Critical behavior of the long-range Ising chain from the largest-cluster probability distribution

Katarina Uzelac,[1] Zvonko Glumac,[2] and Ante Aničić[1]
[1]*Institute of Physics, P.O. Box 304, Bijenička 46, HR-10000 Zagreb, Croatia*
[2]*Faculty of Electrical Engineering, Kneza Trpimira 2B, 31 000 Osijek, Croatia*
(Received 14 April 2000; revised manuscript received 14 July 2000; published 20 February 2001)

Monte Carlo simulations of the one-dimensional Ising model with ferromagnetic interactions decaying with distance r as $1/r^{1+\sigma}$ are performed by applying the Swendsen-Wang cluster algorithm with cumulative probabilities. The critical behavior in the nonclassical critical regime corresponding to $0.5<\sigma<1$ is derived from finite-size scaling analysis of the largest cluster.

DOI: 10.1103/PhysRevE.63.037101 PACS number(s): 05.50.+q, 64.60.Cn

The calculation of the critical behavior of the Ising model with long-range (LR) interactions decaying with distance with a power law $1/r^{d+\sigma}$ is not an easy task, even in one dimension, where a phase transition at finite temperature occurs for $0<\sigma\leqslant 1$ [1,2]. Exact analytical expressions for the critical exponents may be derived for $\sigma\leqslant 0.5$ [3], corresponding to the classical regime, while for $\sigma>0.5$ only approximate results exist. Various analytical and numerical approaches have been applied, from direct numerical calculations on finite chains [4] to several approaches based on the renormalization group (RG) and scaling [5–10]. The nonlocal character of the interactions reduces the efficiency of most of the standard approaches so that the values of critical exponents obtained by all these methods differ considerably.

In numerous cases of phase transitions in systems with short-range interactions, a useful complementary tool for obtaining both qualitative and quantitative results is provided by Monte Carlo (MC) simulations in combination with finite-size scaling. Such systematic studies were lacking for LR models until recently. When applied to models with LR interactions, the standard MC approaches based either on the Metropolis or on various cluster algorithms are particularly time consuming, since the number of operations per spin flip is proportional there to the size of the system. Recently, this problem was successfully resolved by Luijten and Blöte [11] who used the cumulative probabilities within the Wolff cluster algorithm [12], which they applied to the Ising and similar models [13–15], reducing the computing time by several orders of magnitude. Their very exhaustive studies concentrate on questions related to the mean-field regime, while very little or no interest has been dedicated yet to the regime of nonclassical critical behavior corresponding to $\sigma>0.5$.

The purpose of this work is to extend the MC studies of the critical behavior of the LR Ising model to the nonclassical regime. At the same time this is a suitable example to examine the efficiency of using only cluster statistics in deriving the critical properties of the LR model.

The one-dimensional (1D) Ising model with LR interactions written in the form of a special case ($q=2$) of the Potts model is described by the Hamiltonian

$$H=-\sum_{i<j}\frac{J}{|i-j|^{1+\sigma}}\delta_{s_i,s_j}, \tag{1}$$

where $J>0$, s_i is a two-state Potts variable at the site i, δ is the Kronecker symbol, and the summation is over all pairs of the system. By the substitution $\delta_{s_i,s_j}=(S_iS_j+1)/2$ and $J_I=J/2$, where $S_i=\pm 1$ and J_I denote the Ising spins and the interaction constant, respectively, one recovers the standard definition of the Ising model. In the mean-field regime $\sigma\leqslant 0.5$ the critical exponents have classical values ($\nu=1/\sigma$, $\eta=2-\sigma$). We focus here on the region $0.5<\sigma<1$, where the critical exponents are nontrivial and known only approximately.

When the shortcut using cumulative probabilities is implemented in the MC simulations, the full extent of the numerical advantage is achieved when only the distribution of spins has to be calculated, while for the energy sampling the reduction in CPU time is less important. Recently the calculation by energy sampling was improved [16] by calculating the energy in momentum space and applying a fast Fourier transform. Our intent here is to avoid the energy sampling by making a more complete study of the cluster statistics. For this purpose we use the Swendsen-Wang cluster algorithm [17]. The implementation of cumulative probabilities in the Swendsen-Wang cluster algorithm is straightforward. Each step of this iterative procedure consists in identifying all the clusters in a given spin configuration of the system, following the rule that two particles belong to the same cluster with the probability $p_{ij}=\{1-\exp[-J(i,j)/k_BT]\}\delta_{s_i,s_j}$, and then flipping all the clusters randomly. The cumulative probabilities are applied at the point of identifying the individual clusters along the same lines as was done [11] for the Wolf single-cluster algorithm, and this reduces the number of required operations per single spin flip by a factor of the system size. Like the Wolf algorithm, the Swendsen-Wang algorithm suppresses the slowing down at criticality, and, although it might be somewhat more costly in CPU time, it gives a more complete insight into the cluster statistics and the related probability distributions, such as the distribution of cluster sizes or that of the largest cluster.

