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CRITICAL BEHAVIOUR OF FRUSTRATED SYSTEMS: MONTE CARLO SIMULATIONS VERSUS RENORMALIZATION GROUP

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We study the critical behaviour 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 behaviour of 3D stacked triangular antiferromagnets (STA) has deserved much attention [1-9] 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 behaviour of its 2D zero temperature, quantum counterparts. The frustration in such systems comes from the fact that – for $N > 1$ component spins – the ground state is non collinear and shows the famous 120^0 structure. It is thus natural to believe that if the transition is second order, they belong to a new universality class. Our present understanding of these systems comes as usual from the renormalization group (RG) calculations, from Monte Carlo simulations and from experiments. The most impressive fact 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 $D = 4 - \epsilon$ [3] 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 $N > 2$. Some experiments find a second order phase transition while others a weak first order. Moreover, the different approaches finding a continuous transition do not find the same exponents, a fact that suggests that the theoretical or numerical approaches may miss some fundamental points (topological defects, breakdown of perturbation theory, etc.).

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. A very weak first order transition is expected for $N = 3$ – a situation very difficult to test numerically. Therefore, instead of studying

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directly the physical ($N = 3$) spin system, we choose to study the following question: is there consensus between the results given by the RG approach based on the Landau – Wilson (ϕ^4 – like) model and those obtained by Monte Carlo simulations for the values of D and N where a fixed point is found?

Note, that the reliability of the RG approach for predicting the 3D critical behaviours is not generic but has been demonstrated for simplest universality classes such as $O(N)$ one. 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 from the resummed 3D RG expansions. 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 theory. It turns out that $N = 6$ is the ideal candidate. Below, we present numerical results for $N = 6$ as well as analytical ones for various N including $N = 6$ and compare them.

Renormalization Group analysis. The relevant Landau – Wilson Hamiltonian reads [3, 16]:

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

The domain of parameters of interest is $u_0 > 0$ and $w_0 > 0$. The calculations are based on the three-loop RG expansions obtained earlier for the more complicated 3D model having three quartic coupling constants [4]. The Padé-Borel resummation of the RG series is performed, Padé approximants [3/1] and [2/1] are used for analytical extension of the Borel transforms for the β-functions and critical exponent γ, respectively. The exponent η is evaluated by direct substitution of the fixed point coordinates into corresponding expansion.

Table 1

N	5	6	7	8	9	10	12	16	20	100
α	0.305	0.275	0.303	0.152	–0.055	–0.157	–0.292	–0.451	–0.553	–0.909
β	0.300	0.302	0.295	0.319	0.354	0.370	0.393	0.418	0.434	0.488
γ	1.095	1.121	1.108	1.211	1.348	1.417	1.506	1.616	1.685	1.935
ν	0.565	0.575	0.566	0.616	0.685	0.719	0.764	0.817	0.851	0.970
η	0.063	0.051	0.042	0.035	0.032	0.030	0.027	0.023	0.019	0.005

For $N > 7$, the fixed point which controls the chiral critical behaviour is found to be a stable node, for $N = 5, 6, 7$ it is 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 values of critical exponents γ and η obtained from the RG series are used to estimate other exponents via scaling relations. The results of our RG

calculations are collected in Table 1 and presented, along with others, in Fig.1 (RGgE). 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 behaviour.

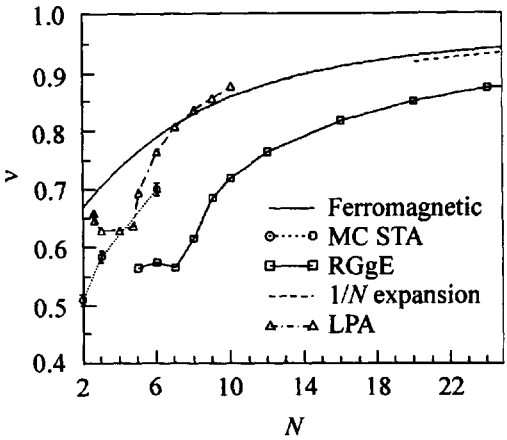

Fig.1. The critical exponent ν for $N = 6$ calculated by the field-theoretical renormalization-group technique (RGgE), by Monte Carlo simulations (MC STA) and by some other methods (see text)

