



Critical exponents and unusual properties of the broken phase in the 3d-RP² antiferromagnetic model.*

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We present the results of a Monte Carlo simulation of the antiferromagnetic RP² model in three dimensions. With finite-size scaling techniques we accurately measure the critical exponents and compare them with those of O(N) models. We are able to parameterize the corrections-to-scaling. The symmetry properties of the broken phase are also studied.

1. Introduction.

AntiFerromagnetic (AF) models exhibit interesting characteristic properties. For instance, AF couplings on non-bipartite lattices, as the triangular Ising model, produce frustration. On bipartite lattices they can produce disordered Ground States, as for the AF three states Potts Model in three dimensions, which belongs to the XY Universality Class. It is then possible to find new Spontaneous Symmetry Breaking (SSB) patterns, and maybe new Universality Classes. Our interest in these models is twofold: they apply to Condensed Matter systems (spin glasses, helical and canted spin systems,³He superfluid phase transition, etc.) and four dimensional Field Theory, as they might offer some insight on the formulation of non asymptotically-free interacting theories. For the AF RP² model, the finite-size scaling analysis close to the transition, strongly suggests that the action's O(3)-symmetry is broken, yielding an SO(3)/{1} SSB pattern. The perturbative prediction for such an SSB pattern is that the transition can either be on the O(4) Universality Class or that it should be first order or tricritical [1].

2. The model.

We consider a system of three components, normalized vectors, placed on the nodes of a cubic

lattice. They interact through a first neighbors coupling

$$S = \beta \sum_{\langle i,j \rangle} (\sigma_i \cdot \sigma_j)^2 . \quad (1)$$

This action presents a global O(3) symmetry, and a local Z₂ one ($\sigma_i \rightarrow -\sigma_i$). From Elitzur's theorem, it follows that we are really studying RP² variables. For positive β , this model suffers a first order phase transition, all spins aligned or anti-aligned with an arbitrary direction. This corresponds to the nematic phase of liquid crystals. At $\beta \approx -2.41$ the system undergoes a second order phase transition [2,3]. The symmetry description is however, more complicated. Let us call the spin placed on (x, y, z) even or odd, according with the parity of $x + y + z$. At $\beta = -\infty$, the ground state consists on all the spins on the, for example, even sublattice, aligned or anti-aligned with an arbitrary direction, while odd spins lie randomly on the perpendicular plane. This state has a remaining O(2)-symmetry, but the symmetry between even-odd sublattices is broken. However, thermal fluctuations induce an interaction between the spins on the plane sublattice, as an alignment allows stronger fluctuations on the other sublattice.

As the natural variable is the tensorial product of σ by itself, we consider the traceless tensorial field

$$T_i^{\alpha\beta} = \sigma_i^\alpha \sigma_i^\beta - \frac{1}{3} \delta^{\alpha\beta} . \quad (2)$$

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We define the normalized non-staggered and staggered magnetizations as

$$\mathbf{M} = \frac{1}{V} \sum_{x,y,z} \mathbf{T}_{(x,y,z)}, \quad (3)$$

$$\mathbf{M}_s = \frac{1}{V} \sum_{x,y,z} (-1)^{x+y+z} \mathbf{T}_{(x,y,z)}. \quad (4)$$

In the simulation we actually measure

$$M = \langle \sqrt{\text{tr} \mathbf{M}^2} \rangle, \quad (5)$$

and the associated susceptibility

$$\chi = V \langle \text{tr} \mathbf{M}^2 \rangle. \quad (6)$$

We have found very useful the measure of the second momentum correlation length defined as

$$\xi = \left(\frac{\chi/F - 1}{4 \sin^2(\pi/L)} \right)^{1/2}, \quad (7)$$

where F is the Fourier transform of the correlation function at minimal non zero momentum, as well as the scaling function (related to Binder's parameter)

$$\kappa = \frac{\langle (\text{tr} \mathbf{M}^2)^2 \rangle}{\langle \text{tr} \mathbf{M}^2 \rangle^2}. \quad (8)$$

The staggered counterparts of the quantities (5-8) are defined analogously.

We have also measured the first and second neighbors energies:

$$E_1 = \frac{1}{3V} \sum_{\langle i,j \rangle} (\sigma_i \cdot \sigma_j)^2, \quad (9)$$

$$E_2 = \frac{1}{6V} \sum_{\ll i,j \gg} (\sigma_i \cdot \sigma_j)^2. \quad (10)$$

E_1 has been used for the Ferrenberg-Swendsen extrapolation method, and for calculating β -derivatives. E_2 is useful to obtain information about the structure of the broken phase.

3. The simulation.

We have used a Metropolis update. Cluster methods are feasible but not efficient.

