ELSEVIER

12 February 1998

PHYSICS LETTERS B

Physics Letters B 419 (1998) 303–310

Antiferromagnetic O(N) models in four dimensions

H.G. Ballesteros [a], J.M. Carmona [b], L.A. Fernández [a], A. Tarancón [b]

[a] *Departamento de Física Teórica I, Facultad de CC. Físicas [1], Universidad Complutense de Madrid, 28040 Madrid, Spain*
[b] *Departamento de Física Teórica, Facultad de Ciencias [2], Universidad de Zaragoza, 50009 Zaragoza, Spain*

Received 8 April 1997
Editor: R. Gatto

Abstract

We study the antiferromagnetic O(N) model in the F_4 lattice. Monte Carlo simulations are applied for investigating the behavior of the transition for $N = 2,3$. The numerical results show a first order nature but with a large correlation length. The $N \to \infty$ limit is also considered with analytical methods. © 1998 Elsevier Science B.V.

PACS: 05.70.Jk; 64.60.Fr; 75.40.Mg; 75.50.Ee
Keywords: Lattice; Monte Carlo; Antiferromagnetic; Phase transitions; O(N) models

1. Introduction

The antiferromagnetic formulations of field theories in four dimensions have been recently paid considerable attention [1–5]. The hope is to give some insight into the well known triviality problem in field theory [6]. Also there are other interesting phenomena as the apparition of new particles [5].

A spin model, in a simple cubic lattice with first neighbor interactions, becomes antiferromagnetic if the coupling is negative. However, with some exceptions [4,7], a simple *staggered* transformation maps the antiferromagnetic phase into the usual ferromagnetic one.

To obtain a non-equivalent antiferromagnetic phase one has to include further couplings or modify the lattice geometry (see for instance ref [8]).

Perhaps the simplest method to obtain non-trivial antiferromagnetism in four dimensions is to work in an F_4 lattice. It is defined by taking out the odd sites (the sum of the coordinates is odd) of a simple hypercubic lattice.

Four dimensional antiferromagnetic O(N) models have been already studied by Monte Carlo(MC) means in this lattice. The O(1) model (Ising model) was considered in Ref. [2]: a weak first order transition was found. A study of the O(4) model appears in Ref. [3]: in the range of the lattice sizes simulated, the behavior pointed to a second order transition.

In this letter we consider the intermediate cases: O(2) and O(3), to know if the order of the transition changes with N. We will give evidence that the transitions are in both cases first order, but the

[1] e-mail addresses: hector, laf@lattice.fis.ucm.es
[2] e-mail addresses: carmona, tarancon@sol.unizar.es

PII S0370-2693(97)01292-6

numerical difficulties grow with N. We also present an analytical study in the $N \to \infty$ limit.

2. The model

We label the coordinates of an F_4 lattice as a set of integers $\{x,y,z,t\}$ such that $x+y+z+t$ is even. We consider the action

$$S = \beta H = -\beta \sum_{\langle i,j \rangle} \mathbf{\Phi}_i \cdot \mathbf{\Phi}_j , \tag{1}$$

where the sum runs over 24 pairs of nearest neighbors and the field, $\mathbf{\Phi}$, is a normalized N component real vector. We work in a hypercubic lattice of size $V = L^4/2$ with periodic boundary conditions.

In the ferromagnetic region ($\beta > 0$) this model is expected to belong to the same universality class of the simple cubic model: it presents a second order transition with mean field critical exponents.

In the antiferromagnetic sector ($\beta < 0$) the system also presents an ordering phase transition, but the structure of the ordered phase is much more complex. In fact, it can be easily checked that the ground state presents frustration. Moreover, the ordered vacuum is not isotropic.

