Critical behavior of frustrated systems: Monte Carlo simulations versus Renormalization Group

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Abstract

We study the critical behavior of frustrated systems by means of Pade-Borel resummed three-loop renormalization-group expansions and numerical Monte Carlo simulations. Amazingly, for six-component spins where the transition is second order, both approaches disagree. This unusual situation is analyzed both from the point of view of the convergence of the resummed series and from the possible relevance of non perturbative effects.

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Frustrated spin systems have been very much studied in their classical as well as quantum aspects. In particular, the critical behavior of 3D Stacked Triangular Antiferromagnets (STA) has deserved much attention since, firstly it has many physical realizations in rare earth materials, secondly it is an archetype for frustrated systems, and thirdly it is directly related to the behavior of its two dimensional zero temperature, quantum counterpart. The frustration in this system comes from the fact that – for \( N > 1 \) component spin systems – the ground state is non collinear and shows the famous 120° structure. It is thus natural to believe that if the transition is second order, it belongs to a new universality class. Our present understanding of these systems comes as usual from theoretical renormalization group (RG) calculations, from Monte Carlo simulations and from experiments. The most impressive fact concerning these systems is that more than twenty years after the first works devoted to their study, there is still no agreement between these approaches. For instance, a calculation made in \( D = 4 - \epsilon \) predicts no stable fixed point for \( N \) in the interval: \( N_{c2} = 2.202 - 0.569\epsilon + 0.989\epsilon^2 < N < N_{c3} = 21.80 - 23.43\epsilon + 7.088\epsilon^2 \) and another made in
$D = 2 + \epsilon$ predicts a fixed point for any $N$ larger than 2. Some experiments find a second order phase transition while others a weak first order. Moreover, the different approaches finding a second order transition do not find the same exponents, a fact that suggests that the theoretical or numerical approaches may miss a fundamental point (presence of topological defects, breakdown of perturbation theory, lattices of too small sizes...).

Our aim in this Letter is to shed light on this problem. We rely on the fact that the three-loop RG calculations made in $D = 4 - \epsilon$ with $\epsilon = 1$ and directly in $D = 3$ find a critical value $N_c(D = 3)$ above which the transition is second order equal to 3.39 [3] and 3.91 [4], respectively. Below it, it is supposed to be first order. We therefore expect a very weakly first order transition for $N = 3$ (and even perhaps for $N = 4$) – a situation very difficult to test numerically. Therefore, instead of studying directly the physical, i.e. $N = 3$, spin system, we choose to study the following question: is there consensus between the results given by the usual RG approach based on the Landau-Wilson ($\phi^4$ - like) model and those obtained by Monte Carlo simulations for the values of $D$ and $N$ where a fixed point is found?

Let us emphasize that the reliability of the RG approach for predicting the three-dimensional critical behaviors is not generic but has been demonstrated for most popular and simplest universality classes such as the usual $O(N)$ and cubic ones. The discrepancy between the perturbative results around $d = 2$ and $d = 4$ is in fact common to a wide class of systems among which the dipole locked phase of $^3$He, electroweak phase transition, smectic liquid crystal, etc. Our study is therefore likely to be relevant to a much wider class of systems than the frustrated magnets.

To tackle with our question, we study in $d = 3$ the largest possible $N$ compatible with numerical possibilities where the usual recipes should work since in this case we are far above the line $N_c(D)$, the proximity of which could be the root of all the problems. Being in principle in the second order region, we expect to compute accurately the critical exponents both numerically and in a RG approach using the usual resummation techniques. The comparison between the results obtained by these two methods should be a test of the most powerful theoretical approaches in this non-ferromagnetic case. We also choose the value of $N$ such that the corresponding system does not show topological defects in order to eliminate a possible reason for the breakdown of perturbation theories. It turns out that $N = 6$ is the ideal candidate. We present in this article numerical results for $N = 6$ as well as analytical ones for many $N$ and compare them.

