 \) (600 samples) up to \( L = 48 \) (100 samples). We computed sample averages of different physical quantities like the free energy and the specific heat, and we analyzed \( T = 0 \) quantities like the number of ground states and of low-lying excited states.

\textit{Low temperature scaling of } \( c_V \) — In the following we mainly analyze the specific heat, \( c_V \), that we compute from the fluctuations of the internal energy \cite{5}.

In the case without disorder, the low \( T \) thermodynamic limit behavior (where \( V \) diverges at fixed low \( T \)) of \( c_V \) is given in Eq. \cite{11}. On the contrary in the finite size limited, \( T \to 0 \) limit (where \( T \to 0 \) at fixed volume), we have that

\[ c_V \equiv \frac{\beta^2}{L^2} \langle [H - \langle H \rangle]^2 \rangle \approx \frac{16 \beta^2 J^2}{g_0} \frac{g_1}{g_0} e^{-4\beta J}. \] \hspace{1cm} (12)

Thus, the scaling in the thermodynamic limit differs from the finite size limited, finite volume low \( T \) scaling, but only in the power of the \( \beta \) prefactor, and not in the argument of the exponential. (This power is related to the logarithmic corrections in the \( L \) scaling of the ratio \( g_1/g_0 \) of Eq. \cite{10}). Disorder completely changes this picture as we shall now make clear.
Let us parametrize the scaling behavior by the argument of the exponential function and by a power for the first subleading correction: \( c_V \approx \beta^P e^{-A \beta J} \). We have seen in the FFM that \( A = 4 \) and that \( P = 2 \) in the naïve, finite size limited scaling while \( P = 3 \) in the scaling regime of the thermodynamic limit. In Fig. 3 we plot \(-T \ln (T^P c_V)\) versus \( T \) for the PD model (with \( p_1 = 1/8 \)). We take here \( P = 2 \), and try to determine \( A \). We proceed in this way since the value of \( A \) is not very sensitive to the value that we assume for \( P \): our conclusions for the value of \( A \) would be unchanged by taking \( P \) up to 10, and would be strengthened by taking \( P < 2 \). \( A \) is given by the intercept of the envelope’s extrapolation to \( T = 0 \). We can distinguish three regions in Fig. (3). The region at very low \( T \) values corresponds to the naïve scaling with \( A = 4 \) as can be seen from the \( T = 0 \) intercept; this region shrinks to zero with increasing lattice size. There is also the high \( T \) region but it is not relevant for critical properties. Finally, the most interesting region is in between the other two; there, one has the scaling in the thermodynamic limit, obtained from the envelope of the set of curves. It is clear from the figure that this scaling is incompatible with \( A = 4 \); in fact, the estimated value for \( A \) decreases with the lattice size (since for higher \( L \) we can determine the envelope to lower \( T \) values), and possibly goes to zero when \( L \to \infty \): such a behavior would imply an algebraic \( T \to 0 \) limit, and not an exponential singularity (it is clear that if this happens \( P \) will become smaller than zero: our best fits are already compatible with a small negative value of \( P \), but since they are not very sensitive to the value of \( P \) we cannot give a quantitative estimate of this effect). We have repeated this analysis for a dilution of 1/4 with similar conclusions: again the curves go down to low values of \( A \), possibly 0. As a final note and to drive home even more the incredibly strong effects of disorder, one can compare the behavior of \( c_V \) in the pure and the PD models: as shown in the inset of Fig. (2) the pure model has both a very clear exponential low temperature limit and small finite size effects; on the contrary in the presence of disorder, \( c_V \) has large finite size effects and the \( \exp(-4\beta J) \) scaling is clearly absent.

The degeneracy of low energy states — In the insets of Fig. (3) we plot \( g_1/g_0 L^2 \) as a function of \( L \) for the FFM and \( \ln(g_1/g_0 L^2) \) (that we get as an output of our exact computation of \( Z \)) as a function of \( L \) for the PD: this is because the first ratio grows logarithmically in \( L \) (see Eq. (10)), while in the presence of quenched disorder, it seems to grow at least exponentially fast with \( L \). The plaquette disorder completely changes the scaling of these quantities and so the low temperature expansion for the pure and the disordered models will
FIG. 3: $-T \ln(T^2 c_V)$ versus $T$ in the PD model with a fraction 1/8 of unfrustrated plaquettes. In the inset: on the left, $\ln(g_1/g_0 L^2)$ versus $L$ for the PD model; on the right, $g_1/g_0 L^2$ versus $L$ for the FFM.

Summary and discussion — Two dimensional frustrated models, with or without disorder, are challenging systems, especially when they have a critical point as Villain’s fully frustrated model does. We first studied in depth his (pure) model: beyond a conjecture for the magnitude of the correlation length, we showed that finite size scaling was anomalous. We also found that the ratio $g_1/g_0$ of the degeneracies of the lowest energy states grows as $L^2$ with multiplicative logarithmic corrections: as a result, the power law in $T$ multiplying the $\exp(-4\beta J)$ scaling of $c_V$ is modified.

We then introduced quenched disorder in the form of a small fraction of randomly positioned unfrustrated plaquettes to find that qualitatively new phenomena arise. For instance, $g_1/g_0$ grows exponentially in $L$ rather than as a power. Following the argument of what occurs in the pure model, this growth breaks the $\exp(-4\beta J)$ scaling of $c_V$, taking one to a form of the type $\exp(-A\beta J)$ with $A$ rather small if non-zero. These effects are striking and show the extreme fragility of the pure system: the universality class of the FFM is completely changed when disorder is introduced.

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[13] This is connected to the fact that finite volume corrections to the ground state entropy are of order $L^{-2}$. In $(f_L - f_\infty)$, the term $e_0$ has no corrections, while $s_0(L) \sim s_0(\infty) + \delta s_0/L^2$, and $\delta s_0$ is the relevant constant.