Probability distributions related to clusters are mostly used in the description of critical properties of geometrical transitions, like percolation [18]. As follows from the graph expansion by Kasteleyn and Fortuin [19], the very basis of the Swendsen-Wang algorithm, this cluster statistics may be related to the thermodynamic quantities of thermal transitions as well. The only important difference is that in perco-

lation one deals with simple geometrical clusters, while in thermal transitions the clusters formed by the *active bonds* (in terms of the cluster algorithm) are considered. In systems with LR interactions, such as the present model, this difference is obvious.

The cluster-related distributions have been much less exploited in the case of thermal transitions, although some detailed studies exist (see, e.g., Refs. [20,21]) for models with short-range interactions. More recently, there has been renewed interest in this subject within a somewhat different context [22,23].

By performing 10^5 MC iterations, which is sufficient for most of the data presented here, chains of size up to a few tens of thousands of sites could be simulated without requiring too much numerical effort on a modest workstation.

We limit our analysis here to the size distribution of the largest cluster, the quantity that remained out of reach within the earlier single-cluster approach. The probability that the largest cluster will be of the size l is defined as

$$P_{max}(l)=\frac{1}{n_{MCS}}N_{max}(l), \tag{2}$$

where $N_{max}(l)$ is the total number of occurrences of the largest cluster of size l during n_{MCS} MC steps (system updates) of the system.

Several thermodynamic quantities of interest may be expressed through the corresponding moments defined as

$$\langle l^k\rangle=\sum_l l^k P_{max}(l). \tag{3}$$

The first moment

$$\langle l\rangle=\sum_l lP_{max}(l) \tag{4}$$

gives the mean size of the largest cluster. Below the critical temperature it describes the order parameter, which is usually defined as the average of the largest component, i.e., $M=(q\langle\max\{m_\alpha\}\rangle-1)/(q-1)$, where m_α denotes the fraction of spins of the system in the state α.

A quantity of interest to consider is Binder's fourth-order cumulant [24] ratio for the largest cluster,

$$R_L(T)=\frac{\langle l^4\rangle}{\langle l^2\rangle^2}, \tag{5}$$

defined in the same way as for the standard order parameter. Differences between the two corresponding distribution functions, however, result in different shapes of the same ratio defined for the two quantities. As may be seen in Fig. 1, the ratio $R_L(T)$ at high temperatures and in the thermodynamic limit tends to 1 and not to 3, while the corresponding probability distribution is expected to be non-Gaussian, as found already in the cases of percolation [25] and the short-range Ising model [21]. However, as in the cases mentioned, these differences should not change the basic scaling properties in the critical regime. At low temperatures and around T_c the behavior of the two ratios coincides. As in the case of the standard order parameter, there is a common crossing point of the curves $R_L(T)$ of different sizes where the ratio (5) almost does not depend on L and which can be identified as the critical temperature. In Fig. 1, $R_L(T)$ is shown in the case $\sigma=0.9$ and for sizes varying from 1000 to 20 000. By taking into account sizes within the range $1000\leqslant L\leqslant 20\,000$, the determination of this crossing point can be made with precision of four digits, which gives an estimated error of 0.2%.

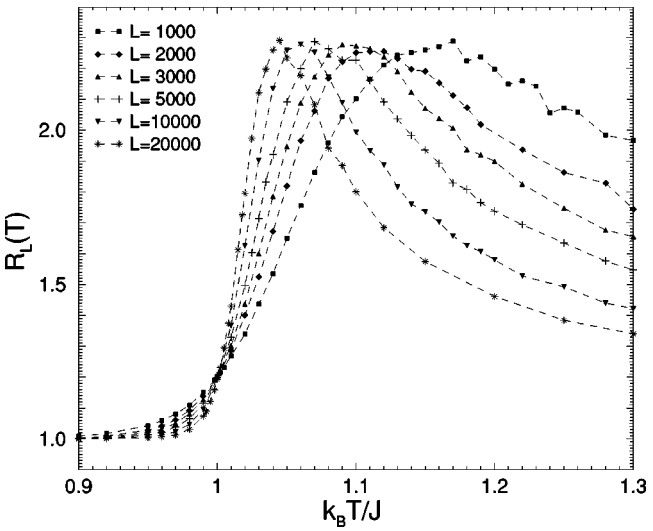

FIG. 1. Ratio $R_L(T)$ for $\sigma=0.9$ and sizes L varying from 1000 to 20 000.

In Table I are presented the critical temperatures for several values of σ in the nonclassical regime $0.5<\sigma<1$ incremented by 0.1, obtained as common crossings of $R_L(T)$. For comparison, we quote the earlier results obtained by numerical calculations [4], the coherent anomaly approach [8,26], finite-range scaling (FRS) [9], and real-space RG [10]. When quoting Ref. [8] we mention only one of the two given sets of results for T_c, which fits better to the later work [26] performed with a significantly improved precision, but, unfortunately, available only for two values of the range considered here.