The independent order parameters we can construct with periodicity 2 are

$$\begin{aligned}
\boldsymbol{M}_{\mathrm{F}} &= \frac{1}{V} \sum_{x,y,z,t} \mathbf{\Phi}_{xyzt}, \\
\boldsymbol{M}^{x}_{\mathrm{A}FH} &= \frac{1}{V} \sum_{x,y,z,t} \mathbf{\Phi}_{xyzt} (-1)^{x}, \\
&\vdots \\
\boldsymbol{M}^{x-y}_{\mathrm{A}FP} &= \frac{1}{V} \sum_{x,y,z,t} \mathbf{\Phi}_{xyzt} (-1)^{x+y}, \\
&\vdots
\end{aligned} \tag{2}$$

where the sums are extended to all the F_4 sites. The dots stand for the other 3 combinations of hyperplanes and 2 of planes.

We label the site $I = 1,\ldots,8$ inside the 2^4 elementary cell with its Cartesian coordinates $X,Y,Z,T = 0,1$. In practice we measure the 8 different magnetizations associated to a given position in the elementary cells, $\boldsymbol{m}_i$, defined as the normalized sum of the magnetization for all 2^4 cells for each of the 8 sites.

$$\boldsymbol{m}_I = \boldsymbol{m}_{XYZT} = \frac{8}{V} \sum_{\substack{x,y,z,t \\ x-X,\ldots \text{ even}}} \mathbf{\Phi}_{xyzt} . \tag{3}$$

The quantities (2) can be expressed as linear combinations of these magnetizations.

The mean magnetization and the susceptibility are defined respectively as

$$M = \left\langle \sqrt{\tfrac{1}{8} \sum_{I=1}^{8} \boldsymbol{m}_I^2} \right\rangle , \quad \chi = \frac{V}{8} \left\langle \sum_{I=1}^{8} \boldsymbol{m}_I^2 \right\rangle . \tag{4}$$

The Binder Cumulants are defined in a such way that $V_M|_{\beta=0} = 0$ and $V_M|_{\beta=\infty} = 1$:

$$V_M^{\mathrm{O}(N)} = \frac{N+2}{2} \left(1 - \frac{8N \left\langle \sum_{I=1}^{8} \left(\boldsymbol{m}_I^2 \right)^2 \right\rangle}{(N+2) \left\langle \sum_{I=1}^{8} \boldsymbol{m}_I^2 \right\rangle^2} \right). \tag{5}$$

For the connected susceptibility we use the definition

$$\chi_{\mathrm{c}} = V \left(\tfrac{1}{8} \sum_{I=1}^{8} \left\langle \boldsymbol{m}_I^2 \right\rangle - M^2 \right). \tag{6}$$

3. Critical behavior

For an operator O that diverges as $(\beta - \beta_{\mathrm{c}})^{-x_O}$, its mean value at a coupling β in a size L lattice can be written, in the critical region, assuming the finite-size scaling ansatz as [9]

$$O(L,\beta) = L^{x_O/\nu} \left(F_O(\xi(L,\beta)/L) + O(L^{-\omega}) \right), \tag{7}$$

where F_O is a smooth scaling function and ω is the universal leading corrections-to-scaling exponent. In order to eliminate the unknown F_O function we can measure at the coupling where F_O presents a maximum as for χ_{c} or for the specific heat C_V. Another method [7] is to study the behavior of the quantities

$$Q_O = O(sL,\beta)/O(L,\beta). \tag{8}$$

We use $V_M L$ as scaling variable [7]. It is direct to obtain

$$Q_O\big|_{Q_{V_M L}=s} = s^{x_O/\nu} + O(L^{-\omega}). \quad (9)$$

We use that $x_\chi = \gamma$ and $x_{\partial_\beta \log(M)} = 1$ to obtain the critical exponents.

The expected FSS behavior of a first-order transition [10] corresponds to apparent exponents: $\nu = 1/d$, $\alpha = 1$, $\gamma = 1$.

