ON THE ORDER OF THE PHASE TRANSITION IN THE 3D THREE-STATE POTTS MODEL WITH ANTI-FERROMAGNETIC NEXT-TO-NEAREST NEIGHBOUR COUPLING

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We investigate the order of the phase transition in the three dimensional, three-state Potts model with anti-ferromagnetic next-to-nearest neighbour (NNN) coupling in a high statistics, finite size scaling study. On L^3 lattices with L ranging from 20 to 48 with the relative strength of the NNN coupling, γ, fixed to -0.2, we find a first order phase transition. The onset of the finite size scaling behaviour seems to occur later compared to the $\gamma=0.0$ case. The discontinuity in the order parameter is of the same magnitude in both cases, while the latent heat decreases by a factor of two.

Recent discussions about the order of the deconfinement phase transition in SU(3) gauge theories in three spatial dimensions [1] brought the issue of the order of the transitions in corresponding spin systems into a sharp focus [2–5]. It is generally expected that the critical behaviour of the former is governed by an effective three dimensional theory of the order parameter, i.e. SU(3) spins, which, in turn, is expected to be related to a corresponding Z(3)-symmetric theory with identical structure of couplings [6]. It is clear that the order of the transition will crucially depend on the type of effective couplings generated. In fact, it has been argued that for the case of SU(3) already a small contribution from an anti-ferromagnetic next-to-nearest neighbour (NNN) coupling in addition to the leading ferromagnetic nearest neighbour (NN) coupling could induce a second order deconfinement phase transition. In particular, the case of a three dimensional three-state Potts model with anti-ferromagnetic NNN coupling was cited as an example for the above scenario. Early numerical simulations of this model on relatively small lattices and with modest statistics seemed to suggest a second order phase transition for $\gamma=-0.2$, where γ is the ratio of the NNN and NN couplings [7]. Later investigations of correlation lengths for this model supported this conclusion [8]. However, a recent study of the thermodynamics of this model on 32^3 and 64^3 lattices claimed a first order phase transition [4]. Unfortunately, this conclusion is based on a rather low statistics study of the flip-flop behaviour of the system in the critical region which is known for its traps [5].

In view of all this, we undertook a detailed high statistics analysis of the three dimensional three state Potts model with $\gamma=-0.2$ on L^3 lattices, with $L=20$, 24, 32, 40 and 48. From our previous analysis of the ferromagnetic case ($\gamma=0.0$) [2], we know that a finite size analysis of various thermodynamic quantities is the best way to decide about the order of the transition. We also found there that it is difficult to decide about the order of the transition on the basis of correlation lengths alone, especially since the scaling behaviour of this quantity near a first order phase transition is only poorly understood.

The hamiltonian for the Potts model with NNN coupling is given by

$$H=\sum_{\substack{\text{NN pairs}\\ \langle j,k\rangle}}\delta_{\sigma_j,\sigma_k}+\gamma\sum_{\substack{\text{NNN pairs}\\ \langle j,k\rangle}}\delta_{\sigma_j,\sigma_k}$$

$$\equiv\sum_{\substack{\text{NN pairs}\\ \langle j,k\rangle}}C_{\mathrm{NN}}+\gamma\sum_{\substack{\text{NNN pairs}\\ \langle j,k\rangle}}C_{\mathrm{NNN}}\,, \qquad (1)$$

where $\sigma_{j(k)}=0$, 1 or 2. The partition function of the system on an L^3 cubic lattice is given by

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$$Z=\sum_{\{\sigma_j\}} \exp(\beta H) \,. \tag{2}$$

For $\gamma=0.0$ the model has been studied in detail [2,9] and a first order phase transition has been established. Here we will consider the case of nonzero NNN coupling. In particular we will concentrate on the case $\gamma=-0.2$, which has been considered previously [4,8] and which is controversial as we have pointed out above. In the following we will study the volume dependence of global observables like the energy density $E=V^{-1}\langle H\rangle$ and the order parameter $\langle S\rangle$, with S defined by

$$S=\tfrac{3}{2}\max(n_0, n_1, n_2)-\tfrac{1}{2} \,. \tag{3}$$

Here $\langle X\rangle$ denotes the thermal expectation value of the observable X with respect to Z, $V=L^3$ is the volume of the box and n_α is defined by

$$n_\alpha=\frac{1}{V}\sum_j \delta_{\sigma_j,\alpha} \,, \quad \alpha=0, 1, 2 \,. \tag{4}$$

