THE MAGNETIC CRITICAL EXPONENT IN THE THREE-STATE THREE-DIMENSIONAL POTTS MODEL

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Received 26 January 1990

We perform a numerical study of the Potts model $q=3$ in three dimensions with nearest neighbour and next to nearest neighbour couplings by means of the finite-size renormalization group method. The analysis of the magnetic critical exponents is complementary to the one of the thermal critical exponent already presented by us and confirms our conclusions that the transition from the disordered phase to the low-temperature ordered phase is first order.

The study of the coupling flow near a fixed point is a crucial aspect of the modern theory of critical phenomena. It provides, in fact, the values of the critical exponents which characterize the universality class of the system under investigation. Analogous methods have been applied in the case when two or more phases co-exist and the exponents extracted.

It is well known from finite-size scaling analysis [1] that at a discontinuity fixed point the inverse thermal exponent, $y_T = 1/\nu$, is equal to the spatial dimensionality of the system, d, and this fact alone allows one to identify the order of the transition as first order.

The idea of the present paper is to show that the renormalization group transformation is a useful tool to discriminate between continuous or second-order transitions and discontinuous but weakly first-order transitions. In a recent letter [2] we presented results concerning the exponent y_T of the Potts three-state model in three dimensions. In the present paper we corroborate the previous conclusions by an analysis of the magnetic critical exponent, y_H.

Let us briefly recall the simple scaling argument, introduced by Fisher and Berker [3], which leads to the relation $y_H = d$. The free energy density at a first-order transition scales as

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0370-2693/90/$ 03.50

$$\lim_{H\to 0} f(H) = H^{d/y_H} f(\pm 1)\,, \tag{1}$$

where H is the field coupled to the order parameter. On the other hand the order parameter discontinuity, ΔM, can be represented by the following relation:

$$\Delta M \sim |H|^{1/\delta}\,, \tag{2}$$

if one assumes for δ, the so-called isothermal exponent, the value ∞. Differentiating eq. (1) with respect to the field and comparing with eq. (2) one obtains the following scaling relation:

$$\frac{d}{y_H} - 1 = \frac{1}{\delta}\,, \tag{3}$$

i.e. $y_H = d$. This relation was verified numerically by means of a recently developed method which combines numerical Monte Carlo simulation, Renormalization group ideas and finite size scaling concepts [4–6].

The three-state Potts [7,8] model is defined by the hamiltonian

$$H = -J_1 \sum_{\substack{\langle i,j\rangle \\ \text{n.n.}}} \delta_{\sigma_i,\sigma_j} - J_2 \sum_{\substack{\langle i,j\rangle \\ \text{n.n.n.}}} \delta_{\sigma_i,\sigma_j}\,, \tag{4}$$

where on each site i belonging to a three-dimensional cubic lattice is defined a Potts variable σ_i, which can take on three different values. The first sum runs over nearest neighbour (n.n.) pairs and the second over the next nearest neighbour (n.n.n.) pairs; the δ is a Kronecker delta, i.e. two sites i and j interact with energies J_1 or J_2 only if they are in the same state. According to the mean field theory the $q=3$ Potts model displays a first-order phase transition in any dimension, d. However, it was proven analytically that in the case $d=2$ and $q\leqslant 4$ the transition is second order. In three dimensions the order of the transition cannot be established analytically for any value of the couplings.

On the other hand, the finite-size real-space renormalization group (FSRSRG) has proved an effective method in determining the order of the transition, as we shall illustrate.

Since the present work is the sequel of a previous letter [2], where we reported the details of the blocking procedure which defines the renormalization transformation, we shall refrain from giving a detailed account of it.

The key idea underlying the present method is to keep track of the dependence of the block variables, which play the role of renormalized couplings, as a function of the original couplings and lattice size.

The finite-size scaling hypothesis allows one to determine the critical exponents by comparing different infrared cutoffs, i.e. different sizes L of the original systems. In order to implement the method one needs to consider block variables such as the magnetization, the energy, their products and their derivatives with respect to the inverse temperature, β, or the external field, h. These derivatives, which control

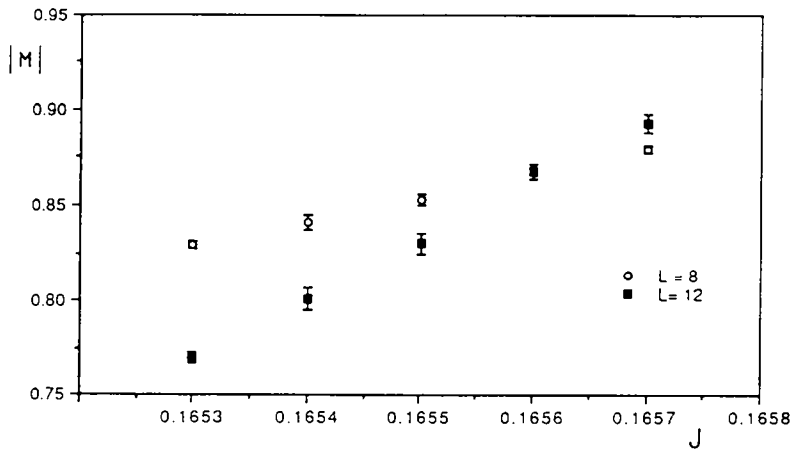

Fig. 1. The absolute block magnetization $\langle |M| \rangle$, as a function of the inverse temperature for the sizes $L=8$ and $L=12$ in the case $J_1 = J_2$.