4. The simulation

We will consider in this letter the cases $N = 2,3$. We have used a Metropolis algorithm followed by N_o overrelaxation steps as update method, N_o depending on the model and lattice size. We have worked in lattice sizes up to 48. We used for the computation the dedicated machine RTNN, consisting in 16 Dual Pentium Pro units. For the largest lattices we parallelized, using shared memory, in each dual motherboard. Every f sweeps we measured the energy, the specific heat and the 8 period-two magnetizations $\boldsymbol{m}_I$. In Table 1 we report the parameters of the simulation at the critical region.

Table 1
Description of the simulation in the critical region for O(2) (upper part) and O(3) (lower part). We report the lattice size, the frequency of measures, number of over-relaxation steps for each Metropolis one, autocorrelation time (τ) for χ, iterations in τ units, and the coupling.

L	f	N_o	$\tau(\chi)$	# of τ	β
4	20	3	0.775(9)	100000	−0.352
6	20	3	1.144(14)	87000	−0.352
8	20	3	1.63(4)	55000	−0.352
12	20	3	3.16(6)	60000	−0.352
16	20	3	6.5(5)	11400	−0.352
24	25	4	15.8(7)	5000	−0.3516
32	24	7	32(1)	1700	−0.3513
48	32	7	85(7)	312	−0.35125
4	20	3	0.871(11)	98000	−0.53
6	20	3	1.19(2)	82000	−0.53
8	20	3	1.52(3)	98700	−0.53
12	20	3	2.07(4)	63000	−0.53
16	20	3	3.15(6)	48000	−0.53
24	24	5	4.99(14)	29000	−0.5287
32	28	6	8.7(4)	5000	−0.5287
48	28	6	21(1)	2000	−0.5286

In order to extrapolate to the neighborhood of the critical point, we used the usual reweighting method [11]. We also simulated at the maxima of the specific heat because the region where the extrapolation was reliable was not large enough. These simulations were about one fourth of the total CPU time.

The errors were computed with a jack-knife method, performing 50 blocks in order to achieve statistical error bars within 10% of precision.

5. The vacuum

For large $|\beta|$, all the magnetizations $\boldsymbol{m}_I$ go to unitary vectors, confirming the assumption of a period 2 vacuum, so that we can restrict our analysis only to a unit cell. We also find that $\boldsymbol{M}_{\mathrm{A}FP}$ is non zero, while $\boldsymbol{M}_{\mathrm{F}}$ and $\boldsymbol{M}_{\mathrm{A}FH}$ vanish.

When $\boldsymbol{M}_{\mathrm{F}} = \boldsymbol{M}_{\mathrm{A}FH} = 0$, it follows that $\boldsymbol{m}_{XYZT} = \boldsymbol{m}_{1-X,1-Y,1-Z,1-T}$. We checked that the cosine between $\boldsymbol{m}_{XYZT}$ and $\boldsymbol{m}_{1-X,1-Y,1-Z,1-T}$ goes to 1, with the expected L^{-4} behavior in the broken phase corresponds to AFP order.

This ordering is also found near the transition. So we can restrict ourselves to study only 4 independent spins.

At $T = 0$ the frustrated ground state is described in [3]; it consists in two couples of antiparallel spins, but the angle between couples is free. The different choices for the couples determine the plane for AFP symmetry breaking.

At $T > 0$ we do not know whether there is a privileged angle or not. It is necessary to determine the pattern of the symmetry breaking.

A very important point is to determine if the two couples are aligned or not. To clarify this point we construct the following tensor:

$$T^{ab} = \tfrac{1}{4} \sum_{K=1}^{4} \boldsymbol{m}_K^a \times \boldsymbol{m}_K^b, \quad (10)$$

where the superindices run for the components of the N vectors and the sum over the four independent magnetizations in the elementary cell. It is clear that if the two couples are aligned, the four tensors as well as the sum tensor can be simultaneously diagonalized, and so we expect in the broken phase a non-zero value for the largest eigenvalue and zero

Table 2
Eigenvalues for the tensor (10) for the O(2) model (upper part) at $\beta = -0.37$ and for the O(3) model (lower part) at $\beta = -0.57$.