In addition we study the corresponding thermal and magnetic response functions, i.e. the specific heat

$$C_V=\frac{1}{V}(\langle H^2\rangle-\langle H\rangle^2) \,, \tag{5}$$

and the susceptibility

$$\chi=V(\langle S^2\rangle-\langle S\rangle^2) \,. \tag{6}$$

We used the standard Metropolis algorithm to simulate the model on periodic cubic lattices of sizes $L=20, 24, 30, 32, 40$ and 48. Typically we performed 5×10^5–2×10^6 iterations at each β value. Expectation values were computed every 10th iteration. To eliminate the remaining time correlations errors have been calculated by dividing the data sample into blocks of various lengths and taking the expectation values on a given block as independent measurements. Fig. 1 shows our results for the order parameter S. It is very suggestive of a discontinuity in it in the thermodynamic limit. Looking at fig. 1, one gets the impression that on smaller lattices the critical region is shifted in an irregular way as a function of lattice size. For instance, the critical coupling for $L=24$ seems to be larger than that for $L=20$, while that for $L=32$ seems to be smaller than that for $L=24$. This irregularity is confirmed by the more detailed analysis discussed below. As a consequence of this irregularity, one expects any leading order finite size scaling analysis to be inadequate on these lattices. Comparing with the results for S obtained in the ferromagnetic case [2], it seems that much bigger lattices ($L\geqslant 32$) are necessary to utilize the tools of finite size scaling theory in this case.

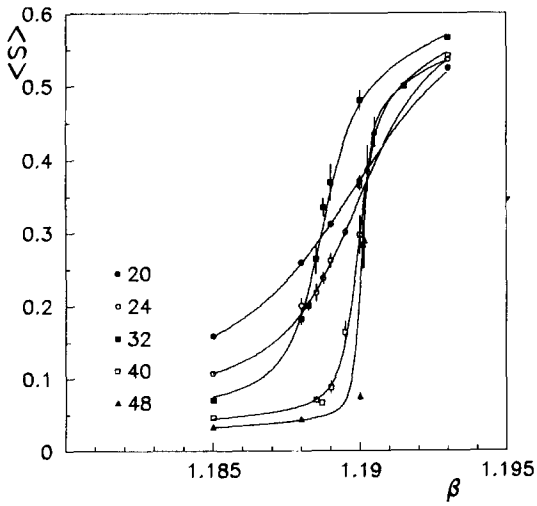

Fig. 1. The order parameter $\langle S\rangle$ versus β on lattices of size L^3 with $L=20$, 24, 32, 40 and 48. The curves shown are obtained by using the method proposed in ref. [10]. The β value choosen for the extrapolations is the one closest to the location of the peak in the magnetic susceptibility given in table 1.

We have studied the time histories of various observables on all the lattice sizes and they display the expected flip-flop behaviour over long runs, as shown for a typical case in fig. 2 where we show the evolution of the order parameter for the 48^3 lattice in the critical region for about 2 million iterations. As elaborated upon in ref. [2], one can exploit the wealth of information hidden in these time histories by analysing the finite size dependence of the probability distributions, $P(S)$. Without repeating the details of the analysis here, we note that we find essentially the same qualitative features: (i) a double peaked probability distribution in the critical region is observed, and (ii) the peaks stay apart and are separated by a deeper valley as the lattice size increases. We, therefore, conclude that even for $\gamma=-0.2$ the model has a first order phase transition, in agreement with ref. [4]. For the gap in S and E we extract from our data on the 48^3 lattice

