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Phase transition in a general continuous Ising model with long-range interactions

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Critical exponents for a one-dimensional general continuous Ising model with long-range ferromagnetic interactions decaying as $1/r^{1+\sigma}$ are calculated using a histogram Monte Carlo technique. A continuous Ising model means that a spin can take any value between -1 and 1. The critical point behavior is investigated. It is found that the system exhibits a second-order phase transition with nonstandard critical exponents; the singularities in the specific heat and susceptibility depend on σ . For $\sigma=1$, there are extremely weak finite size effects: the first-order and the second-order cumulants of the order parameter yield $\nu=2.42(1)$. The susceptibility exponent $\gamma=2.259(9)$. Results for $\sigma=0.7$ will be shown and discussed. © 1999 American Institute of Physics. [S0021-8979(99)28608-2]

I. INTRODUCTION

It is known that long-range forces can induce critical behavior in one- and two-dimensional systems where it would otherwise be absent. There have been some analytical studies as well as a number of numerical results on the critical behavior of these systems. The one-dimensional (1D) Ising model with algebraically decaying long-range interactions has been investigated extensively during the last 2 decades. It is known that it exhibits long-range order at finite temperature if $\sigma \le 1$ and no phase transition if $\sigma > 1$. ¹⁻⁵ Detailed properties of the spherical model with long-range interactions have been discussed by Joyce.⁶ It should be noted, however, that there is no specific information on the critical exponents of such systems. The critical exponents of a general system with an n-component order parameter were calculated by Fisher et al.7 using a renormalization group method. These exponents depend on the values of n, σ and d. For $\sigma > 2$, they take values of short-range exponents for all d. A renormalization group expansion in $1-\sigma > 0$ was done by Kosterlitz⁸ who obtained $1/\nu = [2(1-\sigma)^{1/2}]$ when $\sigma \rightarrow 1$ in one dimension. In the case of the Ising model, the critical temperature T_c and critical exponents were evaluated by Glumac and Uzelac^{3,4} using the transfer matrix with finiterange scaling rather than finite-size scaling. This evaluation has been also made by finite chain extrapolations.⁹

While the Ising case has been widely investigated, non-Ising models have not received much attention. Glumac and Uzelac¹⁰ have investigated the 1D q-state Potts model up to q=64 using a transfer matrix method with a cutoff at 20 atomic distances. Priest and Lubensky¹¹ and Theumann and Gusmao¹² have used renormalization group expansion in $\epsilon = 3 \sigma - d$ to calculate critical exponents of the Potts model.

In the case of long-range d-dimensional systems, with the exception of the early work for d=1 with very small sizes (up to 15 spins), Monte Carlo (MC) techniques have not been used due to the long computing time required. The

In this article we present some simulation results for a 1D continuous Ising model using the standard MC simulation and the MC histogram method. We start in Sec. II with a presentation of the results obtained by traditional MC simulation. In Sec. III we present the results of the MC histogram method. The values of different critical exponents are shown. One of our most striking results is the absence of a first-order transition which is found for the short-range interaction Potts model with large q in two and three dimensions. Concluding remarks are given in Sec. IV.

II. RESULTS OF TRADITIONAL MONTE CARLO SIMULATIONS

The 1D continuous Ising model that we shall consider is defined as

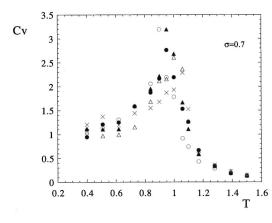
$$\mathcal{H} = -\sum_{\langle i,j\rangle} J_{ij} \sigma_i \sigma_j, \tag{1}$$

where σ_i is a classical Ising spin at site i and takes all values between -1 and 1, and $J_{ij} = 1/(|i-j|^{d+\sigma})$.