Eigenvalue	χ^2/d.o.f.	Value
λ_{max}	0.16	0.20346(15)
λ_{min}	0.13	$-0.0(2.2)\times 10^{-6}$
λ_{max}	0.11	0.18986(7)
λ_{med}	0.89	$2.3(2.7)\times 10^{-7}$
λ_{min}	0.05	$-1.7(1.2)\times 10^{-6}$

values (up to L^{-4} effects) for the rest $(N-1)$ of them.

If this holds true, we also expect in the critical region a $L^{-2\beta/\nu}$ behavior for the biggest one and a L^{-4} for the others. This will be checked in the next section.

In Table 2 we show the eigenvalues for both models in the broken phase. We note that the largest one goes to a non-zero value while the rest go to zero. The fit parameters are obtained with a linear extrapolation in L^{-2} for the former case and in L^{-4} for the latter.

6. Critical exponents

A determination of the critical exponents is obtained by studying the height of the peaks of C_V and χ_c. For a first order transition both quantities should diverge as the volume ($\alpha/\nu = 4, \gamma/\nu = 4$). For small lattices it is usual to find the apparent critical exponents of a *weak first order transition*: $\alpha/\nu = 1, \gamma/\nu = 1$ (see Ref. [12]), which are precursors of a first order transition.

To analyze the divergence of C_V a bilogarithmic plot is not adequate due to the presence of a non-negligible constant term. In order to compare with the first order behavior it is better to plot C_V and χ_c as a function of several powers of L. This is done in

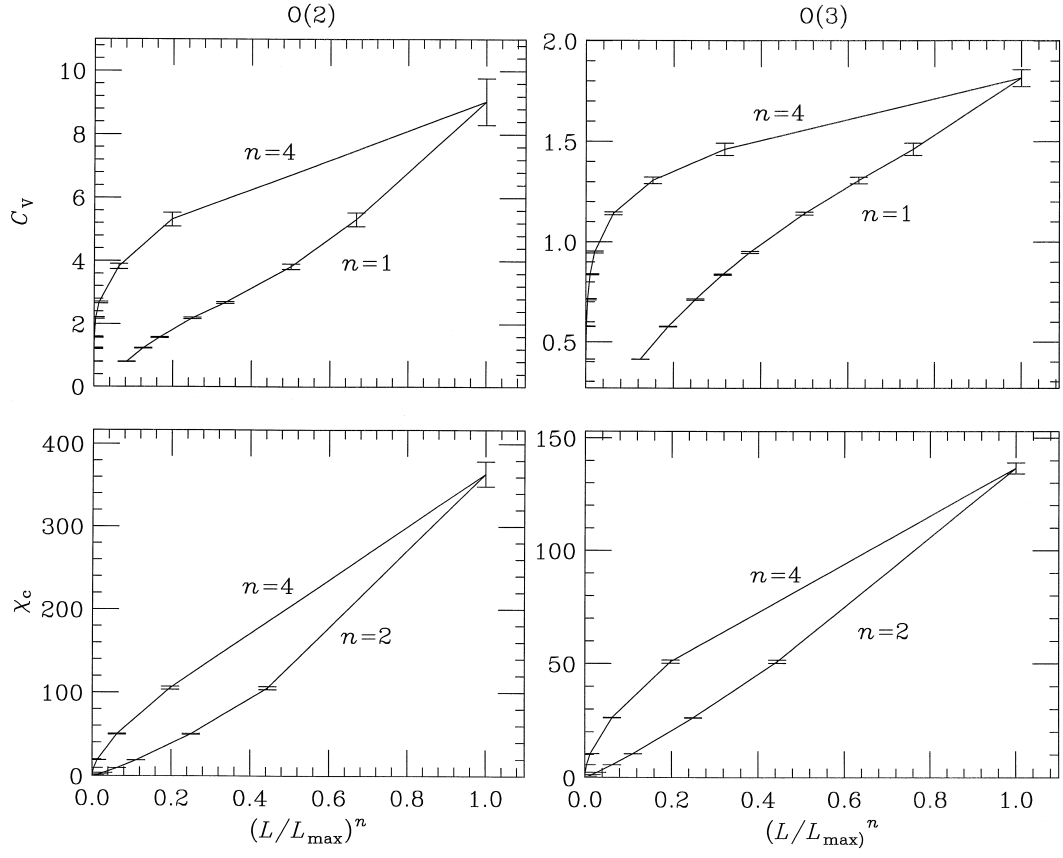

Fig. 1. Specific heat and connected susceptibility for O(2) and O(3) as a function of several powers of the lattice sizes.

