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Short Communication

Critical behavior of the antiferromagnetic Heisenberg model on a stacked triangular lattice

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Abstract. — 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: $\gamma/\nu = 2.011 \pm 0.014$, $\nu = 0.585 \pm 0.009$. These results contradict a perturbative $2 + \epsilon$ Renormalization Group calculation that points to Wilson-Fisher O(4) behaviour. While these results may be coherent with $4 - \epsilon$ results from Landau-Ginzburg analysis, they show the existence of an unexpectedly rich structure of the Renormalization Group flow as a function of the dimensionality and the number of components of the order parameter.

1. Introduction.

There is at present 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 or-

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order below a transition point $T_c$. 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 evidence [4-7] for a continuous transition in the case of the Heisenberg antiferromagnet on a stacked triangular lattice. The exponents found are not compatible with those of the $O(4)$ vector model in three dimensions. 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:

$$H = \sum_{\langle ij \rangle} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j.$$  \hspace{1cm} (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 $\widehat{J}(\mathbf{Q})$ 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 [9] 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 $18^2 12, 24^2 16, 30^2 20, 36^2 24$ and $48^2 32$ with 4 to $8 \times 10^8$ Hybrid Overrelaxation sweeps. Both simulations concentrate in the immediate vicinity of the transition.
CRITICAL BEHAVIOR OF AN HELIMAGNET

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

$$M_L(\beta) = \frac{1}{3} \sum_a < |S_a| >,$$

(2)

the susceptibility:

$$\chi_L(\beta) = \frac{L^2 L_z}{3} \left( \sum_a < S_a^2 > - < |S_a| >^2 \right),$$

(3)

and the fourth-order cumulant:

$$B_L(\beta) = 1 - \frac{1}{3} \sum_a < S_a^4 >.$$

(4)

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

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

(5)

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

(6)

$$\frac{\partial B_L(\beta)}{\partial \beta} \bigg|_{\beta=\beta_c} \sim L^{1/\nu}$$

(7)

$$\frac{\partial}{\partial \beta} \ln M_L(\beta) \bigg|_{\beta=\beta_c} \sim L^{1/\nu}$$

(8)

The extrapolation, from the $\beta$ value used for the simulation, to $\beta_c$ is done using the Ferrenberg-Swendsen technique [10]. 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). An alternative strategy would be to evaluate exponents from the finite size scaling of the maxima of $\chi_L(\beta), M_L(\beta), \frac{\partial}{\partial \beta} B_L(\beta)$ and $\frac{\partial}{\partial \beta} \ln M_L(\beta)$. It would however require to perform simulations at four $\beta$ values, close to the four ($L$ dependent) points where these quantities reach their maxima, otherwise accuracy would be lost. The statistical analysis is done with respect to 20 bins, using first-order bias-corrected jackknife (see e.g. Ref. [11] and Refs. 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 $\beta_c$ are obtained by solving the equations:

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

(9)

The results can be found in the second column of table I. 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 (the quoted error is deliberately on the safe side)

$$\beta_c = 1.0443 \pm 0.0002.$$

(10)

We use this value to compute $\chi_L(\beta_c), M_L(\beta_c), \frac{\partial}{\partial \beta} B_L(\beta)$ and $\frac{\partial}{\partial \beta} \ln M_L(\beta)$ in order to estimate $\gamma/\nu, \beta/\nu$ and $\nu$. Results can be found in table I. We quote separately the estimated “direct"
Table I. — Critical temperature and critical exponents estimates, using equations (9, 5, 6, 7) and (8) respectively. First two lines are CM-2 data, next lines the CRAY data. The first column gives the linear sizes of the 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.

<table>
<thead>
<tr>
<th></th>
<th>$\beta_c$</th>
<th>$\gamma/\nu$</th>
<th>$D - 2\beta/\nu$</th>
<th>$\nu$</th>
<th>$\nu$</th>
</tr>
</thead>
<tbody>
<tr>
<td>24-12</td>
<td>1.04401 (38)</td>
<td>2.009 (14) (04)</td>
<td>2.030 (07) (07)</td>
<td>0.651 (22) (03)</td>
<td>0.604 (10) (01)</td>
</tr>
<tr>
<td>48-24</td>
<td>1.04462 (21)</td>
<td>2.033 (18) (14)</td>
<td>1.998 (09) (25)</td>
<td>0.590 (20) (04)</td>
<td>0.576 (10) (04)</td>
</tr>
<tr>
<td>24-18</td>
<td>1.04452 (40)</td>
<td>2.010 (26) (06)</td>
<td>2.011 (08) (10)</td>
<td>0.605 (30) (03)</td>
<td>0.608 (17) (02)</td>
</tr>
<tr>
<td>30-24</td>
<td>1.04388 (36)</td>
<td>1.994 (36) (11)</td>
<td>2.021 (13) (16)</td>
<td>0.578 (35) (03)</td>
<td>0.583 (19) (03)</td>
</tr>
<tr>
<td>36-30</td>
<td>1.04408 (37)</td>
<td>1.988 (55) (16)</td>
<td>2.020 (18) (21)</td>
<td>0.605 (55) (12)</td>
<td>0.607 (30) (04)</td>
</tr>
<tr>
<td>42-36</td>
<td>1.04485 (25)</td>
<td>2.083 (68) (14)</td>
<td>1.984 (20) (31)</td>
<td>0.528 (48) (06)</td>
<td>0.548 (28) (06)</td>
</tr>
<tr>
<td>48-42</td>
<td>1.04427 (30)</td>
<td>1.986 (61) (18)</td>
<td>2.004 (22) (39)</td>
<td>0.639 (69) (05)</td>
<td>0.577 (27) (03)</td>
</tr>
<tr>
<td>48-18</td>
<td>1.04432 (06)</td>
<td>2.011 (07) (12)</td>
<td>2.010 (03) (21)</td>
<td>0.590 (09) (06)</td>
<td>0.588 (04) (03)</td>
</tr>
<tr>
<td>all</td>
<td>$N/A$</td>
<td>2.011 (07) (12)</td>
<td>2.011 (02) (19)</td>
<td>0.585 (07) (06)</td>
<td>0.585 (04) (04)</td>
</tr>
</tbody>
</table>

