PHASE DIAGRAM OF THE Z(3) SPIN MODEL IN THREE DIMENSIONS

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We use a variational method to study the phase structure of the three-dimensional Z(3) spin model with nearest neighbour and next nearest couplings. The system shows a rich phase diagram. The order and location of the corresponding phase transitions in the ferromagnetic region is compared with a Monte Carlo analysis and found in good agreement with the analytical prediction. We have also found that a region where the phase transition is second order does exist.

In this letter we present a comparison between a variational and a Monte Carlo study of the Z(3) spin model [1,2] in three dimensions. This system has interesting applications in condensed matter physics, and recently its properties have been the subject of renewed interest [3]. It is conjecured, in fact, that this model belongs to the same universality class as the SU(3) lattice gauge theory (LGT) at finite temperature [4,5]. One argues that the order–disorder transition in the Z(3) model is of the same type as the deconfining transition in the SU(3) LGT and thus the approach to the respective transition points should be characterized by the same critical indices [6].

In spite of the apparent simplicity of the model, the study of its phase diagram is a very complex problem and the order of the transition has not yet been firmly established in three dimensions.

When to the standard nearest neighbour coupling a next nearest neighbour coupling is added [7–9], the phase diagram of the system becomes more complex. In the present paper we use both analytical and numerical approaches in order to investigate the phase diagram of the Z(3) Potts model. The interest in studying the whole space defined by the two coupling constants is twofold. First, we are interested in the existence of antiferromagnetic phases. Second, we want to see the possible changes of the order of the transition as the couplings are changed. This possibility is especially important, since it has been conjectured that the correspondence between the deconfining transition in SU(3) and the Z(3) order–disorder transition can require a coupling in the latter of the next nearest neighbour type [10].

We define our model in a three-dimensional cubic lattice. In every site, i, we considered a Z(3) variable $\boldsymbol{s}_i$, that we write as a two-dimensional vector, which can take up three equivalent orientations in a plane:

$$\boldsymbol{s} \equiv (1,0),\ (-\tfrac{1}{2}, \tfrac{1}{2}\sqrt{3}),\ (-\tfrac{1}{2}, -\tfrac{1}{2}\sqrt{3}). \tag{1}$$

The partition function can be written as

$$\mathcal{Z} = \sum_{\{\boldsymbol{s}\}} \mathrm{e}^{-H} \tag{2}$$

with

$$H = \sum_{\substack{|i-j|=1 \\ i<j}} J_1 \boldsymbol{s}_i \boldsymbol{s}_j + \sum_{\substack{|i-j|=\sqrt{2} \\ i<j}} J_2 \boldsymbol{s}_i \boldsymbol{s}_j. \tag{3}$$

In order to describe the phase behaviour of the system, an appropriate order parameter is the magnetization $s = \langle s_x \rangle$, i.e. the projection of the spin along a fixed direction in the plane, say the x direction. Since the exact calculation of the free energy is an extremely difficult task, we have applied to the Potts model a classical method of statistical mechanics, originally devised to deal with the study of the Ising model [11,12]. This method, due to Kirkwood, pro-

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vides a systematic way to go beyond the so-called mean field approximation (MFA). We shall not report the details of the generalization of Kirkwood's method to the present case, which will be given in a forthcoming paper and limit ourselves to write down the final expression of the free energy as a function of the order parameter s:

$$F/V = F_0(s, m=0)/V - s^2 X_1 + (-\tfrac{1}{2} + \tfrac{1}{2}s^2 + s^3 - s^4) X_2 + (-\tfrac{1}{6} + \tfrac{1}{2}s^2 - \tfrac{5}{3}s^3 + 4s^5 - \tfrac{8}{3}s^6) X_3 + \dots , \quad (4)$$

where

$$F_0 = \tfrac{1}{3}(1+2s)\log[\tfrac{1}{3}(1+2s)] + \tfrac{2}{3}(1-s)\log[\tfrac{1}{3}(1-s)] \quad (5)$$

and

$$X_n = (\tfrac{1}{2}J_1)^n z + (\tfrac{1}{2}J_2)^n z_A . \quad (6)$$

Expression (4) has been obtained by considering the cumulant expansion of the free energy up to the third order in the coupling constants. Note that the first line of (4) constitutes the result corresponding to the MFA, whereas the following terms represent higher order corrections. In the case of the Ising model with a single ferromagnetic coupling the expression for the free energy up to the second order in J is identical to the expression one obtains by means of the Onsager cavity field method.