Fig. 1. We remark that in the O(2) case for L in the interval [8,24] ([12,32] for O(3)) there is an excellent linear fit for $n = 1$ which is the value predicted in a weak first order transition. This frequently produces a misunderstanding of the order of the transition. However, it is clear from Fig. 1 that this is a transient effect: for the larger lattices the divergences are faster than linear, and presumably they would reach the first order behavior for very large lattices.

The susceptibility also shows a fast divergence. Although we are not able to observe the asymptotic first order behavior the trend seems rather clear.

A more accurate measure of the critical exponents can be obtained from Eq. (9). We have always used the ratio $s = 2$. In Fig. 2 we plot several determinations of exponents using different operators. We remark that there is a systematic error in the α/ν determination because of the analytic term in C_V. We observe no asymptotic behavior in all cases although the values in the larger lattices are hardly compatible with a second order transition.

In the upper right part of Fig. 2 we plot the exponents related with each of the eigenvalues of the matrix (10). While the maximum eigenvalues should behave as $L^{-2\beta/\nu}$ (with $\beta/\nu = 0$ for a first order transition), the others should go to zero as L^{-d}. The latter can be used as a control of when the asymptotic regime is reached. We observe that we are far from this regime but the first order limit seems rather clear.

A comparison between the curves for O(2) and O(3) shows a roughly similar shape, differing in a horizontal shift that corresponds to multiplying the lattice size by a factor near 2. This fact can be understood as a correlation length at the critical point which is twice larger for O(3) than for O(2).