We have measure the integrated and exponential autocorrelation times for E_1 , χ and χ_s . The

integrated times satisfy $\tau_{E_1}^{\text{int}} < \tau_{\chi}^{\text{int}} < \tau_{\chi_s}^{\text{int}}$ (for instance, in the larger lattice the ratio is 1:3:7). However, the exponential times are almost equal, and they are near $\tau_{\chi_s}^{\text{int}}$. So, we have confidence that the latter is the larger autocorrelation time. Further details can be found in refs. [3].

In table 1 we present the number of Monte Carlo iterations performed at each lattice size, together with the corresponding autocorrelation time. The expected behavior $\tau \propto L^2$ is well satisfied.

Table 1

Number of Monte Carlo sweeps performed for different lattice sizes. Measures have been taken every 10 sweeps. We have discarded in each case about $200\tau_{\chi_s}^{\text{int}}$ iterations for thermalization.

L	MC sweeps($\times 10^6$)	$\tau_{\chi_s}^{\text{int}}$	# of $\tau_{\chi_s}^{\text{int}}$
6	6.71	7.37(3)	910,000
8	17.07	11.41(4)	1,496,000
12	6.51	24.9(2)	261,000
16	22.14	44.5(3)	498,000
24	8.77	107(3)	82,000
32	28.51	175(6)	163,000
48	3.93	410(20)	9,600

4. Finite size scaling techniques.

For an operator, O , with critical exponent x_O , we have

$$\langle O(L, \beta) \rangle = L^{x_O/\nu} (F_O(\xi(L, \beta)/L) + O(L^{-\omega})).$$

Order $\xi(\infty, \beta)^{-\omega}$ terms, are negligible in the critical region.

Measuring at two lattice sizes L and sL and computing the quotient

$$Q_O = \frac{\langle O(sL, \beta) \rangle}{\langle O(L, \beta) \rangle}, \quad (11)$$

we can eliminate the scaling function F_O just by choosing the β value such that the ratio between correlation lengths is s , obtaining

$$Q_O|_{Q_{\xi=s}} = s^{x_O/\nu} + O(L^{-\omega}). \quad (12)$$

5. Exponents

To compute the ν exponent we consider operators like the β derivatives of the correlation length or the logarithm of the magnetization ($x_{d\xi/d\beta} = \nu + 1$, $x_{d \log M/d\beta} = 1$). In table 2 we present in the second column the results obtained from $Q_{d\xi_s/d\beta} | Q_{\xi_s} = 2$. The values using other operators involving ξ are similar but slightly worse. In the case of operators involving magnetizations, the statistical errors are smaller, but the finite-size effects are greater. We do not find any significant deviation between the staggered and non-staggered channels what supports the equality $\nu = \nu_s$ necessary to define a single continuum limit.

In the case of magnetic exponents, we expect a different behavior for the staggered and non-staggered channels. We obtain the respective η_s and η exponents from $\gamma_{(s)}/\nu$ or $\beta_{(s)}/\nu$ using the scaling relations $\eta_{(s)} = 2 - \gamma_{(s)}/\nu$ or $\eta_{(s)} = 2 - d + 2\beta_{(s)}/\nu$. The quality of the results depends on the observable measured. With a good selection of both the O operator and the definition of correlation length the corrections-to-scaling terms can be largely reduced. We should remark that the operator used to measure the correlation length in practice can be any quantity that scales linearly with L at the critical point, such as κL . However, the more interesting property of the method we use is that even if the operator O is a rapidly varying function of the coupling at the critical point, as the magnetization or the susceptibility are, the statistical correlation between Q_O and Q_ξ allows a very precise measure of the critical exponents.

In table 2, (col. 3), we display the results for η_s using χ_s as operator and ξ_s as correlation length. Regarding η exponent the use of ξ or ξ_s as correlation length produce large corrections-to-scaling. We have realized that those effects are strongly reduced when using κL as the *correlation length* operator (see col. 4).

6. Scaling corrections

At very large volume, scaling functions for different lattices, such as ξ_s/L , ξ/L , κ or κ_s should

Table 2

ν , η_s and η exponents obtained from (12) using as operators $d\xi_s/d\beta$, χ_s and χ respectively. As correlation length we take ξ_s in all cases but the latter where we have used κL . The pairs are of type $(L, 2L)$.

