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Stiefel models of frustrated antiferromagnets

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Abstract. Lattice nonlinear σ models, where the Stiefel manifold $O(n)/O(n-p)$ is attached to each lattice site are introduced to analyse phase transitions in frustrated antiferromagnets, with non-collinear spin orderings. A Monte Carlo study of these models in three dimensions indicates either first-order transitions or second-order ones corresponding to new universality classes. There is evidence for a defect mediated transition in some two-dimensional models. None of the results can be reproduced by *RG* techniques ($2+\varepsilon$ and 4-ε expansions).

1. Introduction

In a phase transition, the nature of the order parameter space, seems to be the crucial feature determining the universal properties of the systems considered, in the critical region. It appears, therefore, natural to describe these properties by considering the simplest model, which retains these symmetries. A general rule for constructing such models is the following. If at high temperature, the symmetry group of the system is G, and at low temperature it is H, then the order parameter space is a manifold G/H. One can then define a lattice model, where to each lattice site is attached an element of this manifold. An interaction between neighbouring sites is then introduced, which favours the tendency of these sites to be in the same state. We have studied a specific class of such models, where the high temperature group is $O(n)$ and the low temperature group is $O(n-p)$. The order parameter space in this case is what is called in mathematics the Stiefel manifold $V_{n,p}=O(n)/O(n-p)$. It can be simply described as a set of p orthogonal unit vectors $\boldsymbol{\sigma}_\alpha$ ($\alpha=1\dots p$) in a n dimensional space. The corresponding Hamiltonian is then defined by

$$H=-\sum_{\langle x,y\rangle}\sum_{\alpha=1}^{p}\boldsymbol{\sigma}_\alpha(x)\cdot\boldsymbol{\sigma}_\alpha(y) \tag{1}$$

where the points x, and y are nearest neighbours on a cubic lattice, and the constraint $\boldsymbol{\sigma}_\alpha(x)\boldsymbol{\sigma}_\beta(x)=\delta_{\alpha\beta}$ is satisfied at each site. When $p=1$, we recover the familiar n component Heisenberg model. When $p=2$ and $n=3$ the manifold is $SO(3)$ and the model should be in the same universality class as certain helical magnets and triangular antiferromagnets, characterized by *non-collinear* spin orderings, like VCl_2 and Ho, Dy for example [1]. We call models described by H, Stiefel models. We have undertaken

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a Monte Carlo study of these models in three dimensions and found that they have either a first-order transition or a continuous phase transition, belonging to new universality class, which in the case $(p=2, n=3)$ appears to be the same as the one found by Kawamura [2] for certain Heisenberg antiferromagnets. We have also studied these models by means of renormalization group techniques ($2+\varepsilon$ and $4-\varepsilon$ dimensions expansions). None of the results of the numerical investigation could be reproduced by *RG* techniques.

An important feature of some of these models is that they possess topologically stable defects: magnetic disclination lines. We find indeed that in three dimensions, the phase transition is associated to a condensation of defects. We have also seen that these defects play an important role in two dimensions, and found good evidence for a defect mediated phase transition, which shows some similarity with the familiar BKT transition, in the $X-Y$ model. A similar transition was detected in a numerical study of the classical Heisenberg antiferromagnet on the triangular lattice [3].

On the analytical side, the following results have been found. In the mean field approximation, where the order parameters $\langle\boldsymbol{\sigma}_\alpha\rangle$ are introduced, the model shows a continuous phase transition, with the classical values of the critical exponents when $p<n$. In order to describe the fluctuations, a Ginsburg–Landau type of Hamiltonian is introduced with an interaction given by the potential

$$V(\varphi)=\lambda_1\sum_{\alpha\beta}(\varphi_\alpha\cdot\varphi_\beta)^2+\lambda_2\sum_{\alpha\beta}\varphi_\alpha^2\varphi_\beta^2+\lambda_3\sum_\alpha[\varphi_\alpha^2]^2 \tag{2}$$

with $\lambda_1\neq 0$ and $\lambda_2\neq 0$, the $\varphi_\alpha(x)$ being p vectors in R^n. There is one stable fixed point $\lambda_1^*\neq 0\lambda_2^*\neq 0\lambda_3^*=0$, if $n\geqslant n_c(p)$, when $p\geqslant 2$ [4, 5]. When $p=2$ for example $n_c=21.8$. A traditional interpretation of these results is that for $n\leqslant n_c$, the transition may be first order. The second tool at our disposal is an expansion in $2+\varepsilon$ dimensions, describing spin wave interactions in the model. Here, however, the situation is much more complicated than in the usual Heisenberg model, where only the temperature is changed in a length rescaling. In the case $p=2$, four coupling constants are needed. This means that if we start with the Hamiltonian, in the continuum limit