The magnetization of the system is the s value which minimizes F. For any value of the parameters we compute numerically the s-value where F has the absolute minimum, which we call $s_{\min}$. We have found three different regions as shown in fig. 1. Within the MFA there are only two regions: broken (ferromagnetic) phase, which corresponds to the upper region in fig. 1 (large J_2) and unbroken phase in the lower region. If only the first correction is considered, then a new broken intermediate phase appears, where the magnetization (that is to say, the value of $s_{\min}$) is negative. When the second correction is also included, then the final diagram consists of three regions: upper region, corresponding to a large positive J_2, with a ferromagnetic behaviour; intermediate region or unbroken phase, and lower region with large negative J_2 or antiferromagnetic region. Let us now clarify these names.

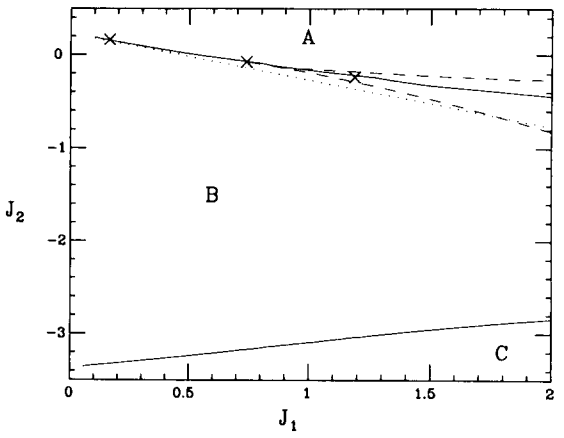

Fig. 1. Phase diagram obtained using eq. (4) in the J_1–J_2 plane. The region A is ferromagnetic, B the unbroken phase and C the antiferromagnetic one. The lines represent the transition points within the MFA (dotted). The results obtained by including the first and second order corrections are represented by dashed and solid lines, respectively. The crosses indicate the Monte Carlo results.

In the unbroken phase $s_{\min}$ is zero everywhere. In the upper "ferromagnetic" region, $s_{\min}$ is positive and goes asymptotically to 1, as the couplings increase. This situation corresponds to a phase where all spins are in the same state, and the order parameter is saturated. In the lower region $s_{\min}$ is negative and its value goes asymptotically to $-\frac{1}{2}$. This solution corresponds to the presence of a minimum, where all the spins are oriented in the negative horizontal direction. This situation is only possible if one half of the total number of spins are in the state with $(-\frac{1}{2}, +\frac{1}{2}\sqrt{3})$, and the remaining one half in the state $(-\frac{1}{2}, -\frac{1}{2}\sqrt{3})$ [see (1)]. Our solution in this case is merely indicative, because in constructing the expression for F we specialized to the case of spatially uniform order. In order to assess the existence of the region characterized by a negative s we performed a Monte Carlo simulation (see below). We found that an ordered region is present and in the stable phase, the spins are alternated in the vertical direction. A more detailed analysis of this region is beyond the scope of this letter, and will be the object of a future study.