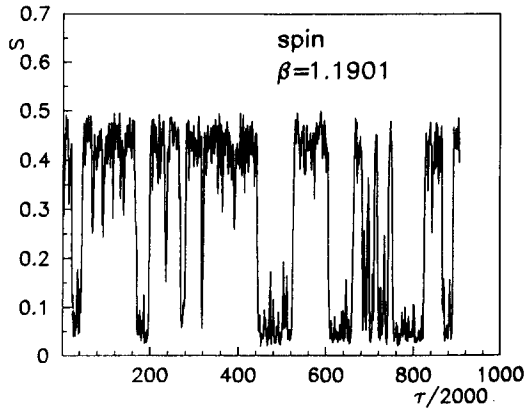

Fig. 2. Time history of the order parameter S as a function of Monte Carlo time on the $L=48$ at $\beta=1.1901$.

$$\Delta S = 0.348 \pm 0.007 ,$$

$$\Delta E = 0.061 \pm 0.001 ,$$

$$\Delta C_{\mathrm{NN}} = 0.047 \pm 0.001 ,$$

$$\Delta C_{\mathrm{NNN}} = 0.066 \pm 0.001 . \qquad (7)$$

We note that the gap in the order parameter and the NN term in the hamiltonian is similar in magnitude to that observed in the case of $\gamma=0.0$, being 0.345(5) and 0.053(3), respectively [#1]. The fact that the magnitude of the discontinuities in these quantities is essentially independent of γ is rather surprising, especially since in the critical region the NN term is only three times as big as the NNN term. Of course, the competing interaction from the NNN term makes the latent heat, $\Delta E = 3\Delta C_{\mathrm{NN}} - 6\gamma\Delta C_{\mathrm{NNN}}$, much smaller in this case, compared to 0.159(9) for $\gamma=0$. Moreover, its influence is also evident in the large shift of β_c; as γ changes from 0.0 to -0.2, β_c changes from ~ 0.55 to ~ 1.19.

Fig. 3 exhibits the susceptibility in units of $1/V$ as a function of β on all our lattices. Again one sees a behaviour characteristic of first order phase transitions. The values of critical couplings obtained from the positions of the peaks are given in table 1; they quantify the irregular behaviour we anticipated from fig. 1. The height of these peaks in susceptibility seems

[#1] We quote here the discontinuities on a 48^3 lattice for both the cases. Results for $\gamma=0$ change only little when extrapolated to infinite volume [2].

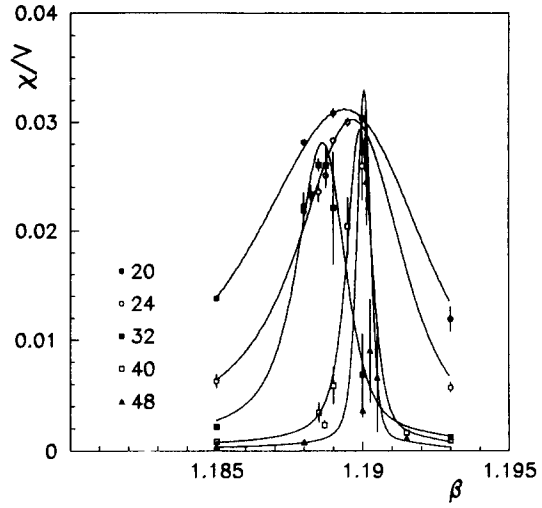

Fig. 3. Same as fig. 1 but for the magnetic susceptibility χ in units of $1/V$.

Table 1
Critical couplings determined on lattices of size L^3 from the peak in the magnetic susceptibility (a), specific heat (b) and the cumulant function V_E (c).

L	(a)	(b)	(c)
20	1.1894(3)	1.1903(3)	1.1900(1)
24	1.1897(2)	1.1901(2)	1.1900(1)
32	1.1885(2)	1.1887(2)	1.1886(1)
40	1.1899(2)	1.1900(2)	1.1900(2)
48	1.1901(1)	1.1901(1)	1.1901(1)

Table 2
Peak values for the magnetic susceptibility (a), specific heat (b) and the cumulant function V_E (c) on lattices of size L^3.