Monte Carlo results. We study six-component spins interacting via the Hamiltonian

$$H = \sum_{(ij)} J_{ij} \mathbf{S}_i \mathbf{S}_j \ , \tag{2}$$

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]: one over-relaxation step per one Metropolis step. This reduces the correlation time and improves 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. The histogram MC technique by Ferrenberg and Swendsen [11] is used to obtain thermodynamic quantities at T close to T_0 from a simulation done at T_0. We have studied our system in the finite size scaling (FSS) region [12] with the simulations done at $T_* = 0.463$. We consider $L^2 \cdot (2L/3)$ systems, where $(L)^2$ is the size of the planes and $2L/3$ is the number of planes. To find the critical temperature T_c, we use Binder's cumulant defined as $U = 1 - < M^4 > /3 < M^2 >^2$ 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 T_c at the intersection of these curves [13]. In Fig.2 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 $(\ln b)^{-1} \to 0$. From these data, we extrapolate the value of T_c (not shown) and obtain $T_c = 0.4636(2)$, while the universal quantity U at T_c is $U^* = 0.6545(15)$. Then we calculate the critical exponents using log-log fit [12, 14]. The estimate of $1/\nu$ is extracted from $V_1 =< ME > / < M > - < E >$, $V_2 =< M^2E > / < M^2 > - < E >$ (Fig.2), while the data for susceptibility

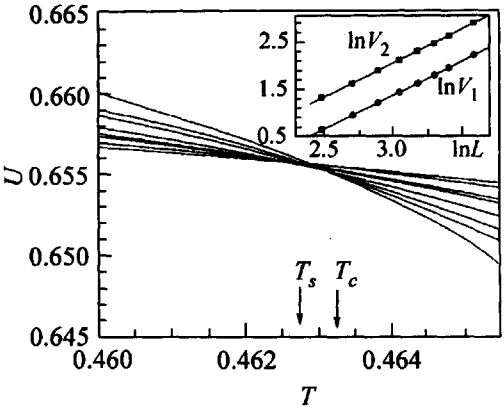

Fig.2. Binder's parameter U as function of the temperature for different sizes L (in the left part of the figure from down to up $L = 12, 15, 18, 21, 24, 27, 30, 36$). The arrows show the estimated critical temperature T_c and the temperature of our simulations T_s. In the inset, the values of V_1 and V_2 are shown 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

$\chi = N < M^2 > /k_BT$ and $< M >$ (not shown) yield the values of γ/ν and β/ν which are found to be 1.975(20) and 0.513(12), respectively. All errors are calculated with the help of the Jackknife procedure [15] and include the influence of the uncertainty in estimating T_c. The final results are summarized in Table 2, with η and α evaluated using scaling relations $\eta = 2 - \gamma/\nu$ and $\alpha = 2 - D\nu$. Note that, contrary to spins with $N = 2$ or $N = 3$, $\eta > 0$. This is due to the fact that for $N = 6$ the RG flow is attracted by a true stable fixed point and not by a local minimum [6, 8, 9].

Table 2

N	α	β	γ	ν	η
6	−0.100(33)	0.359(14)	1.383(36)	0.700(11)	0.025(20)

Discussion. The predictions of the RG analysis for six-component spins listed in Table 1 do not agree with the Monte Carlo results given in Table 2. General situation is illustrated by Fig. 1 where our MC and RG results for ν, along with those given by the Local Potential Approximation (LPA) [6] and the $1/N$ expansion [16], are presented; the six-loop RG estimates for the ferromagnetic case [17] are also plotted for comparison.

Since our numerical results are well converged, it seems unlikely that Monte Carlo study of much larger systems would resolve the discrepancy with the RG predictions. To clear up the origin of this discrepancy, we analyze the structure of the RG series employed. Of prime importance is the vicinity of the chiral fixed point for $N = 5, 6, 7$ when this point is a focus. Contrary to the (unstable) fixed point governing the $O(N)$-symmetric behavior, the chiral point lies very close to the w axis being far from the u axis. 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 β-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:

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

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

The coefficients in (3), (4) do not decrease monotonically with increasing their numbers, and the expansion (4) has coefficients with irregular signs. Hence, the RG series for β-functions would not demonstrate a good summability near the chiral fixed point and are

hardly believed to yield precise numerical results. Moreover, the Padé-Borel approximant for β_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 the chiral fixed point coordinate u^* given by our series remains positive preventing the RG expansions from losing Borel summability in the domain of interest. Hence, we do not face here this problem as it occurs when systems with quenched disorder are studied [18]. This keeps calculations of the higher-order contributions to the RG functions meaningful and desirable.

