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CRITICAL BEHAVIOR OF THE ANTIFERROMAGNETIC HEISENBERG MODEL ON A STACKED TRIANGULAR LATTICE

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We estimate, using a large-scale Monte Carlo simulation, the critical exponents of the antiferromagnetic Heisenberg model on a stacked triangular lattice. We obtain the following estimates: $\gamma/\nu = 2.01 \pm .03$, $\nu = .79 \pm .03$. These results are compatible with a transition in the Wilson-Fisher $O(4)$ universality class, as predicted by a $2+\epsilon$ Renormalization Group calculation. As a consequence we are able to obtain a satisfactory picture of the critical behaviour of Heisenberg helimagnets, solving thus a long-standing puzzle.

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1 INTRODUCTION

There is at the present time a satisfactory understanding of the critical behaviour of physical systems where the rotation symmetry group O(N) is broken down to O(N-1) at low temperatures. Several theoretical tools are available to estimate the critical exponents and there is good agreement between these estimates. The Wilson-Fisher fixed point which describes the critical physics can be smoothly followed between two and four dimensions: for $N \geq 3$ the $2+\epsilon$ and $4-\epsilon$ renormalization group expansion merge in a continuous manner.

The situation is much more complicated when the rotation symmetry is *fully* broken in the low-temperature phase. A prominent example is found in the so-called helimagnetic systems where Heisenberg spins are in a spiral arrangement below the critical temperature. It is an interesting question, both theoretically and experimentally, to know the corresponding universality class. A widely studied prototypical model is the antiferromagnetic Heisenberg model on a stacked triangular lattice, which is simple and display commensurate helimagnetic order below a transition point T_c. At the present time, there is little consensus in the literature regarding critical phenomena associated with this model [1].

This topic has been investigated by use of a $D = 4-\epsilon$ renormalization group calculation[2]. The corresponding Ginzburg-Landau theory for a N-component vector model involves two N-component bosonic fields. It is found that for N large enough the transition is second order and not governed by the Heisenberg O(2N) Wilson-Fisher fixed point but by a different fixed point which is also non-trivial for $D < 4$. For smaller N, this new fixed point disappears and there is no stable fixed point which is an indication for a fluctuation-induced first-order transition. The dividing universal line between second-order and first-order behaviour is found to be $N_c(D) = 21.8 - 23.4\epsilon + O(\epsilon^2)$. The rapid variation of N_c leaves us rather uncertain about the fate of the case $D = 3$. Clearly more information is needed about the $N_c(D)$ line in the (number of components-dimension)-plane.

A $D = 2+\epsilon$ renormalization group study has been performed for a system of Heisenberg spins[3] by use of a non-linear sigma model defined on a homogeneous non-symmetric coset space $O(3)\times O(2)/O(2)$. It was found that near two dimensions the system undergoes a second order transition which is governed by the O(4) usual Wilson-Fisher fixed point. In fact the symmetry

$O(3) \times O(2)/O(2)$ is dynamically enlarged at the critical point to $O(3) \times O(3)/O(3)$ and $O(3) \times O(3)$ is O(4). This mismatch between the expansions near four dimensions and near two dimensions is quite unusual and does not happen in the well-studied $O(N) \to O(N-1)$ critical phenomena. As a consequence, the $D = 3$ case remains elusive and a direct study in three dimensions is called for.

Some preliminary Monte Carlo (MC) simulations have shown some evidence [4] for a continuous transition in the case of the Heisenberg antiferromagnet on a stacked triangular lattice. However the exponents found are not compatible with those of the O(4) vector model in three dimensions. This fact is difficult to reconcile with RG studies which predict a O(4) transition ($D = 2 + \epsilon$). It is the purpose of this article to shed light on this discrepancy by means of a MC study of the model. We did a large-scale simulation with much better statistics than previous attempts. As a consequence we are able to pin down the transition temperature in a very precise manner and to obtain reliable estimates of critical exponents.