L	(a)	(b)	(c)
20	0.031(1)	0.0022(1)	0.00492(6)
24	0.030(4)	0.0017(3)	0.00399(60)
32	0.028(2)	0.0012(1)	0.00285(9)
40	0.029(5)	0.0010(2)	0.00249(57)
48	0.032(6)	0.0011(3)	0.00252(60)

to scale as V: We have used the probability distributions of the hamiltonian to extrapolate to nearby β values [10] in order to extract the height and the position of the peak on the various lattices. The results for the extrema in the susceptibility are given in table 2. The error estimates have been obtained by using

the extrapolations from several nearby β values in the critical region. Also given in these tables are similar estimates from the specific heat which too exhibits a peak that scales with volume. However, in this case the scaling behaviour clearly sets in only for $L \geqslant 32$.

A characteristic feature of a first order phase transition is the multiple valued nature of thermodynamic quantities at β_c. This feature can be exploited by looking at cumulants of these variables [11,12]. A simple observable is, for instance, constructed from cumulants of the hamiltonian

$$V_E(\beta) = \frac{\langle H^4 \rangle}{\langle H^2 \rangle^2} - 1 \,. \tag{8}$$

This observable has the property of approaching zero for any single valued distribution, which in the infinite volume limit is well approximated by a gaussian distribution. For a first order transition, on the other hand, one expects

$$\lim_{V \to \infty} V_E(\beta_c) = 1 - 4 \frac{E_-^2 E_+^2}{(E_-^2 + E_+^2)^2} , \tag{9}$$

where E_+ and E_- are the limiting value of the energy density in the infinite volume limit when β_c is approached from above and below, respectively. A first order transition thus would be signaled by a peak in the cumulant $V_E(\beta)$ at β_c, which persists in the infinite volume limit. Of course, the usefulness of this observable strongly depends on the size of the latent heat, $\Delta E = E_+ - E_-$, as can be seen from eq. (9). Our results for $V_E(\beta)$ are given in fig. 4. One sees a clear peak, which shifts on the different lattices in a way consistent with the irregularities in β_c found from other thermodynamic observables. The values for β_c obtained from the location of the peak as well as the value, $V_E^{\max}$, at the maximum are also given in the tables 1 and 2, respectively. We note that on the larger lattices, $L \geqslant 32$, $V_E^{\max}$ seems to saturate at a non-zero value. In fact, for $L = 48$ we obtain $V_E^{\max} = 0.0025 \pm 0.0006$, which is in good agreement with the value 0.0022 ± 0.0002 we obtain from eq. (9) using our results for $E_+ = 1.331(1)$ and $E_- = 1.270(1)$ and also with a straightforward $1/V$ extrapolation of our finite volume results to the infinite volume limit.

Finally, we would like to discuss our results on correlation lengths in this model. For the case of a ferromagnetic Potts model, i.e. $\gamma = 0.0$, we have presented an extensive analysis of the correlation

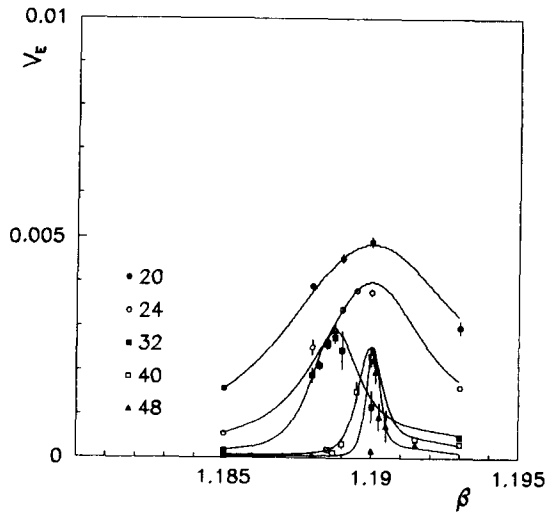

Fig. 4. Same as fig. 1 but for the ratio of cumulants V_E, defined in eq. (8).

functions. We will, therefore, be brief here, concentrating on the important features relevant to the $\gamma = -0.2$ case. The correlation functions $\Gamma(r)$ which we measured are defined by

$$\Gamma(r) = \frac{1}{6L} \left\langle \sum_{i=1}^{L} \bar{s}_i \bar{s}_j^{\dagger} \right\rangle . \tag{10}$$