Renormalization Group calculations. Let us first show our results obtained from the renormalization group analysis. The Landau-Wilson Hamiltonian relevant to the STA system is:

$$H = \frac{1}{2} \int d^3x \left[ r_0^2 \phi^2 + \nabla \phi \nabla \phi^* + \frac{u_0}{2} \phi \phi^* \phi \phi^* + \frac{w_0}{2} \phi \phi^* \phi \phi^* \right]. \quad (1)$$

The domain of parameters of interest is $u_0 > 0$ and $w_0 > 0$. The calculations are based on the three-loop RG equations obtained earlier for the more complicated model having three independent quartic coupling constants [4]. They are carried out directly in $d = 3$ and a Padé-Borel resummation of the relevant expansions is performed. Padé approximants [3/1] and [2/1] are employed for analytical continuation of the Borel transform series for the $\beta$-functions and critical exponent $\gamma$, respectively. The Fisher exponent is evaluated by direct substitution of the fixed point coordinates into the corresponding expansion.
The fixed point of the RG flow diagram which controls the non-trivial (chiral) critical behavior is found. For \( N > 7 \) it turns out to be a stable node, for \( N = 5, 6, 7 \) this point manifests itself as a stable focus. The latter scenario looks quite new, i.e. is observed for the first time in STA systems, while the former one has been already discussed (see, e.g., [4]). The estimates of critical exponents \( \gamma \) and \( \eta \) for various \( N \) are obtained from corresponding RG series. Making use of well-known scaling relations yields numerical values of the others. The results of our RG calculations are collected in Table 1 and presented, along with the other data, in Fig. 3. As is seen, critical exponents as functions of \( N \) demonstrate a cusp between \( N = 7 \) and \( N = 8 \) that reflects the abovementioned change of type of the fixed point governing the critical behavior.

**Monte Carlo results.** We present now our MC simulations. We use six-component spins interacting via the Hamiltonian

\[
H = \sum_{(ij)} J_{ij} S_i S_j ,
\]

(2)

where the sum runs over all neighbors of the stacked triangular lattice (STA) and the interaction is chosen antiferromagnetic (\( J > 0 \)). In the ground state the spins are planar with the three spins at the corners of each triangle forming a 120° structure. We use the standard Metropolis algorithm in combination with the over-relaxation algorithm [10]. Between each Metropolis we use one over-relaxation step. This allows us to reduce the correlation time and obtain better statistics. For each size we use some hundred thousand steps to equilibrate our system and up to five millions steps to thermalize for the bigger sizes. We have repeated these simulations for different initial configurations (ordered or random) to make sure that our results do not depend on them. We use the histogram MC technique developed by Ferrenberg and Swendsen [11]. From a simulation done at \( T_0 \), this technique allows us to obtain thermodynamic quantities at \( T \) close to \( T_0 \). We have studied our system in the finite size scaling (FSS) region [12] and our simulations have been done at \( T_s = 0.463 \). We consider \( L^2 \times (2L/3) \) systems, where \((L)^2\) is the size of the planes, and \(2L/3\) is the number of planes in the \( z \) axis. First, to find the critical temperature \( T_c \), we use Binder’s cumulant defined as

\[
U = 1 - \frac{< M^4 >}{(3 < M^2 >^2)}
\]

(3)

where the order parameter \( M \) is calculated in partitioning our lattice in three sublattices with only collinear spins and by summing each magnetization. We record the variation of \( U \) with \( T \) for various system sizes and then locate the intersection of these curves. We compare the values of \( U \) for two different lattice sizes \( L \) and \( L' = bL \), making use of the condition [13]

\[
\frac{U_{bL}}{U_L} \bigg|_{T=T_c} = 1.
\]

(4)

In Fig. 4, \( U \) is plotted as a function of the temperature for different sizes from \( L = 12 \) up to \( L = 36 \). Due to the presence of residual corrections to finite size scaling, one actually needs to extrapolate the results of this method for \( \ln b \rightarrow 0 \). From these data, we extrapolate the value of \( T_c \) (not shown) and obtain: \( T_c = 0.4636(2) \). We estimate the universal quantity \( U \) at \( T_c \) (\( U^* \)) as \( U^* = 0.6545(15) \). With the value of \( T_c \) we calculate the critical exponents using
log-log fit [2,3]. We obtain from $V_1 = \langle ME \rangle / \langle M \rangle - \langle E \rangle$, $V_2 = \langle M^2 E \rangle / \langle M^2 \rangle - \langle E \rangle$, (Fig. 2), estimates of $1/\nu$, from the susceptibility $\chi = N \langle M^2 \rangle / (k_BT)$ (not shown) estimates of $\gamma/\nu$, and from $<M>$ (not shown) an estimate of $\beta/\nu$. Combining these results we obtain respectively, $\nu = 0.700(11)$, $\gamma/\nu = 1.975(20)$, and $\beta/\nu = 0.513(12)$. All our errors are calculated with the help of the Jackknife procedure [14] and include the influence of the uncertainty in estimating $T_c$. The results are summarized in Table I where the value of $\eta$ has been calculated with the hyperscaling relation $\gamma/\nu = 2 - \eta$. We note that, contrary to spins with two or three components, $\eta$ is positive. This is due to the fact that for $N = 6$ the Renormalization Group flow is attracted by a true stable fixed point and not simply by a local minimum [13].