Can an account for higher-order terms in the RG expansions significantly improve the situation? In principle, yes. Indeed, the true chiral fixed point location may differ substantially from that given by the three-loop approximation and lie in the domain of the RG flow diagram where the series for β-functions can be properly resummed. Higher-order terms may shift calculated fixed point coordinates toward their exact values thus making the RG series better summable at criticality. To clear up whether such a situation really takes place, higher-order RG calculations have to be performed.

There is up to now only one other theoretical approach that allows quantitative calculations in $D = 3$: the LPA method based on a truncation of the Wilson RG equations. Even when missing the field renormalization, this method is non perturbative since it is not based on a weak coupling expansion. However, although in our case the results obtained within the LPA are closer to the MC data than their RG analogs, they show an unexpected dependence of ν with N at small N. Moreover, used around $D = 2$, this approach contradicts the perturbative results obtained from the Non Linear Sigma (NLσ) model that are, in this dimension, well confirmed by simulations [19]. 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, it is desirable that the next order be computed.

Let us now remark that even if the 3D physics was well reproduced by our analysis, it would remain that a coherent picture of the frustrated systems behaviour would require to understand the discrepancy between the NLσ model approach and the Landau – Wilson one. A striking difference between both approaches is that near $D = 2$ the low temperature expansion of the NLσ model predicts that a new "current" term of the form $(\phi^* \nabla \phi)^2$ is relevant [2]. 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 $D = 4$, 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 (1) is incomplete in 3D. As it was suggested for the Abelian Higgs transition, this could be interpreted as the necessity to have recourse to the NLσ model description abandoning that of the Landau – Wilson model. Note, however, that it is very doubtful that the analysis made around $D = 2$ can be extended straightforwardly for any N up to $D = 3$ since i) for 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 [20] – and since ii) an $O(4)$ behaviour has neither been seen experimentally nor numerically for $N = 3$ and $D = 3$. Thus, the perturbative analysis of the NLσ model fails also for $D > 2$. However, it remains that a coherent picture of

the behaviour of frustrated systems for all N and D should include the results of the NLσ 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 results presented above and explain why otherwise powerful methods do not work properly here. 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 RG calculations and improvement of the LPA method.

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1. *Magnetic Systems with Competing Interactions (Frustrated Spin Systems)*, Ed. H.T.Diep, World Scientific, Singapore, 1994.
2. P.Azaria, B.Delamotte, F.Delduc, and Th.Jolicoeur, Nucl. Phys. **B408**, 585 (1993).
3. S.A.Antonenko, A.I.Sokolov, and V.B.Varnashev, Phys. Lett. **A208**, 161 (1995).
4. S.A.Antonenko and A.I.Sokolov, Phys. Rev. **B49**, 15901 (1994).
5. M.F.Collins and O.A.Petrenko, Can. J. Phys. **75**, 605 (1997).
6. G.Zumbach, Phys. Rev. Lett. **71**, 2421 (1993); Nucl. Phys. **B413**, 771 (1994).
7. H.Kawamura, J. Phys.: Condens. Matter **10**, 4707 (1998).
8. D.Loison and K.D.Schotte, Eur. Phys. J. **B5**, 735 (1998).
9. D.Loison and K.D.Schotte, Eur. Phys. J. **B14**, 125 (2000).
10. M.Creutz, Phys. Rev. **D36**, 515 (1987).
11. A.M.Ferrenberg and R.H.Swendsen, Phys. Rev. Lett. **61**, 2635 (1988); **63**, 1195 (1989).
12. N.Barber, in *Phase Transition and Critical Phenomena*, Vol.8, Eds. C.Domb and J.L.Lebowitz, Academic, New York, 1983.
13. K.Binder, Z. Phys. **B43**, 119 (1981).
14. A.M.Ferrenberg and D.P.Landau, Phys. Rev. **B44**, 5081 (1991).
15. B.Efron, *The Jackknife, The Bootstrap and other Resampling Plans*, SIAM, Philadelphia, PA, 1982.
16. H.Kawamura, Phys. Rev. **B38**, 4916, (1988); **42**, 2610 (1990).
17. S.A.Antonenko and A.I.Sokolov, Phys. Rev. **E51**, 1894 (1995).
18. A.J.Bray, T.McCarthy, M.A.Moore et al., Phys. Rev. **B36**, 2212 (1987); A.J.McKane, Phys. Rev. **B49**, 12003 (1994); B.N.Shalaev, S.A.Antonenko, and A.I.Sokolov, Phys. Lett. **A230**, 105 (1997).
19. B.W.Southern and A.P.Young, Phys. Rev. **B48**, 13170 (1993).
20. M.Tissier, D.Mouhanna, and B.Delamotte, Phys. Rev. **B61**, 15327 (2000).