

Critical Behavior of Frustrated Systems: Monte Carlo Simulations versus Renormalization Group¹

D. Loison*, A. I. Sokolov**, B. Delamotte***, S. A. Antonenko**,
K. D. Schotte*, and H. T. Diep****

* Institut für Theoretische Physik, Freie Universität Berlin, 14195 Berlin, Germany

** St. Petersburg Electrotechnical University, St. Petersburg, 197376 Russia

e-mail: ais@sokol.usr.etu.spb.ru

*** Université Paris 7, 75251 Paris Cedex 05, France

**** Université de Cergy-Pontoise, 95302 Cergy-Pontoise Cedex, France

Received August 28, 2000

We study the critical behavior of frustrated systems by means of the Padé–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 nonperturbative effects. © 2000 MAIK “Nauka/Interperiodica”.

PACS numbers: 75.10.-b; 64.60.Ak; 64.60.Cn; 05.10.Ln

Frustrated spin systems have been very much studied in their classical and quantum aspects. In particular, the critical behavior 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 behavior 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 noncollinear and shows the famous 120° 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, and others, a weak first-order transition. Moreover, the different approaches to 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 and 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 the physical ($N = 3$) spin system directly, we choose to study the following question: whether there is 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 3D critical behaviors is not generic but has been demonstrated for simplest the universality classes such as $O(N)$. The discrepancy between the perturbative results around $D = 2$ and $D = 4$ is, in fact, common to a wide class of systems, among which there are the dipole-locked phase of ^3He , electroweak phase transition, smectic liquid crystal, etc. Our study is therefore likely to be relevant to a much wider class of systems than frustrated magnets.

To tackle 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 compari-

¹ This article was submitted by the authors in English.

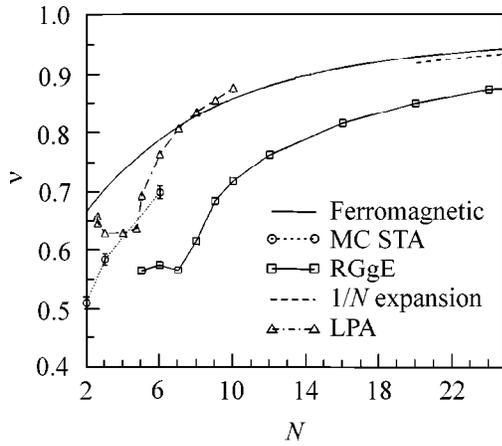


Fig. 1. The critical exponent ν for $N = 6$ calculated by the field-theoretical renormalization-group technique (RGgE), by Monte Carlo simulations (MC STA), and by some other methods (see text).

son between the results obtained by these two methods should be a test of the most powerful theoretical approaches in this nonferromagnetic 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 the analytical ones for various N , including $N = 6$, and compare them.

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

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

The domain of parameters of interest is $u_0 > 0$ and $w_0 > 0$. The calculations are based on the three-loop RG expansions obtained earlier for the more complicated 3D model with three quartic coupling constants [4]. The Padé–Borel resummation of the RG series is performed, and Pade 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 the corresponding expansion.

For $N > 7$, the fixed point, which controls the chiral critical behavior, is found to be a stable node; and for $N = 5, 6, 7$ it is a stable focus. The latter scenario looks quite new; i.e., it is observed for the first time in STA systems, while the former one was 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 $N = 8$, which reflects the above-mentioned change in the type of fixed point governing the critical behavior.

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

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

where the sum runs over all neighbors of the stacked triangular lattice (STA) and the interaction is chosen to be 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 overrelaxation algorithm [10]: one overrelaxation step per one Metropolis step. This reduces the correlation time and improves the statistics. For each size, we use several hundred thousand steps to equilibrate our system and up to five millions steps to thermalize for the larger 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 $T_s = 0.463$. We consider $L^2(2L/3)$ 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 $U = 1 - \langle M^4 \rangle / 3 \langle M^2 \rangle^2$, where the order parameter M is calculated by partitioning our lattice into three

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

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 $(\ln b)^{-1} \rightarrow 0$. 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 a log–log fit [12, 14]. The estimate of $1/\nu$ is extracted 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), while the data for susceptibility $\chi = N \langle M^2 \rangle / k_B T$ and $\langle M \rangle$ (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].