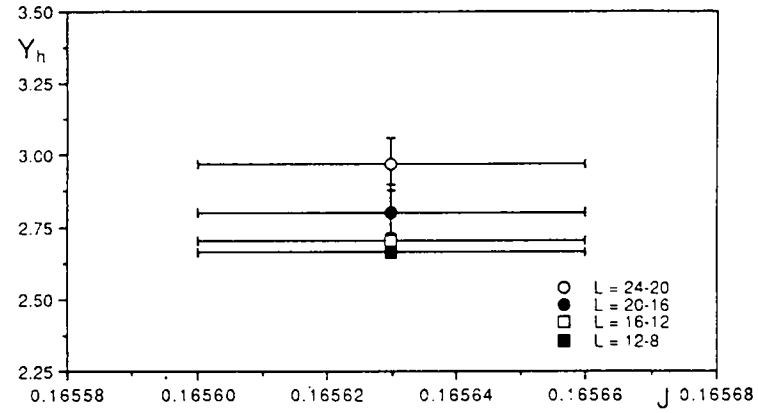

Fig. 2. The magnetic critical exponent y_H as extracted from different pairs of sizes in the case of $J_1 = J_2$.

the coupling flow under renormalization group transformation, are computed from appropriately defined correlation functions that we extract from our Monte Carlo simulation.

We performed simulations of cubic systems of linear size $L = 8, 12, 16, 20, 24, 28, 32$. We used a highly optimized multispin code, storing eight independent lattices in a single 32-bit word. The Metropolis algorithm was employed and we performed thorough checks against possible problems caused by a bad thermalization or correlation among the measures. In addition we tested the presence of the "flip-flop" process between the different phases in every run we performed. All the errors are calculated (with a jackknife method) as fluctuations of the eight independent samples corresponding to the eight lattices mentioned above. The overall CPU time we used is over 900 h of IBM 3090. More details (as the number of thermalization or measurement sweeps for every lattice) were reported in our previous paper [2].

As shown in fig. 1 the couplings strongly depend on the size of the system. Their intersection locates the matching point. In order to calculate the magnetic critical exponent one defines the following ratio:

$$y_H = \frac{\ln\{[\mathrm{d}\langle M(L')\rangle/\mathrm{d}h]/[\mathrm{d}\langle M(L)\rangle/\mathrm{d}h]\}}{\ln(L'/L)} \qquad (5)$$

evaluated at zero field, h. $\mathrm{d}\langle M(L)\rangle/\mathrm{d}h$ is the derivative of the block magnetization M with respect to the magnetic field, relative to the volume L^3. In fact, we do not compute the derivative directly, but from the connected correlation function between M and the original magnetization.

In figs. 2 and 3 we display the dependence of the

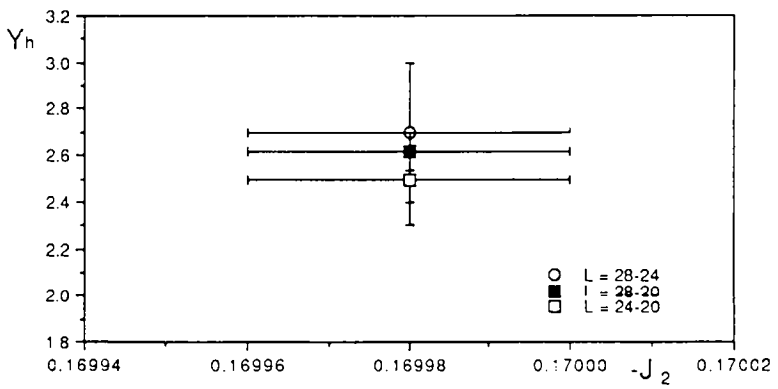

Fig. 3. The magnetic critical exponent y_H computed from different pairs of sizes in the case of $J_1 = 1$ and $J_2 < 0$.

exponent y_H on the size for the ferromagnetic system with $J_1 = J_2$ and for the one with $J_1 = 1$ and J_2 negative ($J_2 = -0.16998(2)$ at the transition), respectively.

The vertical error represents the MC uncertainty on the determination of the exponent whereas the horizontal error represents the uncertainty on the location of the transition inverse temperature. In both cases one notices a systematic drift towards larger values of the magnetic exponent, y_H, as the volume increases. This phenomenon is (partly) due to the fact that one needs sizes definitely larger than the correlation length associated to the first-order transition to see the appropriate scaling properties. Phase transitions exhibiting such a slow approach to the asymptotic scaling laws have been termed weakly first order. Finally y_H seems to settle around the value $3 (= d)$ as expected in the case of a first-order phase transformation. We also remark that the magnetic critical exponent converges to d faster than the thermal exponent as the sizes of the system increase.

In conclusion we have studied the finite-size behaviour of thermodynamic averages of the three-state Potts model in three dimensions and found that for two different values of the couplings J_1 and J_2 it exhibits first-order-like behavior. More specifically we have determined the magnetic critical exponent, y_H. The analysis presented fully confirms the results [9,10] previously published and shows that the finite-size scaling renormalization group is a powerful tool in determining the order of the transition.

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