$$H=\frac{1}{2}\int\sum_{\mu=1}^{d}\sum_{\alpha=1}^{p}(\partial_\mu\boldsymbol{\sigma}_\alpha)^2(x)\,d^dx \tag{3}$$

the renormalization will lead us to a more general Hamiltonian

$$H=\frac{1}{2}\int\sum_{\mu}\sum_{\alpha\beta}^{p}\{B_{\alpha\beta}(\partial_\mu\boldsymbol{\sigma}_\beta)(\partial_\mu\boldsymbol{\sigma}_\alpha)+c[(\partial_\mu\boldsymbol{\sigma}_1)\cdot(\boldsymbol{\sigma}_2)]^2\}\,d^dx$$

where

$$B_{\alpha\beta}=B_{\beta\alpha}. \tag{4}$$

The bracketed expression has a geometric interpretation; it is the most general $O(n)$ invariant metric on the manifold. The renormalization group gives a flow in the parameter space $\{B, c\}$ in terms of the curvature tensor associated to this metric [6]. In our case, to first order in ε, the equation read

$$\dot{B}=\varepsilon B+\frac{1}{2\pi}\left\{\left(3-n-\frac{c}{f}\right)1+\frac{B}{2f\det B}(c^2+2c\operatorname{tr}B)\right\}$$
$$\dot{f}=\varepsilon f-\frac{n-2}{2\pi}\left[2+\frac{1}{2\det B}(c^2+2c\operatorname{tr}B)\right] \tag{5}$$

where

$$f = c + \mathrm{tr}\, B. \tag{6}$$

These equations have a fixed point $B^* = b1$ and f^*, from which one deduces the exponent ν for the correlation length: $\nu = 1/\varepsilon$, the same as for the Heisenberg model. The exponent η has also been computed. One finds

$$\eta = \frac{\varepsilon}{2(n-2)} \left[2 + \left(\frac{n-1}{n-2} \right)^2 \right]. \tag{7}$$

When $n = 3$, one finds that these exponents are those of a 4-component Heisenberg model (η being the abnormal dimension of an operator of angular momentum $l = 1$, in the Heisenberg case). These results are confirmed to second order in ε. An $O(4)$ symmetry has been dynamically generated. In this case, we recover the results of Azaria, Delamotte and Jolicoeur [7], which were the first to analyse nonlinear σ models of this type. There is a simple geometric way to understand these results, which points to their limitations. The manifold $SO(3)$ is isomorphic to the manifold RP^3, the sphere S^3 with opposite points identified. The $2+\varepsilon$ expansions probes only the local structure of these manifolds described by their curvature and cannot distinguish the Stiefel model $V_{3,2}$ from the Heisenberg model S^3, and this is why all these models have the same critical exponents in this $2+\varepsilon$ expansion. Globally however these manifolds are quite different and physically this difference is revealed by the existence of defects in the Stiefel model, absent in the 4-component Heisenberg model.

In fact the isomorphism between $SO(3)$ and RP^3 can be used to construct a new representation of the Stiefel model $V_{3,2}$. To each rotation $g_x \in SO(3)$, characterized by an angle θ_x and a unit vector $\boldsymbol{n}_x$, we can associate a unit vector $\boldsymbol{R}_x$ in R^4, given by

$$\boldsymbol{R}_x = \left(\sin \frac{\theta_x}{2} \boldsymbol{n}_x, \cos \frac{\theta_x}{2} \right). \tag{8}$$

In this representation, the Hamiltonian of the Stiefel model $V_{3,2}$ becomes

$$H = -2 \sum_{\langle x,y \rangle} \{ (\boldsymbol{R}_x \cdot \boldsymbol{R}_y)^2 + (\boldsymbol{R}_x, J\boldsymbol{R}_y)^2 \} \tag{9}$$

where J is a 4×4 matrix given by $J = 1 \otimes \sigma_y$. In this representation, the chiral $SO(3)$ model described by the Hamiltonian

$$H = -\sum_{\langle x,y \rangle} \mathrm{tr}\, g_x^{-1} g_y \tag{10}$$

can be seen to be equivalent to the RP^3 model [13] since its Hamiltonian becomes

$$H = -4 \sum_{\langle x,y \rangle} (\boldsymbol{R}_x \cdot \boldsymbol{R}_y)^2 + Nd. \tag{11}$$

Although the $2+\varepsilon$ expansion predicts the same critical behaviour for these two models, as well as the chiral $O(3)$ model, we find numerically a continuous transition for the Stiefel model $V_{3,2}$ but a first order transition for the two others.