Discussion. The predictions of the renormalization-group $g$-expansion technique for $N = 6$-component spins listed in Table I do not agree with the Monte Carlo results given in Table I. We have plotted in figure 3 the results for $\nu$ from the MC data, the RG $g$-expansion (this work), the Local Potential Approximation method (LPA) [1] and the $1/N$ expansion [10] (first order). The six-loop RG results for the ferromagnetic case [7] are also plotted for comparison. The interesting point is that these results are obtained by methods representing the state of the art in the field of critical phenomena. When applied to the systems belonging to the $O(N)$ universality classes they indeed fit very well together. Let us emphasize that our numerical results are well converged and it seems unlikely that a non trivial behavior shows up at much larger system sizes THAT would resolve the discrepancy with the RG $g$-expansion results.

In order to clear up what can be an origin of the marked discrepancy, we analyze the structure of the RG expansions employed. The main attention is paid to the vicinity of the chiral fixed point of the RG flow for $N = 5, 6, 7$ when this point is a focus. Contrary to the (unstable) fixed point governing the $O(N)$-symmetric critical behavior, the chiral point lies very close to the $w$ axis being far from the $u$ axis. In particular, for the case of interest $N = 6$ its coordinates are: $u^* = 0.0665, w^* = 1.6025$. In this region, the structure of the series of the $\beta$-functions turns out to be unexpectedly irregular. As an example, we present here two “cuts” of the Borel-transformed expansion for $\beta_u(u, w)$ running through the chiral fixed point which clearly demonstrate such irregularity:

$$\beta_u^B(u, 1.6025) = -0.3607 + 0.7774u - 0.5004u^2 + 0.0339u^3 - 0.0055u^4, \quad (5)$$

$$\beta_u^B(0.0665, w) = 0.0643 - 0.0132w - 0.1960w^2 + 0.0346w^3 + 0.0010w^4. \quad (6)$$

The coefficients in these formulas do not decrease monotonically with increasing their numbers, and the expansion in powers of $w$ is not alternating having coefficients with irregular signs. Therefore, the RG series for $\beta$-functions would not demonstrate a good summability near the chiral fixed point and, subject to Padé-approximant-based analytical continuation and subsequent Borel integration, they are hardly believed to yield precise numerical results. Moreover, the Padé-Borel approximant for $\beta_u$, taken at the chiral fixed point, as a function of the Borel variable $t$ has a pole at $t = 61.8$ which is not dangerous practically but reflects the series poor summability. The difference between numerical results obtained within RG and MC approaches may be caused by an unfavorable structure of the RG expansions. On the other hand, for all $N$ studied the chiral fixed point coordinate $u^*$ given by the resummed three-loop series remains positive preventing the RG expansions from losing Borel summability in the domain of interest. Hence, fortunately, we do not face here this serious problem.
that may spoil a perturbative RG analysis, as it occurs, say, when systems with quenched disorder are investigated \[18\]. This keeps calculations of the higher-order contributions to the RG functions of the model Eq.(1) meaningful and desirable.

Can an account for four-loop or higher-order terms in the RG expansions significantly improve the situation? In principle, yes. The point is that the exact coordinates of the chiral fixed point may differ substantially from those given by the three-loop approximation and lie in the domain of the RG flow diagram where the perturbative expansions of $\beta$-functions can be properly resummed. Higher-order terms added to the three-loop series may shift calculated fixed point coordinates toward their exact values thus making counterparts of the series (4-5) better summable. To clear up whether such a situation really takes place, higher-order RG calculations have to be performed. Until this is done, an alternative scenario, i.e., the case when higher-order terms do not improve the summability, cannot be excluded.

There is up to now only one other theoretical approach that allows quantitative calculations in $D = 3$: the LPA method that consists in a truncation of the Wilson RG equations. Note that even if the LPA is missing the field renormalization and thus the anomalous dimension $\eta$, it is non perturbative since it is not based on a weak coupling expansion. However, although in our case the results obtained within this method are closer to the MC data than those obtained at the three-loop RG approximation, they show an unexpected dependence of $\nu$ with $N$ at small $N$. Moreover, used around $d = 2$, this approach contradicts the perturbative results obtained from the Non Linear Sigma model that are, in this dimension, well confirmed by simulations \[20\]. They are anyway not enough accurate to draw a conclusion in $d = 3$. Since the LPA is known to be the first order of a systematic derivative expansion of the effective action, it is desirable that the next order be computed.