We thus focus on the classical spin model defined by the classical Heisenberg Hamiltonian:

$$H = \sum_{<ij>} J_{ij} \; \mathbf{S}_i \cdot \mathbf{S}_j . \tag{1}$$

The exchange interaction J_{ij} is nonzero ($J_{ij} = 1$ in what follows) between nearest-neighbors of a stacked triangular lattice and the spins are three-component unit vectors. The classical ground state is found by minimizing the Fourier transform $J(\mathbf{Q})$ of the couplings J_{ij}. The spins adopt a planar arrangement on a three-sublattice structure with relative angles 120 degrees.

2 The simulation

We made two successive sets of Monte Carlo simulations of this model, using slightly asymmetric lattices (with periodic boundary conditions) of shape $L^2 L_z$, where L is the linear size inside the planes, and $L_z = 2/3L$ the stacking size.

The first set of simulations was run on a CM-2 8K massively parallel computer. We made runs on lattices of size 12^2 8 (with a total of 600 000 Monte Carlo sweeps of the lattice), 24^2 16 (with a total of 1 500 000 sweeps) and

$48^2\ 32$ (with a total of 1 570 000 sweeps). In the first case we used the Heat-Bath algorithm, in the later two cases we used an Hybrid Overrelaxation algorithm[5] where each Heat-Bath sweep is followed by an energy conserving sweep. The next set of simulations was run on CRAY vector computers on lattices of size $24^2 16$, $30^2 20$, $36^2 24$ and $48^2 32$ with 4 to 8 10^6 Hybrid Overrelaxation sweeps. Both simulations concentrate in the immediate vicinity of the transition.

Let us note by $\mathbf{S}_a$ the total spin per site for sublattice a ($a \in [1, 2, 3]$), we measured the magnetization:

$$M_L(\beta) = \frac{1}{3} \sum_a < |\mathbf{S}_a| >, \tag{2}$$

the susceptibility:

$$\chi_L(\beta) = \frac{L^2 L_z}{3} \quad \sum_a < \mathbf{S}_a^2 > - < |\mathbf{S}_a| >^2, \tag{3}$$

and the fourth-order cumulant:

$$B_L(\beta) = 1 - \frac{1}{3} \sum_a \frac{< \mathbf{S}_a^4 >}{< \mathbf{S}_a^2 >^2}. \tag{4}$$

Our strategy to extract the critical exponents was first to estimate the value of the critical temperature β_c, as the point where $B_L(\beta)$ is L independent and then to estimate the exponents from the following set of equations:

$$\chi_L(\beta_c) \sim L^{\gamma/\nu}, \tag{5}$$

$$M_L(\beta_c) \sim L^{-\beta/\nu}, \tag{6}$$

$$\left.\frac{\partial B_L(\beta)}{\partial \beta}\right|_{\beta=\beta_c} \sim L^{-1/\nu}. \tag{7}$$

The extrapolation, from the β value used for the simulation, to β_c is done using the Ferrenberg-Swendsen technique [6]. This technique is invaluable to extrapolate in a neighborhood of size $\sim 1/L^{1/\nu}$ (We understand that, when used blindly outside such a tight range, it may give wrong results). The statistical analysis is done with respect to 20 bins, using first-order bias-corrected jackknife (see e.g. Ref.[7] and references therein). The first 20 % of each run is discarded for thermalization.

¿From simulations of lattices of increasing sizes $L_1 < L_2 < \ldots$, converging estimators of β_c are obtained by solving the equations:

$$B_{L_{i-1}}(\tilde{\beta}) = B_{L_i}(\tilde{\beta}). \qquad (8)$$

L values	β_c	γ/ν	$D-2\beta/\nu$	ν
24-12	1.0440 (4)	2.009 (14) (04)	2.030 (07) (07)	.68 (02) (00)
48-24	1.0446 (2)	2.033 (18) (14)	1.998 (09) (25)	.77 (03) (01)

Table 1: CM-2 runs: critical temperature and critical exponents estimates. The first column gives the linear sizes of the two lattices used. The two numbers inside parenthesis are the estimates of the statistical errors, direct and induced, on the last digits of the number on their left.