2. The Monte Carlo simulations

The algorithm

We are using two recently available methods for the Monte Carlo simulations. First, a multi-histogram method due to Ferrenberg and Swendsen [8] is employed in order to compute the various observables in function of the temperature. Then, we use a cluster update due to Wolff [9] for the Heisenberg model, biased according to [10] in order to avoid the formation of too large clusters in the low temperature phase. In this paper, we will only discuss problems specific to the Stiefel model. Let us consider a general translation invariant Hamiltonian given as a sum over the links of the lattice

$$-\beta H = -\sum_{\langle x,y\rangle} h(\varphi(x), \varphi(y)) \tag{12}$$

in which the 'energy' function is symmetric $h(\varphi, \psi) = h(\psi, \varphi)$. For the Stiefel model, the energy is $h(\varphi, \psi) = \beta \operatorname{Tr} \varphi^{+}\psi$. In order to build a cluster algorithm, we define the linear operator R on φ given by $R = 1_n - 2P$ and P is a projector chosen at random. The operator R is in $O(n)$ and corresponds to a reflection through the hyperplane perpendicular to the P subspace. Then, the probability to activate a link $\langle x, y\rangle$ is given by

$$p(\langle x, y\rangle) = 1 - \exp\{\min[0, h(R\varphi(x), \varphi(y)) - h(\varphi(x), \varphi(y)]\}. \tag{13}$$

The only degree of freedom left in the algorithm is the dimension, $\dim(P)$, of the P subspace. For the Heisenberg model, as done by Wolff [9], it seems natural to take $\dim(P) = 1$. For the Stiefel model $V_{n,2}$, we tried $\dim(P) = 1$ and $\dim(P) = 2$. We found that, the algorithm with $\dim(P) = 1$ gave a much lower autocorrelation time. Nevertheless, even in the better case $\dim(P) = 1$, the autocorrelation time grows badly around the critical temperature, and it seems that this algorithm does not get rid of the critical slowing down. As discussed in [11, 12], this seems related to the non-ferromagnetic interaction of the underlying Ising model.

All simulations were done on a cubic lattice of side L, with periodic boundary conditions. The program was written for a first exploration of these models, but was not optimized for a high precision study. The errors on the curves presented here (estimated either by computing the number of independant measurements for a given temperature or by adding new simulations in the set of histograms) are of a few percent or better. An estimation of the errors on the critical exponents is much more tricky. A subjective estimate based on the finite size scaling would give typically 5% on v or γ.

Definition of the observables

Quantities of interest are the energy per link $h = \langle H\rangle / dL^d$, the specific heat $C_v = \partial\langle H\rangle/\partial T$, and the susceptibility $\chi = \langle \Sigma_{\alpha x}\, \boldsymbol{\sigma}_\alpha(0) \cdot \boldsymbol{\sigma}_\alpha(x)\rangle$. The correlation length ξ is defined as follows. We compute the Fourier transform $G(k)$ of the two point correlation function

$$G(k) = \sum_{\alpha x} e^{ikx} \langle \boldsymbol{\sigma}_\alpha(0) \cdot \boldsymbol{\sigma}_\alpha(x)\rangle \tag{14}$$

for $k^2 = (2\pi/L)^2$. For small k, we expect $G(k)^{-1} = \chi^{-1}(1 + k^2\xi^2)$ and take this as a definition of ξ.

A problem specific to the $V_{3,2} \approx SO(3) \approx RP^3$ models is the definition of defects on a lattice. We already solved this problem in the general RP^{n-1} case [13]. For the $SO(3)$ case, we simply use the mapping given by equation (8), to reduce the problem to the RP^3 case.

Let us consider the loop ∂P around an elementary plaquette of the lattice. We define the density of defects by

$$D=\tfrac{1}{2}\left\{1-\left\langle \text{sign} \prod_{\langle x,y\rangle \partial P} (\boldsymbol{R}_x\cdot\boldsymbol{R}_y)\right\rangle\right\}. \tag{15}$$

In the same way, we can introduce a topological order parameter μ by

$$\mu=\left\langle \text{sign} \prod_{\langle x,y\rangle\in\mathscr{L}} (\boldsymbol{R}_x\cdot\boldsymbol{R}_y)\right\rangle \tag{16}$$

where $\mathscr{L}$ is a loop of length L across the sample.