Let us now remark that even if the three-dimensional physics was well reproduced by our calculations, it would remain that a coherent picture of the critical thermodynamics of the frustrated systems would require to understand the discrepancy between the NL$\sigma$ model approach and the Landau-Wilson one. A striking difference between both approaches is that near two dimensions the low temperature expansion of the NL$\sigma$ model predicts that a new “current” term of the form $(\phi^* \nabla \phi)^2$ is relevant \[3\]. This term appears to be fundamental since for $N = 3$ it allows to find a fixed point with an $O(4)$ symmetry. Being highly non renormalizable near four dimensions, it is irrelevant and forgotten. There is thus another scenario than the numerical unreliability of the three-loop RG approximation, namely, that the Landau-Wilson Hamiltonian Eq.(1) itself is incomplete in three dimensions (remember that the presence of topological defects cannot be invoked here since there are no such defects for $N = 6$). As it was suggested for the Abelian Higgs transition, this could be interpreted as the necessity to have recourse to the NL$\sigma$ model description and to abandon that of the Landau-Wilson model. Note, however, that it is very doubtful that the analysis made around two dimensions can be extended straightforwardly for any $N$ up to $d = 3$ since i) for $N = 3$-component spins the $O(4)$ fixed point found in $D = 2 + \epsilon$ has been shown to disappear in a non trivial dimension strictly smaller than three in a closely related model – the principal chiral model \[21\] – and since ii) an $O(4)$ behavior has neither been seen experimentally nor numerically for $N = 3$ and $d = 3$. Thus, the perturbative analysis of the NL$\sigma$ model fails also above two dimensions. However, it remains that a coherent picture of the behavior of frustrated systems for all $N$ and $d$ should include the results of the NL$\sigma$ model and therefore explain why and when the current term starts to be relevant.
as a function of $N$ and $d$. If this happens to be around $d = 3$ for $N \sim O(1)$, it could perturb the RG $g$-expansion results presented here and explain why otherwise powerful methods do not work properly in our case. In any case, we believe that our results for $N = 6$ constitute a clear challenge for the theoretical approaches which is perhaps not out of reach from higher order calculations and/or improvement of the LPA method.

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### TABLES

| N  | α   | β   | γ   | ν   | η   |
|----|-----|-----|-----|-----|-----|
| 5  | 0.305 | 0.300 | 1.095 | 0.565 | 0.0632 |
| 6  | 0.275 | 0.302 | 1.121 | 0.575 | 0.0507 |
| 7  | 0.303 | 0.295 | 1.108 | 0.566 | 0.0421 |
| 8  | 0.152 | 0.319 | 1.211 | 0.616 | 0.0355 |
| 9  | -0.055 | 0.354 | 1.348 | 0.685 | 0.0325 |
| 10 | -0.157 | 0.370 | 1.417 | 0.719 | 0.0305 |
| 12 | -0.292 | 0.393 | 1.506 | 0.764 | 0.0273 |
| 16 | -0.451 | 0.418 | 1.616 | 0.817 | 0.0226 |
| 20 | -0.553 | 0.434 | 1.685 | 0.851 | 0.0192 |
| 24 | -0.623 | 0.444 | 1.734 | 0.874 | 0.0167 |
| 100| -0.909 | 0.488 | 1.935 | 0.970 | 0.0046 |

**TABLE I.** Critical exponents calculated by RG

| N  | α    | β    | γ     | ν    | η     |
|----|------|------|-------|------|-------|
| 6  | -0.100(33)\(^1\) | 0.359(14) | 1.383(36) | 0.700(11) | 0.025(20)\(^2\) |

**TABLE II.** Critical exponents obtained by MC. \(^1\)calculated with \(\alpha = 2 - d\nu\). \(^2\)calculated with \(\eta = 2 - \gamma/\nu\).
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FIG. 1. Binder’s parameter $U$ as function of the temperature for different sizes $L$ (in the left part of the figure from down to up $L=12, 15, 18, 21, 24, 27, 30, 36$). The arrows show the estimated critical temperature $T_c$ and the temperature of our simulations $T_s$.

FIG. 2. Values of $V_1$ and $V_2$ as function of $L$ in a ln-ln scale at $T_c$. The value of the slopes gives $1/\nu$ and we obtain $\nu= 0.698(12)$ for $V_1$ and $0.702(13)$ for $V_2$. The smallest size ($L = 12$) is not included in our fits.
FIG. 3. $\nu$ for different methods (see text).