Here $\bar{s}_i = L^{-2} \sum \exp(2\pi i \sigma)$ is the average spin on the plane i, and $r = |i-j|$ denotes the distance between the planes i and j along one of the principal axes of the lattice. Forming ratios

$$R(r) = \frac{\Gamma(r)}{\Gamma(r+1)} , \tag{11}$$

and using an ansatz inspired by the behaviour of Γ on an infinite lattice that takes into account the periodicity of the L^3 lattice,

$$\Gamma(r) = A\{\exp(-mr) + \exp[-m(L-r)]\} , \tag{12}$$

we extract a distance-dependent mass $m(r)$ for each β and L. At large r, these masses develop a plateau from which one easily obtains the correlation length $\xi = 1/m$. Fig. 5 shows our results for the asymptotic values of m as a function of β. For lattices of size $L \geqslant 32$, one observes the characteristic crossing pattern which separates regions of different finite size behaviour for this observable. While such a pattern is suggestive of a first order phase transition, one is

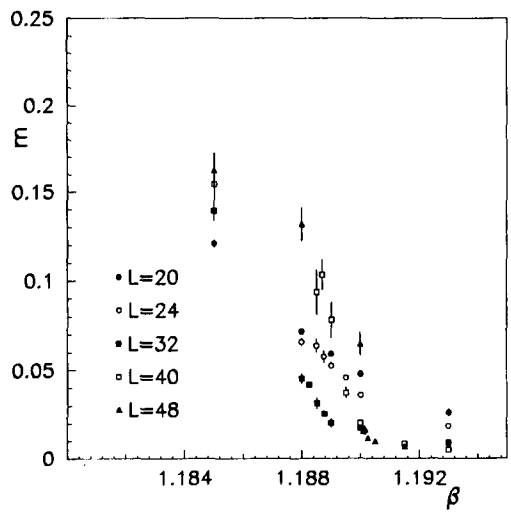

Fig. 5. Same as fig. 1 but for the inverse correlation length $m = 1/\xi$.

clearly unable to establish it quantitatively, as found in similar studies of correlation length for the $\gamma = 0.0$ case also. In particular, no finite size scaling study of $\beta_{c,L}$ or any determination of the critical exponent seems to be feasible for the data in fig. 5. Indeed, if the phase transition were to be first order, as we have shown here to be the case, it is not even clear what the corresponding critical exponent should be.

We also attempted to extract the physical mass gap m_c at the critical point. We divided the data sample on our larger lattices into two separate samples for the symmetric and broken phase, respectively. Using connected correlation functions in the broken phase we found consistent results for m_c in both phases. For lattices with $L \geqslant 32$ we find that the mass gap stays finite, i.e. shows only small size dependence and the correlation length $\xi = 1/m$ is much smaller than the size of the lattice. We find $\xi(\beta_c) \simeq 14$.

In conclusion, we simulated the three dimensional three-state Potts model with a relative NNN coupling of -0.2 on L^3 lattices with L up to 48. Our investigations of thermodynamic observables led us to the conclusion of a first order phase transition on basis of finite size scaling analysis. In particular, we find a rise in susceptibility and the specific heat at the critical point which is consistent with a linear growth in V and the cumulant, defined in eq. (8), shows a peak which seems to persist in the infinite volume limit. We are, however, unable to check quantitatively whether β_c has the expected finite size scaling behaviour corresponding to a first order phase transition. The difficulties are evident from table 1. The estimated discontinuity in the order parameter is surprisingly the same as for the case of $\gamma = 0.0$, although the latent heat does go down significantly. Also the onset of finite size scaling behaviour seems to be somewhat later which may presumably tie in with the larger physical correlation length we found in this case.

Clearly it would be interesting to investigate whether the phase transition remains first order for smaller values of γ. For $\gamma \leqslant -0.25$ the model has a rich phase structure with a spontaneous breaking of rotational symmetry [13]. Work in this direction is in progress.

Note added. After completion of this work we learned about concurrent studies of the three dimensional three-state Potts model with anti-ferromagnetic NNN coupling [14,15]. The conclusions of these groups agree with ours. In particular the need for very large lattice to reach a regime where finite size scaling can be applied for the model with $\gamma = -0.2$ is evident from the renormalization group analysis presented in ref. [14].

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