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. The 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 a 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 $N = 6$ of interest, its coordinates are $u^* = 0.0665$ and $w^* = 1.6025$. In this region, the structure of the series of 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 this irregularity:

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

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

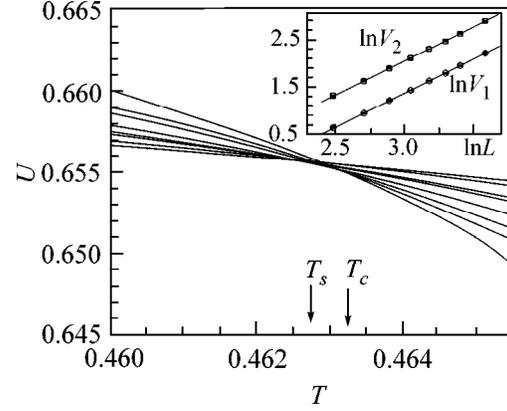


Fig. 2. Binder’s parameter U as a function of the temperature for different sizes L (in the left part of the figure from bottom to top $L = 12, 15, 18, 21, 24, 27, 30, 36$). The arrows show the estimated critical temperature T_c and the temperature of our simulations T_s . In the inset, the values of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

The coefficients in Eqs. (3) and (4) do not decrease monotonically with an increase in their numbers, and 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 in practice but reflects the poor summability of the series. The difference between numerical results obtained within the 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, here we do not face this problem, as 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. The higher order terms may shift

Table 2

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

the calculated fixed point coordinates to 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.

Up to now, there is only a single different theoretical approach that allows quantitative calculations for $D = 3$: the LPA method based on a truncation of the Wilson RG equations. Even when missing the field renormalization, this method is nonperturbative, 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 analogues, they show an unexpected dependence of v on N at small N . Moreover, used around $D = 2$, this approach contradicts the perturbative results obtained from the Nonlinear Sigma ($NL\sigma$) model, which are, in this dimension, well confirmed by simulations [19]. They are, in any case, not accurate enough 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 is well reproduced by our analysis, a coherent picture of frustrated system behavior would still require one to understand the discrepancy between the $NL\sigma$ model approach and the Landau–Wilson one. A striking difference between both approaches is that near $D = 2$ the low-temperature expansion of the $NL\sigma$ 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 one to find a fixed point with an $O(4)$ symmetry. Being highly nonrenormalizable near $D = 4$, it is irrelevant and forgotten. There is thus a scenario other than the numerical unreliability of the three-loop RG approximation; namely, the Landau–Wilson Hamiltonian (1) is incomplete in 3D. As was suggested for the Abelian Higgs transition, this could be interpreted as the necessity to have recourse to the $NL\sigma$ 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 for $D = 2 + \epsilon$ was shown to disappear in a nontrivial dimension strictly smaller than three in a closely related principal chiral model [20] and ii) an $O(4)$ behavior was seen neither experimentally nor numerically for $N = 3$ and $D = 3$. Thus, the perturbative analysis of the $NL\sigma$ model also fails for $D > 2$. 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 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 to the theoretical approaches, which is perhaps not out of reach from higher order RG calculations and improvement of the LPA method.

This work was supported in part by the Alexander von Humboldt Foundation (D.L.), the International Science Foundation (A.I.S., grant no. p99-943), and the Ministry of Education of Russian Federation (A.I.S., grant no. 97-14.2-16). B. Delamotte and D. Loison are grateful to G. Zumbach for discussions.

REFERENCES

1. *Magnetic Systems with Competing Interactions (Frustrated Spin Systems)*, Ed. by H. T. Diep (World Scientific, Singapore, 1994).
2. P. Azaria, B. Delamotte, F. Delduc, and Th. Jolicoeur, *Nucl. Phys. B* **408**, 585 (1993).
3. S. A. Antonenko, A. I. Sokolov, and V. B. Varnashev, *Phys. Lett. A* **208**, 161 (1995).
4. S. A. Antonenko and A. I. Sokolov, *Phys. Rev. B* **49**, 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. B* **413**, 771 (1994).
7. H. Kawamura, *J. Phys.: Condens. Matter* **10**, 4707 (1998).
8. D. Loison and K. D. Schotte, *Eur. Phys. J. B* **5**, 735 (1998).
9. D. Loison and K. D. Schotte, *Eur. Phys. J. B* **14**, 125 (2000).
10. M. Creutz, *Phys. Rev. D* **36**, 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*, Ed. by C. Domb and J. L. Lebowitz (Academic, New York, 1983), Vol. 8.
13. K. Binder, *Z. Phys. B* **43**, 119 (1981).
14. A. M. Ferrenberg and D. P. Landau, *Phys. Rev. B* **44**, 5081 (1991).
15. B. Efron, *The Jackknife, the Bootstrap and Other Resampling Plans* (SIAM, Philadelphia, 1982).
16. H. Kawamura, *Phys. Rev. B* **38**, 4916 (1988); **42**, 2610 (1990).
17. S. A. Antonenko and A. I. Sokolov, *Phys. Rev. E* **51**, 1894 (1995).
18. A. J. Bray, T. McCarthy, M. A. Moore, *et al.*, *Phys. Rev. B* **36**, 2212 (1987); A. J. McKane, *Phys. Rev. B* **49**, 12003 (1994); B. N. Shalaev, S. A. Antonenko, and A. I. Sokolov, *Phys. Lett. A* **230**, 105 (1997).
19. B. W. Southern and A. P. Young, *Phys. Rev. B* **48**, 13 170 (1993).
20. M. Tissier, D. Mouhanna, and B. Delamotte, *Phys. Rev. B* **61**, 15 327 (2000).