L values	β_c	γ/ν	$D-2\beta/\nu$	ν
30-24	1.0439 (4)	1.994 (37) (12)	2.022 (13) (16)	.79 (07) (01)
36-30	1.0441 (4)	1.988 (55) (16)	2.020 (18) (21)	.74 (09) (02)
42-36	1.0448 (3)	2.083 (68) (14)	1.984 (20) (31)	.90 (14) (02)
48-42	1.0443 (3)	1.986 (61) (18)	2.004 (22) (39)	.70 (08) (01)
48-24	1.0443 (1)	2.011 (11) (15)	2.010 (04) (25)	.78 (02) (01)

Table 2: CRAY runs: critical temperature and critical exponents estimates. The first column gives the linear sizes of the two lattices used. The two numbers inside parenthesis are the estimated statistical errors, direct and induced, on the last digits of the number on their left.

The results can be found in the second column of Tab.1 (resp. Tab.2) for the CM-2 (resp. CRAY) data. Within our statistical accuracy, all estimates are compatible, there is neither any clear lattice size dependence, nor any discrepancy between the two sets of runs. Our final estimate is thus:

$$\beta_c = 1.0443 \pm .0002. \qquad (9)$$

We use this value to compute $\chi_L(\beta_c)$, $M_L(\beta_c)$ and $\left.\frac{\partial B_L(\beta)}{\partial\beta}\right|_{\beta=\beta_c}$, in order to estimate γ/ν, β/ν, and ν itself. Results can be found in Tab.1 (Tab.2) for the CM-2 (CRAY) runs. We quote separately the estimated "direct" statistical errors computed from the dispersion of the results from the 20 bins, and the errors induced by the uncertainty on the determination of β_c, computed as the (absolute value of the) difference between the values obtained using our best estimate of β_c and the values using the one standard deviation estimate. Our final numbers are $\gamma/\nu = 2.01 \pm .03$, $D - 2\beta/\nu = 2.01 \pm .03$, $\nu = .79 \pm .03$, obtained from linear fits of the CRAY data for $\ln(\chi_L(\beta_c))$, $\ln(M_L(\beta_c))$ and $\ln(\left.\frac{\partial B_L(\beta)}{\partial\beta}\right|_{\beta=\beta_c})$ respectively. The results of the fits are stable against omitting the smallest lattice data.

We observe that hyperscaling is verified within errors, and as usual in three dimensions, η is very small ($\eta \sim .01$). The value for ν is compatible with the value for the $O(4)$ fixed point[9] ($\nu \sim .75$). We have thus obtained excellent evidence for a continuous transition in the $D = 3$ case and we have shown that the critical exponents are perfectly compatible with the RG prediction of the $2 + \epsilon$ expansion. The specific heat exponent α is *negative* due to the large value of ν, like in the usual Heisenberg model (non-canted) in D=3. Our results are in marked disagreement with the lower statistics Monte Carlo results of Ref.[4] ($\nu = .59 \pm .02$). The methods of analysis are different. Ref.[4] uses data taken in a wide region around the transition point and adjust the values of the critical exponents using the old fashioned "data collapsing" method. This method has the disadvantage to give much weight to points with large value of $(\beta - \beta_c)L^{1/\nu}$. We extract the exponents directly from data reweighted to β_c. We have also a much higher statistics: we use 8×10^6 heat-bath + energy-conserving sweeps whereas [4] uses 6-20 times 20000 sweeps of a less efficient algorithm. Our estimated statistical error on the determination of β_c is one order of magnitude smaller than the one in ref.[4].