Statistical errors computed from the dispersion of the results from the 20 bins, and the errors induced by the uncertainty on the determination of $\beta_c$, computed as the (absolute value of the) difference between the values obtained using our best estimate of $\beta_c$ and the values using the one standard deviation estimate from equation (10). The last line in table I gives the results of linear fits of the CRAY data for $\ln(\chi_L(\beta_c))$, $\ln(M_L(\beta_c))$, $\ln(\frac{\partial}{\partial \beta} B_L(\beta)\big|_{\beta=\beta_c})$ and $\ln(\frac{\partial}{\partial \beta} \ln M_L(\beta)\big|_{\beta=\beta_c})$ respectively. The results of the fits are stable against omitting the smallest lattice data. The $\chi^2$ is equal to 1.5, 3.7, 1.9 and 4.5 respectively (we expect $\chi^2 \approx 4$). Such values mean that linear fits give good representation of the data for $L \geq 18$ (with the current accuracy).

Our final numbers are $\gamma/\nu = 2.011 \pm 0.014$, $D - 2\beta/\nu = 2.011 \pm 0.019$, $\nu = 0.585 \pm 0.009$. We observe that hyperscaling is verified within errors, and $\eta$ is very small ($|\eta| \approx 0.01$). The value for $\nu$ is clearly not compatible with the value for the O(4) fixed point [13] ($\nu \approx 0.75$).

Published Monte Carlo results for $\nu$ are $0.53 \pm 0.02$ [4], $0.53 \pm 0.03$ [5], $0.55 \pm 0.03$ [6] and $0.59 \pm 0.02$ [7]. Our results are in good agreement with the most recent results (and with the result $0.57 \pm 0.02$ from a model of commensurate Heisenberg helimagnet [8]). The methods of analysis are quite different. Reference [7] 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 $\beta_c$. We have also a much higher statistics: we use $8 \times 10^6$ heat-bath + energy-conserving sweeps whereas [7] uses 6-20 times 20000 sweeps of a less efficient algorithm. Our estimated statistical error on the determination of $\beta_c$ is one order of magnitude smaller than the one in reference [7].

3. Conclusion.

Let us first summarize the knowledge obtained from perturbative RG studies as a function of the dimensionality and the number of components of the order parameter.

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
\( D = 4 \).

1) Large-\( N \) studies [12] indicate that the stable fixed point found above \( N_c(D) \) persists smoothly in the region \( N = \infty \) and \( 2 < D < 4 \).

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 \( O(N) \times O(2)/O(N-2) \times O(2) \) [14]. 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.

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 \( N_c(D) \). This line may intersect 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 \( D = 3 \). A possibility would be that the critical behaviour we observe is described by the fixed point found in the neighborhood of \( D = 4 \).

However one has to note that the sigma model approach shows that this fixed point is \( O(4) \) for \( N = 3 \). This is clearly ruled out by our data. The simplest scenario suggested by i-iii above is wrong. It may be that the whole sigma model approach breaks down 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]. One may invoke the peculiar vortices present in the model [16] since \( \Pi_1(\text{SO}(3)) = \mathbb{Z}_2 \) that form loops in \( D = 3 \) as responsible of the breakdown of the sigma model. However vortices are also excluded from the perturbative calculations near \( D = 4 \) and thus it would be difficult in this case to believe in what is found perturbatively. It may be also that the fixed point found in \( 2 + \epsilon \) expansion is destabilized by some operators containing high powers of gradients [15].

We have thus obtained the critical behaviour of a magnet with a canted ground-state. This calls for a deeper understanding of the Renormalization Group behaviour of canted systems since there is no obvious relationship between the different perturbative approaches, contrary to the case of collinear vector magnets. 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.

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Note added in proof:

Results compatible with our's have been obtained by D. Loison [17].

References