A transition line separates different phases, and we focus our interest on the study of the order of the transition along this line. In the unbroken phase the minimum of F is at $s=0$, whereas in the ordered phase $s_{\min}$ has a non-zero value. If $s_{\min}$ jumps discontin-

uously from the disordered phase to the ordered phase, then the transition is first order (note that $s_{\min}$ in the magnetization of the system, which can be obtained as a first derivative of Z with respect to a magnetic field coupled to the spins). Instead, if $s_{\min}$ evolves continuously (but not its derivative) we are in the presence of a second order phase transition. By expanding the free energy in powers of the order parameter s,

$$\frac{F}{N} = \sum_{n=0}^{\infty} B_n s^n, \tag{7}$$

one obtains

$$N^{-1}\partial^2 F/\partial s^2|_{s=0} = 2B_2 + 6B_3 s + \dots . \tag{8}$$

A second order transition is present only when both B_2 and B_3 vanish simultaneously. Within the MFA the above condition can never be fulfilled. Thus the transition is always first order along the transition line. If the first correction is included, a point appears where the transition is second order (at $J_1 = 0.7$, $J_2 = -0.058$).

We remark that within this approach only a finite number of points where this phenomenon can occur is possible. To obtain a whole *region* where the transition is second order an infinite number of corrections would be needed. However, even within this approach in the vicinity of the point where the transition is second order, a region is present where the behaviour is very similar to a critical one. We shall make this point clearer by considering the behaviour of the correlation length, ξ, close to the transition point. The correlation length is a measure of the amplitude of the quadratic fluctuations of the system around $s_{\min}$ and is divergent at a true critical point, as the one we found.

Close to this point ξ is finite, and strictly speaking the transition is first order. However, the evolution of ξ when higher order corrections are considered is a hint for a divergence in the limit of the exact solution of the model. We have plotted this behaviour in fig. 2.

The validity of the previous approximation scheme was tested against the Monte Carlo method. We employed a heath bath algorithm to update 8 parallelized lattices storing the set of 8 spins (one on each lattice) in a single 32 bit word. We use the random number generator of ref. [13]. The study of the data

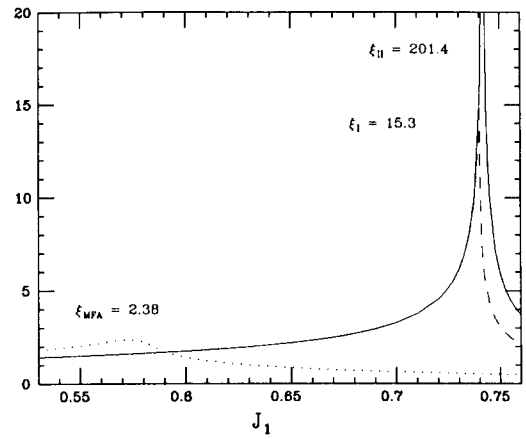

Fig. 2. Correlation length according to the MFA (dotted line), and variational method with first order correction (dashed line) and second order corrections (solid line), as a function of J_1, and $J_2 = -0.1 J_1$. The numbers on the plot indicate the maximum values of ξ respectively for the MFA (ξ_{MFA}), the first (ξ_I) and the second (ξ_{II}) correction.

from the 8 independent lattices allows us to obtain a good control of statistical errors and thermalization time.

We performed simulations with lattices of size $8\times8\times8$ and $16\times16\times16$ and the analysis of the data showed that the results relative to the quantities under investigation were rather insensitive to the above change. This fact is indicative that finite size effects are not very relevant.

For every value of the parameters (and for every of the 8 parallelized lattices) we have run up to 2500 Monte Carlo iterations in the 16^3 lattice and 5000 in the 8^3 one, after discarding 1000 for thermalization, with a more dense distribution of the points close to the phase transition.

We focused our attention on the expectation value of the magnetization and the energy. We explored the (J_1, J_2) plane along lines with $J_2 = \gamma J_1$, keeping γ constant. We selected three different values of γ ($\gamma = 1$, -0.1, -0.2), because these correspond to three qualitatively different behaviours in the analytical approach. For every value of the parameters, we computed the transition point, $\langle E \rangle$ and $\langle |\boldsymbol{M}| \rangle$, where

$$\boldsymbol{M} \equiv \frac{1}{V} \sum_{i=1,V} \boldsymbol{s}_i .$$

Because of the tunnelling effect, $\langle \boldsymbol{M} \rangle$ turns out to be

zero. This problem can be avoided by computing the mean value of the norm of $\boldsymbol{M}$. This quantity is no longer zero in the unbroken phase, but scales as $1/V$. In the broken phase this quantity is (with corrections of order $1/V$) the true value of $|\langle \boldsymbol{M} \rangle|$ in the absence of the tunnelling effect. We determine the position of the transition point as the locus where the specific heat shows a maximum.