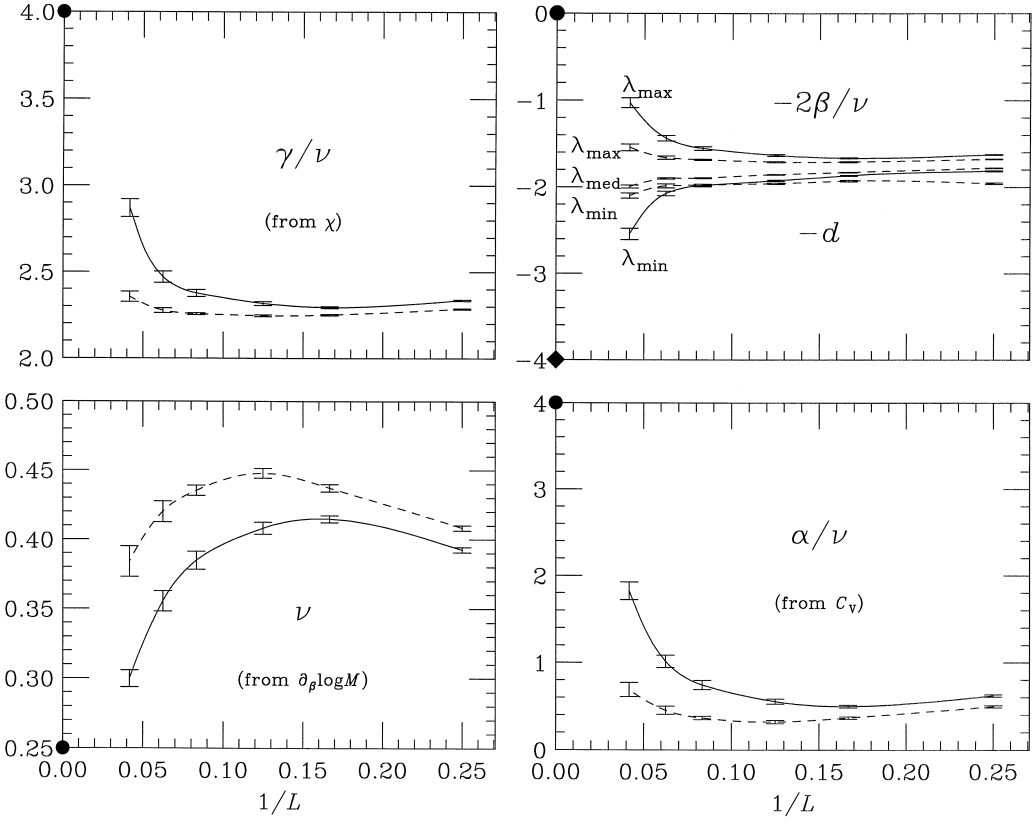

Fig. 2. Critical exponents for O(2) (solid lines) and O(3) (dashed ones) measured through the relation (9). The filled circles (diamond for the non-maximum eigenvalues) mark the first order limit.

7. Critical point and energy histograms

To calculate an estimation for the critical coupling we study the β_L values where $V_M(2L,\beta_L) = V_M(L,\beta_L)$. In both models, these β_L for the largest lattices are compatible within the error bars. We can fit to the functional form $\beta_c^L - \beta_c(\infty) \propto L^{-x}$ in order to estimate the error bars. We perform these fits with the full covariance matrix. In both cases we obtain fitting for $L \geq 6$ a wide valid range for x and very good χ^2 ($\chi^2/\text{d.o.f.} = 1.9/2$ for O(2) and $\chi^2/\text{d.o.f.} = 0.8/2$ for O(3)). The results are compatible with the values for the largest lattices. We get

$$\beta_c(\infty)^{O(2)} = -0.351216(10) \tag{11}$$

$$\beta_c(\infty)^{O(3)} = -0.52857(2). \tag{12}$$

Finally let us comment on the energy distribution of the configurations. A direct check of the first order character of a transition is the observation of a latent heat. Unfortunately, a sharp double peak structure can be observed only when the lattice size is much larger than the correlation length at the critical point. In Fig. 3 we show the energy histograms for both models at β_c. In the O(2) case we note that the width of the energy distribution is nearly constant for the larger lattices, being an indication of the existence of a two peak distribution that cannot be resolved. In the O(3) case, up to $L = 48$ there is not a similar behavior.

8. The N → ∞ limit

The partition function of the model can be written as

$$Z = Z_0 \int \prod_j d^N \boldsymbol{\Phi}_j \, \delta\left(\boldsymbol{\Phi}_j^2 - 1\right) e^{-N\beta' H}$$

$$= Z_0 \int \prod_j d^N \boldsymbol{\Phi}_j \frac{N\, d\alpha_j}{2\pi} e^{N\{\sum_j (i\alpha_j + \lambda_j)(1 - \boldsymbol{\Phi}_j^2) - \beta' H\}}, \tag{13}$$

where $\beta' = \beta/N$, and Z_0 is a normalization factor such that $Z \to 1$ when $\beta \to 0$. We have introduced