Other topological defects come from the fact that the manifold $V_{n,n}\approx O(n)$ is composed of two sheets. This is expressed by $\Pi_0(V_{n,n})=Z_2$. The associated Z_2 symmetry breaking is measured by the quantuty

$$\pi_0^2=\left\langle\left(\frac{1}{L^d}\sum_x \det(\sigma(x)\right)^2\right\rangle. \tag{17}$$

In order to fit the critical exponents around the transition, we use the finite scaling hypothesis (FSS), in the form

$$\begin{aligned}&\xi(T,L)/L=f(L/\xi_\infty)\\&\chi(T,L)/L^{\gamma/\nu}=f'(L/\xi_\infty)\end{aligned} \tag{18}$$

where ξ_∞ denotes the infinite volume correlation length. We proceed in a similar way for the other observables, with the corresponding critical exponents. In the parameters fitting, we also impose that when the correlation length is sufficiently small compared to the size of the system, the observables must tend to the infinite volume limit, that is

$$\begin{aligned}&\xi(T,L)\to\xi_\infty \qquad \text{for } \xi/L<\tfrac{1}{4}\\&\chi(T,L)\to\chi_\infty \qquad \text{for } \xi_\infty/L<\tfrac{1}{4}.\end{aligned} \tag{19}$$

For the three-dimensional systems, the critical temperature and the exponents ν are computed on the specific heat by imposing the scaling relation $\alpha=2-d\nu$. Then, the other critical exponents are computed, with fixed T_c and ν.

Three-dimensional systems

The series of Stiefel model $V_{n,2}$ offers a good opportunity to test the renormalization group results. We studied numerically in three dimensions, the five models $V_{2,2}\approx O(2)$, $V_{3,2}\approx SO(3)$, $V_{3,3}$, $V_{4,2}$ and $V_{5,2}$. These values of n and p are precisely in the domain where the $4-\varepsilon$ expansion failed. According to the standard line of arguments, these models are expected to have a first-order phase transition. Another reason is bound to the defects of the models classified by the following homotopy groups

$$\begin{array}{lll}\Pi_1(V_{3,2})=Z_2 & \Pi_1(V_{4,2})=0 & \Pi_1(V_{5,2})=0\\ \Pi_2(V_{3,2})=0 & \Pi_2(V_{4,2})=Z & \Pi_2(V_{5,2})=0\\ \Pi_3(V_{3,2})=Z & \Pi_3(V_{4,2})=Z\times Z & \Pi_3(V_{5,2})=Z_2.\end{array} \tag{20}$$

This means that in three dimensions, the model $V_{3,2}$ possesses line defects and configuration defects (instantons), $V_{4,2}$ point defects, and $V_{5,2}$ configuration defects (instantons). Because of the general relation $\Pi_j(V_{n,p})=0$ for $j<n-p$, the first three homotopy groups for the manifold $V_{n,2}$ are trivial for $n\geqslant 6$.

The simulations for the $V_{4,2}$ and $V_{5,2}$ models show a clear second-order phase transition with exponents given in table 1. The scaling is fulfilled up to a very good accuracy. Obviously, for these two models, a first-order transition is to be excluded.

We made extensive numerical simulations for the $SO(3)$ model, and obtained clear evidence for a continuous phase transition. The specific heat is shown in figure 1. The critical exponents are very close to those of a tricritical point. Even using finite size scaling, it is difficult to exclude the mean field values, $\nu=\frac{1}{2}$ and $\gamma=1$, with some logarithmic corrections [7]. These exponents clearly differ from those of the four component Heisenberg model, predicted by the $2+\varepsilon$ expansion; ($\beta=0.25$ compared to $\beta=0.39$, for example). In figure 2, the density of defects D and the topological order parameter μ are drawn. We see clearly the usual signatures of a phase transition, with the increase in the number of defects through the critical region, and with μ which is a topological order parameter, even for a three-dimensional system. The discomforting feature for this model is its poor FSS accuracy. In particular, the susceptibility can only be accommodated with a negative η exponent, if we assume valid the scaling relation $\gamma=\nu(2-\eta)$. This is a nonsense, which may indicate some strong finite size corrections.