We simulated systems with linear sizes in the L =50-900 range. We took into account all interactions without cutoff that were permitted by the periodic boundary conditions. The maximum system size was limited to L = 900 in order to curtail the computing time due the presence of longrange interactions. A MC step (MCS) per site for a longrange Ising model involves $O(L^2)$ operations. The equilibrating time is from 100 000 to 200 000 MCS/site and the averaging time is from 500 000 to 1 000 000 MCS/site. Simulations of the model were carried out for σ =0.7 and 1. The values were chosen in the nonclassical regime $0.5 < \sigma \le 1$ where the critical exponents are expected to depend not only on σ but also on n and d, unlike in the case of classical regime $(0 < \sigma < 0.5)$. The magnetization per site M, energy per site U, specific heat C_n , and susceptibility χ were measured as functions of the temperature T. The results of U vs T (not shown) show a single inflection point suggesting the

absence of reliable MC results, in particular for the non-Ising case, has motivated the present work.

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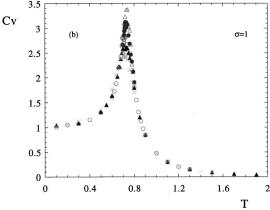


FIG. 1. Temperature and size dependence of the specific heat for σ =0.7 (a) and (b) 1. Open circles, closed triangles, closed circles, open triangles, and crosses are for L=50, 100, 150, 400, and 900, respectively.

occurrence of a continuous transition. In Fig. 1, we show C_v calculated from energy fluctuations as a function of T for σ =0.7 and 1, each with several lattice sizes. For σ =1 a very small size dependence is observed, whereas for σ =0.7 we have found that the critical temperature T_c has a size dependence. This is shown in Table I.

III. CRITICAL EXPONENTS

A. Method

The MC histogram method¹³ is known to be a very accurate way to determine critical exponents. Contrary to traditional MC calculations, it does not need prior knowledge of T_c with high precision. We have used our previous results to localize the transition temperature $T_c(L)$ where the histogram measurements are performed for each size. The following quantities have been calculated: magnetization M, total

TABLE I. Transition temperatures $T_c(L)$ associated with the peak position of C_n for all L studied.

σL	50	100	150	400	900
0.7	0.94	0.95	0.96	1.02	1.06
1	0.71	0.71	0.71	0.71	0.71

TABLE II. Estimates of critical exponents using the MC histogram method.

σ	ν	γ	β	α	η	$d_{ m eff}$	T_c
0.7	1.795(5)	1.26(1)	0.29(1)	0.16(1)	1.30(1)	1.03(1)	1.08
			0.26(1) 0.084(1)	0.21(1) $-0.34(1)$			
1	2.42(1)	2.26(1)	. ,	-0.41(1)	1.07(1)	0.97(1)	0.70

energy E, specific heat C_v , susceptibility χ , first-order cumulant of energy C_U , and nth order cumulant of the order parameter V_n for n=1 and 2, defined as

$$\begin{split} \langle M \rangle &= \sum_i \ \langle \sigma_i \rangle, \langle E \rangle = \langle \mathcal{H} \rangle, \\ C_v &= (1/k_B T^2) (\langle E^2 \rangle - \langle E \rangle^2), \\ \chi &= (1/k_B T) (\langle M^2 \rangle - \langle M \rangle^2), \quad C_U = 1 - (\langle E^4 \rangle / 3 \langle E^2 \rangle^2), \\ V_n &= \langle \left[\partial \ln M^n / \partial (1/k_B T) \right] \rangle = (\langle M^n E \rangle / \langle M^n \rangle) - \langle E \rangle. \end{split}$$

The mean values, which are functions of M and of powers of E, may be calculated as continuous functions of temperature using the histogram obtained at $T_c(L)$ as follows:

$$\langle E^n f(M) \rangle = \frac{\sum_E E^n \langle f \rangle(E) H(E) \exp(-\Delta k_B E)}{\sum_E H(E) \exp(-\Delta k E)},$$
 (2)

where H(E) is the histogram measured at $T_c(L)$ and $\langle f \rangle \times \langle E \rangle$ are the mean values of the corresponding function of M calculated at $T_c(L)$ for each fixed value of energy. For large values of L, these quantities are expected to scale with L as follows: $V_1 \propto L^{-1/\nu}$, $V_2 \propto L^{-1/\nu}$, $C_U = CU_{T_c(\infty)} + AL^{-\alpha/\nu}$, $M_{T_c(\infty)} \propto L^{-\beta/\nu}$, $C_v = C_0 + C_1 L^{\alpha/\nu}$, $\chi \propto L^{\gamma/\nu}$, and $T_c(L) = T_c(\infty) + C_A L^{-1/\nu}$.