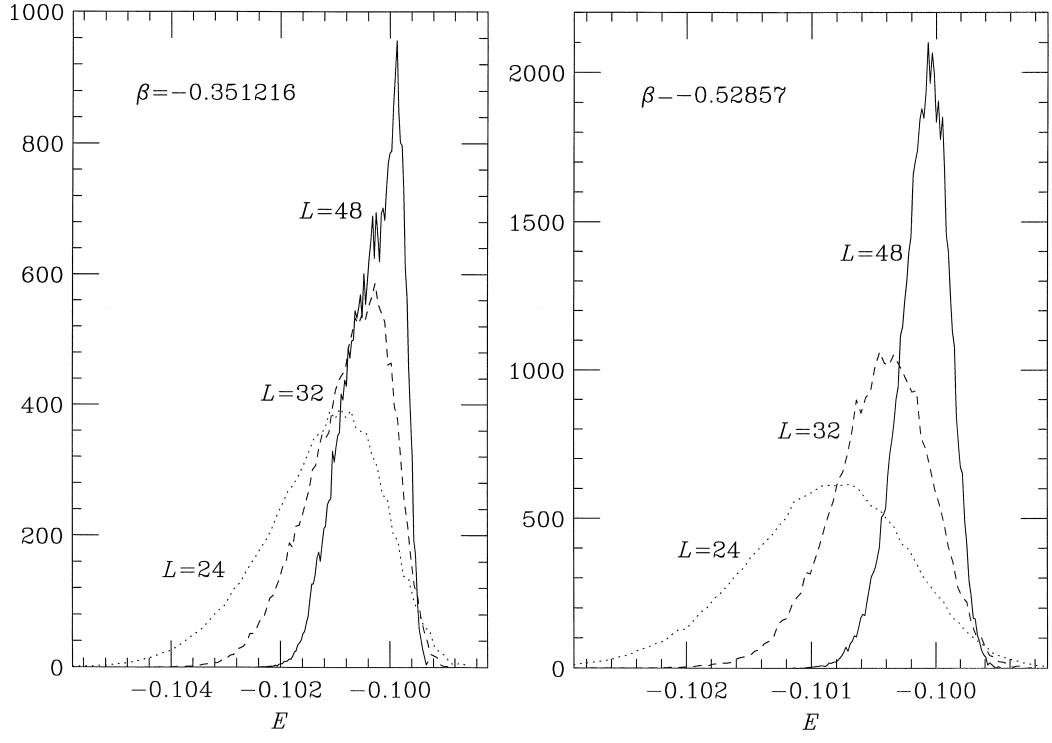

Fig. 3. Normalized energy histogram at $\beta_c(\infty)$ for both models.

the conjugate parameters α_j, λ_j to give an integral representation of the constraint $\boldsymbol{\Phi}_j^2 = 1$ [13].

Writing the quadratic form in the exponent of Eq. (13) as

$$\frac{-1}{2} \sum_{n,m} \phi_n Q_{nm} \phi_m, \tag{14}$$

the integration over $\boldsymbol{\Phi}$ yields

$$Z = Z_0 \left(\frac{2\pi}{N} \right)^{1/2(N-2)V} \times \int \prod_j d\alpha_j \, \mathrm{e}^{N/2\{\sum_j 2(\lambda_j + \mathrm{i}\alpha_j) - \mathrm{Tr}\ln Q\}}. \tag{15}$$

In the limit $N \to \infty$, a variational equation with respect to $2(\lambda_k + i\alpha_k)$ gives

$$1 = \left(Q^{-1}\right)_{ii}. \tag{16}$$

In order to study the disorder-AF transition in the F_4 lattice ($\beta < 0$), we perform a change of variables which transforms the plane-AF vacuum (suppose $x - y$) into a ferromagnetic one defining

$$\boldsymbol{\Phi}'_{xyzt} = (-1)^{x+y} \boldsymbol{\Phi}_{xyzt}. \tag{17}$$

Q matrix changes and then the propagator, Q^{-1}, reads

$$G(p) = \frac{1}{(-\beta')} \frac{1}{\xi^{-2} + 4(2 + g(p))}, \tag{18}$$

where

$$g(p) = \cos p_x \cos p_y + \cos p_z \cos p_t - \cos p_x \cos p_z - \cos p_x \cos p_t - \cos p_y \cos p_z - \cos p_y \cos p_t, \tag{19}$$

and ξ is defined from (translationally invariant) auxiliary fields as

$$2(\lambda_i + \mathrm{i}\alpha_i) \equiv (-\beta')(\xi^{-2} + 8). \tag{20}$$

From the variational Eq. (16) we obtain β'_c imposing $\xi = \infty$:

$$\beta'_c = \int \frac{d^4p}{(2\pi)^4} \frac{1}{-8 - 4g(p)} = -0.178972. \tag{21}$$

In Table 3 we compare (21) with MC results for $N = 1,2,3,4$. The good agreement between the simulations for these values of N and the analytical limit when $N \to \infty$ points to the absence of an abrupt change of the critical properties as a function of N. Exactly at $N = \infty$ the order of the transition is not clear, because the divergence in the correlation length can simply be caused by the Goldstone bosons of the symmetry breaking.