Table 1. Critical exponents for $d=3$

Model	T_c	ν	α	γ	η	$\beta^2_{\pi_0}$
$SO(3)=V_{3,2}$	1.532	0.515 (10)	0.46 (3)	1.1 (1)	−0.10 (5)	
$V_{4,2}$	1.12	0.57	0.29	1.1	0.05	
$V_{5,2}$	0.88	0.59	0.23	1.1	0.14	
Kawamura $n=2$	1.45	0.53 (3)	0.40 (10)	1.10 (10)	−0.1	0.8 (1)
Kawamura $n=3$	0.95	0.55 (3)	0.34 (10)	1.10 (10)	0.0	
$O(2)=V_{2,2}$	2.445	0.41	0.77	0.95 (5)	−0.3	0.35
$O(3)=V_{3,3}$	1.6825	0.37	0.9	0.9	−0.4	

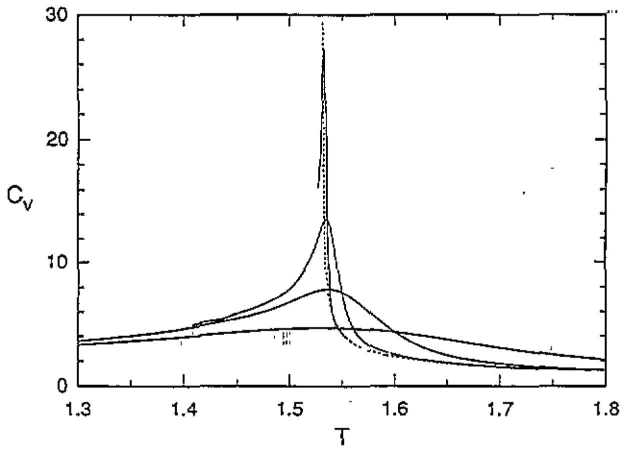

Figure 1. The specific heat C_ν for the $SO(3)$ model at three dimensions $d=3$, size $L=4, 8, 16, 32$. The dashed curve is the usual power law singularity with $T_c=1.5315$, $\nu=0.515$ and $\alpha=2-d\nu$.

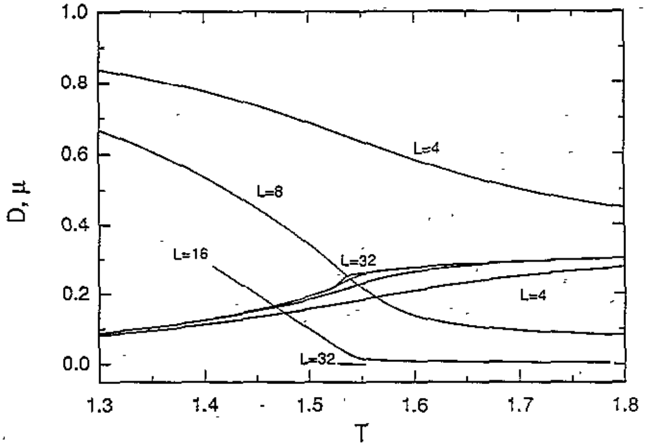

Figure 2. The density of defects D and the topological order parameter μ for the $SO(3)$ model at three dimensions.

The $V_{2,2} \approx O(2)$ and $V_{3,3} \approx O(3)$ models appear to be very different. The numerical simulations are much more difficult because there are more vectors, because the bias, as proposed in [10], does not help to reduce the autocorrelation time in the low temperature phase, and because the autocorrelation time grows very badly at transition. For the $O(2)$ model, the specific heat shows a very strong singularity and the FSS, as explained above, gives $\nu = 0.4$, a value close to $\frac{1}{3}$ which should signal a first-order transition; but it is not possible to fit correctly the data with an exponent $\nu = \frac{1}{3}$. The FSS applied to the susceptibility gives $\gamma \approx 1$, and using the above scaling relation, we obtain the strongly negative value $\eta = -0.3$. However, the probability distribution of energy at the transition has a double bump shape, advocating a first-order transition. For the $O(3)$ model, the first-order character of the transition is even more pronounced. Proceeding with the FSS as for the $O(2)$ model, we obtain $\nu = 0.37$ and $\eta = -0.4$. In both cases, the transition occurs with the Z_2 symmetry breaking. It seems that, generically, the $O(n)$ models in three dimensions will have first-order transition. This indicates that the absence of fixed point in the $4-\varepsilon$ expansion for some Stiefel model is related to a true singularity for $p = n$.