Then we estimated ν independently from V_1 and V_2 . With these values we calculated γ from χ . We estimated $T_c(\infty)$ by using the last expression for each observable. Using this value of $T_c(\infty)$, we calculated β from $M_{T_c(\infty)}$. The Rushbrooke scaling law $\alpha+2\beta+\gamma=2$ allows us to obtain α . Finally, using the hyperscaling relationship, we can estimate

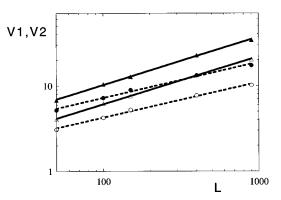


FIG. 2. Determination of the critical exponent ν from the slope of V_1 (open symbols) and V_2 (closed symbols) vs L in the ln-ln scale, the triangles and the circles correspond, respectively, to σ =0.7 and 1. The errors are smaller than the size of the data points.

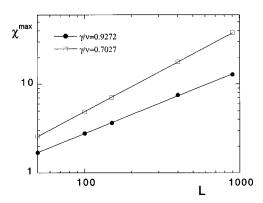


FIG. 3. Determination of the critical exponent γ from the slope (γ/ν) of $\chi_{\rm max}$ vs L in the ln-ln scale. The errors are smaller than the size of the data points.

the effective dimension of this model $d_{\text{eff}} = (2 - \alpha)\nu^{-1}$ and the exponent η from the scaling law $\gamma = (2 - \eta)\nu$.

B. Results

We performed MC histogram calculations for L=50, 100, 150, 400, and 900 at the $T_c(L)$ obtained in Sec. II. Between 3 and 5 million MCS/sites were performed for each lattice size. The results show that the transition is clearly of second order. The asymptotic value of C_U tends towards 2/3 for large L (not shown). Figure 2 presents the minima of V_1 and V_2 as functions of L in the ln-ln scale. The data lie nicely on a straight line whose slope is $1/\nu$. We obtain $\nu = 1.795(5)$ and $\nu = 2.42(1)$ for $\sigma = 0.7$ and 1, respectively. The errors were estimated from the line-fitting procedure. Systematic errors from estimates of $T_c(L)$ were much smaller. The maximum of χ vs L is shown in Fig. 3 for σ =0.7 and 1. The slope of each line yields the value of γ/ν . Using the values of ν we obtain γ . Now, using the values in Table I we obtain by scaling $T_c(\infty)$. Plotting $M_{T_c(\infty)}$ vs $L^{-\beta/\nu}$ in the ln-ln scale (not shown), we obtain β/ν directly. Using the Rushbrooke relationship, we obtain α indirectly. The scaling relationship then gives the effective dimensionality $d_{\rm eff}$. The criticals exponents are summarized in Table II where the values in the second lines of β and α are those obtained by first using $\alpha = 2 - d\nu$ with d = 1 and then calculating β with $\beta = (2 - \gamma - \alpha)/2$. Although the orders of magnitude and the sign of these deduced values are in qualitative agreement with those in the first line, we believe that the latter values are more reliable due to the fact that only one scaling relation is used.

IV. CONCLUDING REMARKS

We have studied the general continuous Ising model with long-range interactions decaying as a power law of distance using the MC histogram method and finite-size scaling. We found the transition to be continuous with the critical exponents obtained. Several remarks regarding our results are in order:

- (1) The very small size dependence when $\sigma=1$ explains the large value of ν .
- (2) We do not, however, find a divergence of ν when $\sigma=1$, which was predicted for the Ising case.⁸
- (3) Our results for ν are not close to those obtained by Glumac and Uzelac: ¹⁰ for q=64 they obtained $\nu=1$ where $\sigma=1$ and for q=16 they reported $\nu=0.22$ for $\sigma=0.7$. These small values of ν are contradict ours if we consider their values of q are large enough to be compared to our case.
- (4) The correction to the expression $\eta = 2 \sigma$ in the nonclassical regime is very small (see values of η).

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