Table 3
Critical couplings divided by N for different O(N) models. We include also the obtained in Refs. [2] and [3].

N	β_c
1	−0.17459(15)
2	−0.175608(5)
3	−0.17619(1)
4	−0.1766(1)

9. Conclusions

In this letter we present a MC study of the four dimensional antiferromagnetic O(2) and O(3) models in the F_4 lattice. We study the critical behavior of these models with FSS techniques. There is an apparent asymptotic behavior which gives false critical exponents for not large enough lattice sizes. This transitory effect can be understood as caused by a large correlation length whose presence can be demonstrated for some observables (as the eigenvalues of the sum tensor of the period-two magnetizations). This must be very carefully controlled, because as we see in our case, the behavior changes drastically when larger lattice sizes are considered, revealing the true first order nature of the O(2), O(3) transitions. We also see that this effect is bigger as N grows, so that for larger values of N, it is very difficult to study numerically the critical properties of the system. However, the great accuracy in the determination of the critical point obtained by the analytical calculation at $N = \infty$ points to a similar qualitative behavior for all values of N.

10. Acknowledgments

We thank to the CICyT (contracts AEN94-0218, AEN96-1634) for partial financial support. We have

employed for the simulations dedicated Pentium Pro machines (RTNN project). J.M. Carmona is a Spanish MEC fellow.

References

[1] G. Gallavotti, V. Rivasseau, Phys. Lett. B 122 (1983) 268.
[2] J.L. Alonso, J.M. Carmona, J. Clemente Gallardo, L.A. Fernández, D. Iñiguez, A. Tarancón, C.L. Ullod, Phys. Lett. B 376 (1996) 148.
[3] I. Campos, L.A. Fernández, A. Tarancón. Phys. Rev. D55 (1997) 2965.
[4] H.G. Ballesteros, J.M. Carmona, L.A. Fernández, V. Martín-Mayor, A. Muñoz Sudupe, A. Tarancón. Phys. Rev. D55 (1997) 5067.
[5] V. Branchina, H. Mohrbach, J. Polonyi, hep-th/9612110; hep-th/9612111.
[6] D.J.E. Callaway, Phys. Rep. 167 no. 5, (1988) 241; R. Fernández, J. Frölich, A.D. Sokal, Random Walks, Critical Phenomena and Triviality in Quantum Field Theory. Springer-Verlag, 1992.
[7] H.G. Ballesteros, L.A. Fernández, V. Martín-Mayor, A. Muñoz Sudupe). Phys. Lett. B378 (1996) 207; Nucl. Phys. B483 (1997) 707.
[8] J.L. Alonso, A. Tarancón, H.G. Ballesteros, L.A. Fernández, V. Martín-Mayor, A. Muñoz Sudupe. Phys. Rev. B53 (1996) 2537.
[9] J.L. Cardy Ed., Finite-Size Scaling. North-Holland, 1988.
[10] M.E. Fisher, A. Nihat Berker. Phys. Rev. B26 (1982) 2507.
[11] A.M. Ferrenberg, R.H. Swendsen, Phys. Rev. Lett. 61 (1988) 2635.
[12] L.A. Fernández, M.P. Lombardo, J.J. Ruiz-Lorenzo, A. Tarancón, Phys. Lett. B 277 (1992) 485.
[13] C. Itzykson and J-M. Drouffe, Théorie statistique des champs. InterEditions, 1989 (Paris), page 138.