It is interesting to compare the present study to the Monte Carlo computations of Kawamura [2], who studied the frustrated Heisenberg model on a stacked triangular lattice, and to the computation of Diep [14], who studied a helical magnet. As discussed in the introduction, it can be argued that these systems should belong to the same universality class, with the same critical exponents. At least, for the frustrated $X-Y$ antiferromagnet, corresponding in principle to our $O(2)$ model, the discrepancy for ν and for the specific heat exponent is rather clear. We must notice that, from the Kawamura results, we would also deduce a negative value for η. But if the $O(2)$ model has a first-order transition, we have no reason to expect universal behaviour. For the frustrated Heisenberg antiferromagnet, corresponding to the $SO(3)$ model, the agreement is only marginal.

Because three dimensions can be reached by a $2+\varepsilon$ expansion, it is also interesting to compare the models RP^3, S^3, $SO(3)$ and $O(3)$ for $d=3$. The RP^n model has a first-order phase transition for all $n \geq 2$. In contrast, the S^n model possesses the usual well known second-order phase transition, the $SO(3)$ model has a second-order phase transition, but with different critical exponents than S^3, and the $O(3)$ model has a first-order transition.

Two-dimensional systems

As argued above, an interesting group of models on which we can test the renormalization group in two dimensions is S^3, RP^3, $SO(3)$ and $O(3)$. These manifolds all have the same local structure and differ only by global quantities (except for $SO(3) \approx RP^3$ where the action differs). We made large Monte Carlo simulations for the RP^3 and $SO(3)$ models. For these two models, although fitting curves is a difficult art, a singularity of the form predicted by the RG in two dimensions $\xi_\infty = c\exp(a/T)$, $\chi_\infty = c'\exp(a'/T)$ clearly has to be excluded. We then try the usual power law form $\xi_\infty = c|t|^{-\nu}$, and a Kosterlitz–Thouless form $\xi_\infty = c\exp(a\sqrt{t})$, $\chi_\infty = c'\exp(a'\sqrt{t})$, with $t = (T - T_c)/T_c$. As already known for the X-Y model, it is difficult to decide between these two forms. A power law fits well, but a KT like divergence fits even better. Without any analytic hint, we would favour this second form. As an example, for the $SO(3)$ model the finite size scaling for the susceptibility is reported in figure 3 for a KT like divergence, in scales suited to test the conditions 18 and 19. Without rescaling, on the raw plot χ versus T, the power law and KT fit are barely distinguishable from the measurements. As for the RP^2 model [13], the transition is clearly associated to the defects for both RP^3 and $SO(3)$. The density of defects D grows across the critical domain and μ is a topological order parameter. Nevertheless, the defects susceptibilities are very different for these two models in the low temperature phase. This indicates that they are not identical.

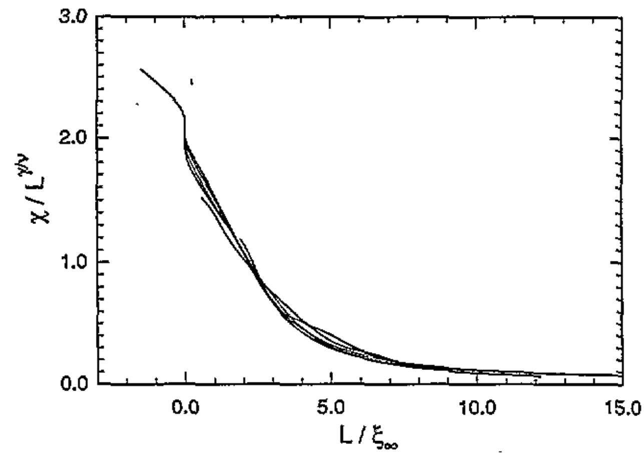

Figure 3. The FSS plot with a KT singularity for the susceptibility χ in the $SO(3)$ model at two dimensions at size $L = 8, 32, 64, 128, 256$. The parameters are $T_c = 0.683$, $a = 1.43$, $\gamma/\nu = 1.7$, $c(\xi) = 0.32$, $c(\chi) = 0.77$.

The $O(3)$ model still has another critical behaviour. As discussed above, the Monte Carlo simulations are much more difficult. Again, a singularity as given by the RG in two dimensions has to be excluded and we would favour a KT like divergence, π_0^2 being a topological order parameter for the transition.

In order to conclude on these two-dimensional numerical simulations of RP^3, $SO(3)$ and $O(3)$ compared to S^3, we clearly obtain four different critical behaviours. The first three systems seem to have a KT like a singularity and only S^3 has a singularity as predicted by the RG in two dimensions [15].

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