L	ν	η_s	η
6	0.786(6)	0.0431(10)	1.332(6)
8	0.785(4)	0.0375(7)	1.332(4)
12	0.789(8)	0.0357(17)	1.321(13)
16	0.786(6)	0.0375(12)	1.340(5)
24	0.77(2)	0.038(5)	1.334(18)

cross at β^c . Scaling corrections shift the crossing point, corresponding to a pair of lattices $(L_1, L_2 = sL_1)$, an amount given by

$$\Delta\beta^{L_1, L_2} \propto \frac{1 - s^{-\omega}}{s^{\frac{1}{\nu}} - 1} L_1^{-\omega - \frac{1}{\nu}}. \quad (13)$$

As the crossing point of correlation lengths and Binder-like parameters tend to the critical point from opposite sides, it is sensible to perform a global fit, with the full covariance matrix to take into account the statistical correlation of all the data. We have fitted our data either fixing the small lattice, L_1 , or an s value. For instance, for $L_1 = 8$, we obtain

$$\begin{aligned} \beta^c &= -2.4085(3), \\ \omega &= 0.86(4), \\ \chi^2/\text{d.o.f.} &= 12.2/14. \end{aligned} \quad (14)$$

Using also the $L_1 = 6$ data or fixing $s = 2$ the results are compatible (see ref. [3]).

After measuring the, universal, corrections-to-scaling exponent ω we can estimate the finite-size effects on the critical exponents using

$$\frac{x}{\nu} - \frac{x}{\nu} \Big|_{(2L, L)} \propto L^{-\omega}. \quad (15)$$

From the results quoted in table 2 we conclude that the values for ν are rather stable when increasing the lattice size, but a proper accounting of finite-size effects is crucial in the case of η exponents for some operators (see also ref. [4] where this method is applied to three dimensional $O(N)$ models).

Anyway, the presence of an L dependence, even when it is not measurable, requires an increasing of the error bars for a safe determination of the systematic error due to finite-size effects. We summarize the results giving the value for the (16,32) pair, with a second error bar that corresponds to the increasing of the error due to the infinite volume extrapolation,

$$\begin{aligned} \nu &= 0.783(5)(6) , \\ \eta_s &= 0.0380(12)(14) , \\ \eta &= 1.339(5)(5) . \end{aligned} \tag{16}$$

Some minor differences between the values in table 2 and (16) exist because here we average between the results of several operators not displayed in the table.

The exponent ν is two standard deviations apart from the value for the three-dimensional O(4) model ($\nu_{O(4)} = 0.755(8)[4]$) what supports that the AF transition in the RP^2 model belongs to a new Universality Class, but the opposite cannot be completely discarded.

7. Vacuum structure

In the $\beta = -\infty$ limit, there is a breakdown of the symmetry between the odd and even sublattices, but a global O(2) symmetry still remains. At the critical region, the presence of fluctuations can change this picture.

To study the structure of the broken phase near the critical point we have analyzed the FSS of two operators

$$A = \langle (\text{tr } \mathbf{M}_s \mathbf{M})^2 \rangle, \tag{17}$$

$$B = \langle \text{tr}[\mathbf{M}_s, \mathbf{M}][[\mathbf{M}_s, \mathbf{M}]^\dagger] \rangle. \tag{18}$$

The A operator depends on the difference of the magnetizations squared of both sublattices ($\text{tr } \mathbf{M}_{\text{even}}^2 - \text{tr } \mathbf{M}_{\text{odd}}^2$), so, if the even-odd symmetry were not broken it should scale as L^{-2d} . The obtained value

$$x_A/\nu = -3.389(15) , \tag{19}$$

agrees with $-2(\beta + \beta_s)/\nu$ and discards a remaining even-odd symmetry.

The B operator measures if the tensors \mathbf{M} and \mathbf{M}_s commute (what is equivalent to the commutation of \mathbf{M}_{even} with \mathbf{M}_{odd}). If they did not, a

simultaneous diagonalization is not possible, and a remaining O(2) symmetry is discarded. The expected FSS for an unbroken O(2) symmetry correspond to $x_B/\nu = -d - 2\beta_s/\nu = 4.04(2)$ while the value obtained numerically is

$$x_B/\nu = -3.406(11) . \tag{20}$$

To check if both breakdowns occur deep in the broken phase, we have studied the second neighbor energy E_2 for each sublattice, as well as the eigenvalues of the magnetization tensors.

The analysis of the E_2 histograms show an unambiguous signature of breakdown of the even-odd symmetry along all the broken phase. It is interesting to remark that the energy of the less aligned sublattice takes for $\beta \rightarrow -\infty$ the value 0.532(5) to be compared with the $\beta = -\infty$ value, 0.5. The presence of fluctuations acts as an effective coupling that favors an alignment.

The intensity of that induced interaction increases when approaching to the critical point. To know where it actually produces a breakdown of the O(2) symmetry, we have studied the eigenvalues of the \mathbf{M} matrix. We have observed that the difference between the two smaller eigenvalues goes to zero when the lattice size grows, for $\beta \leq -4$. At $\beta = -3$ a nonzero value is not completely excluded but we would need lattice sizes larger than 48 to obtain a reliable measure. In order to clarify this point, we project to study an extended model where an explicit second neighbor coupling is added.

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