In the $\gamma = 1$ region where the MFA result is very close to the results obtained by including the corrections, the agreement is impressive. The first correction improves the zero order result, and the successive correction is hardly noticeable. This gives us confidence of being close to the exact solution and we feel that in this region the transition is truly first order.

In the $\gamma = -0.1$ case the situation is quite different (see fig. 3). The MFA result improves upon adding the first correction. In fact, the Monte Carlo results are very well reproduced by applying the first correction beyond the MFA. The second correction does not improve the analytical result for the energy and the location of the critical point, but the discrepancy is small. On the other hand, it slightly improves the values of the magnetization. Thus, we conclude that the analytical method converges pretty well, since the predictions are not very sensitive to the order at which the cumulant expansion is truncated. We argue that the exact result (the infinite order cumulant expansion) should not be very different from our result for this value of γ. Notice that $\gamma = -0.1$ is above the point where the first correction predicts a second order transition.

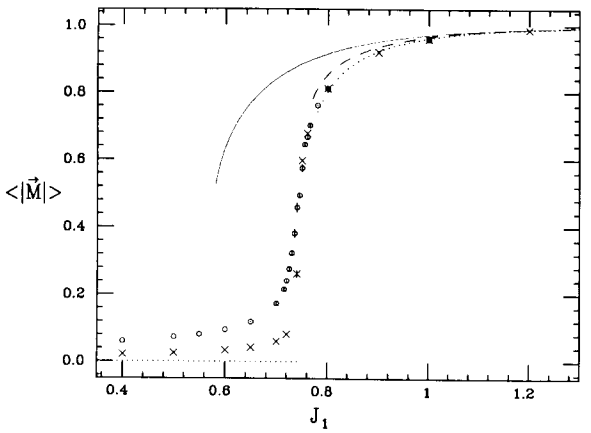

Fig. 3. Monte Carlo and analytical results for the magnetization, $\langle |\boldsymbol{M}| \rangle$, as a function of J_1, and $J_2 = -0.1 J_1$. The circles represent the MC results relative to the 8^3 lattice whereas the crosses those relative to the 16^3 lattice. The thin line stands for the MFA solution, the dashed line for the first correction and the dots for the second correction.

The situation for $\gamma = -0.2$ is different. Evaluating the free energy with the first correction beyond MFA the transition point is predicted with a very high precision (see fig. 1), but this agreement disappears if the next order in the expansion is considered. This phenomenon is understood by recalling that the truncated expansion in the coupling parameter is no longer convergent. This fact is unfortunate since this region is very interesting in view of the correspondence with QCD. It has been conjectured that such a correspondence is obtained by introducing a large antiferromagnetic next nearest neighbour coupling [10].

In conclusion, we have introduced an analytical approach to investigate the order of the transition in the Z(3) spin model in three dimensions. We have found that when the next nearest neighbour coupling J_2 is positive the transition is first order. On the other hand, for small negative J_2 the analytical method is accurate, and a point is found where the transition turns out to be second order. For larger negative values of J_2 the analytical treatment no longer works, due to the slow convergence of the cumulant expansion. In order to assess this situation we performed a Monte Carlo simulation in these three different regions. In the large positive J_2 the agreement is impressive even at the lowest order. In the intermediate region, we found that by including all the corrections, up to the third order, we obtain the best predictions. In contrast, in the region with large negative J_2 we found the Monte Carlo results show a discrepancy with those obtained by means of the variational approach, and even the higher order corrections proved to be insufficient to remedy this state of affairs. Finally, Monte Carlo results seem to indicate that for moderately large negative values of γ the system undergoes a second order phase transition.

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