3 Conclusion

In view of the present evidence for O(4) behaviour at $D = 3$ we are led to suggest the phase diagram shown in Fig.1 between two and four dimensions and for models with three or more components. Let us first summarize the

knowledge obtained from perturbative RG studies:
i) There is a universal line $N_c(D)$ separating a first-order region from a second-order region near $D = 4 - \epsilon$. Its slope is known from RG studies[2] as well as the critical value N_c for $D = 4$.
ii) Large-N studies[8] have shown that the stable fixed point found above $N_c(D)$ persists smoothly in the region $N = \infty$ and $2 < D < 4$: the top boundary line of Fig.1.
iii) Smoothness along the $D = 2$ vertical axis can be shown by studying the nonlinear sigma model suited to the N-vector model: it is built on the homogeneous space $O(N) \times O(2)/O(N-2) \times O(2)$[10]. One finds a single stable fixed point for *all* values of $N \geq 3$. In the large-N limit the exponents from this sigma model are the same as those of the linear model: this happens at the upper left corner of Fig.1.

If we believe in the perturbative RG results, then necessarily the universal line $N_c(D)$ can only intersect the horizontal axis $N = 3$ between D=2 and D=4. The simplest hypothesis is then that the plane (N, D) is divided in two regions by the line $N_c(D)$ as shown in fig.1. This line intersects the $N = 3$ axis at a critical dimension D_c. Our Monte-Carlo results thus imply that D_c is between three and four dimensions since we observe a continuous transition at D=3. Since in addition we have evidence for O(4) behaviour this means that nothing dramatic happens between the neighborhood of D=2 and D=3. We note that the stable fixed point that governs the whole second-order domain reduces to a known fixed point (of the Wilson-Fisher $O(N)$ family) *only* in the N=3 case where there is a peculiar symmetry enlargement[10]. This is consistent with the fact that the stable fixed point found near D=4 above the line $N_c(D)$ does not belong to the Wilson-Fisher family. Our results seem to exclude the intriguing proposal[3] $D_c = 3$ or very close to 3, a logical possibility for which there is no compelling argument. We note that the phase diagram we propose is in agreement with all known RG results and does not require the addition of any new fixed point, unseen in perturbation theory. Our results also give support to the validity of the $2 + \epsilon$ expansion, a fact that is far from being obvious since perturbative treatment of a sigma model neglects global aspects. Previous studies indeed have performed, as usual, only perturbation theory for spin-wave excitations[3].

We have thus obtained a simple picture of the critical behaviour of a magnet with a canted ground-state. In the physical case, we predict that Heisenberg helimagnets will belong to the O(4) universality class (the exponent η belonging to a tensor representation[10]). We note for the future that it would be interesting to obtain the critical behaviour of the XY canted systems, much more relevant to the experimental situation.

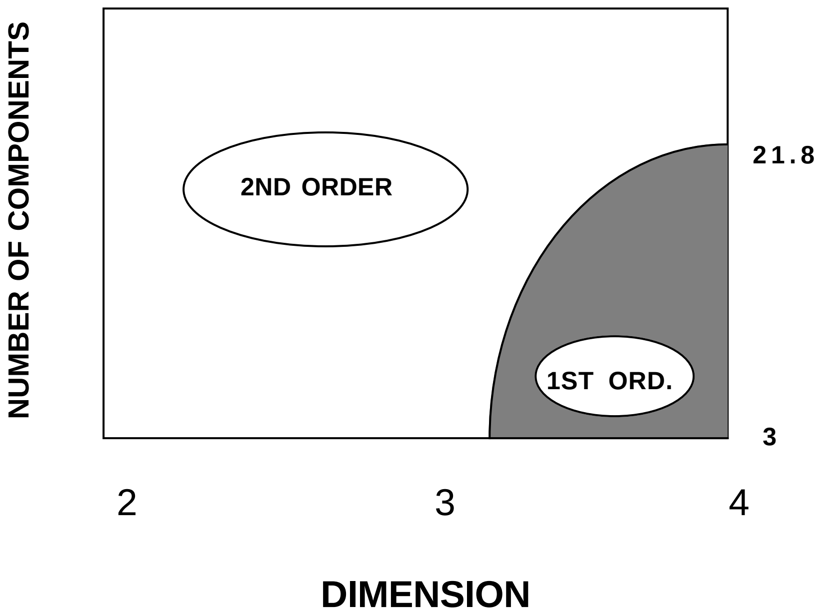

Figure 1: Phase diagram of the D-dimensional $O(N)$ canted model, in the (N, D)-plane.

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