Near T_c (i.e., in the regime $L<\xi$), the moments (3) and their ratio (5) should obey finite-size scaling. Thus

$$R_L(T)=L^x f(L^{1/\nu}\tau), \tag{6}$$

where $\tau=(T-T_c)/T_c$ is the reduced temperature. Since $R_\infty(T_c)$ is finite, $x=0$.

TABLE I. Comparison of results for the critical temperature T_c to earlier results by Nagle and Bonner [4], Monroe *et al.* [8], FRS [9], Cannas and Magalhães [10], and Monroe [26]. $J=k_B$.

σ	This work	[4]	[8]	[9]	[10]	[26]
0.6	1.770 ± 0.003	1.766	1.7885	1.7718		
0.7	1.463 ± 0.003	1.458	1.491	1.4635	1.28	1.466850
0.8	1.2155 ± 0.002	1.212	1.2585	1.2150		
0.9	1.001 ± 0.001	1.0015	1.058	1.0027	0.77	1.018845

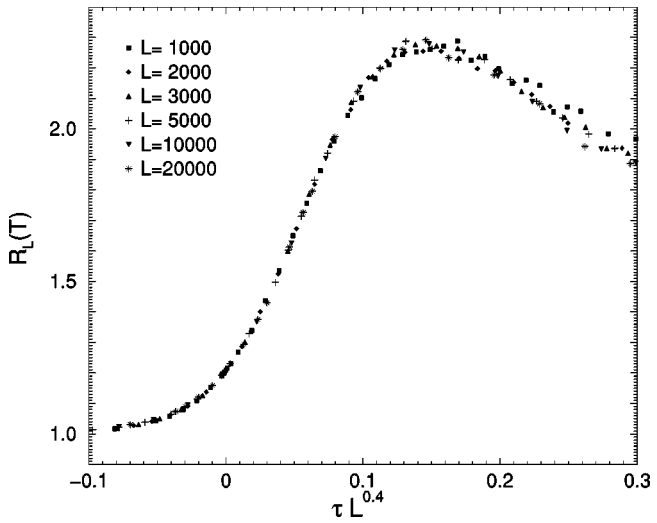

FIG. 2. Ratio $R_L(T)$ for $\sigma=0.9$ versus reduced temperature τ scaled with $L^{1/\nu}$.

It turns out that the critical exponent ν may be estimated with rather good precision by a simple tuning of the unknown exponent $1/\nu$ in Eq. (6) until the curves collapse in the vicinity of the crossing point. In Fig. 2 we present the curves from Fig. 1, collapsed after taking $1/\nu=0.40$. The results for ν^{-1} obtained by collapsing fits for other considered values in the interval $0.5<\sigma<1$ are given in Table II.

In order to reduce the degree of arbitrariness of such fits we require the curves to be indistinguishable in the region of temperatures around T_c, up to the temperature of the maximum of $R_L(T)$, T_{max}. This temperature may be related to the finite-size crossover temperature up to which the finite-size scaling equation (6) should hold. In Fig. 1 one can observe that the maximum of $R_L(T)$ shrinks and shifts toward T_c with increasing L. A rough fit of the difference $T_{max}-T_c$ to the power-law form $(1/L)^{\phi}$ gives the values of ϕ that roughly correspond to $1/\nu$ for a given σ, as expected for the finite-size crossover exponent [27]. The interval of tuning in which the curves remain indistinguishable determines the error margins of the values obtained for the exponent ν^{-1}, which increase with decreasing σ but do not exceed 4% in the considered range of σ's.

Alternative calculations of the exponent, e.g., by using the derivatives of moments, turn out to be less advantageous. (The purely numerical derivative would require a much higher numerical precision and consequently far more extensive runs; the derivative obtained by histogram interpolations or by mixed moments would require an energy sampling and an increased numerical precision in addition.) We also mention at this point that the calculations of Binder's cumulant ratio may equally be performed for the standard order parameter using the Wolff cluster algorithm. One advantage of the approach that uses the Swendsen-Wang cluster algorithm is that it has similar precision and efficiency in both low- and high-temperature regimes, which improves the scaling fit.

The degree of precision of the data obtained permits comparison to results by other approximate methods. These results, which are quite few, are quoted in Table II in chronological order and correspond to numerical calculations on finite chains using Padé series extrapolations [4], ϵ expansion near $2\sigma=d$ [5], the coherent anomaly method [8], finite-range scaling [9], and real-space RG [10]. In Refs. [4] and [8] only the numerical data for the exponents γ and β are available. The exponent ν may be expressed in two ways, which, due to the approximate character of the results, do not give identical values. *a* labels the values obtained from the scaling relation $\nu=\gamma/(2-\eta)$ and the exact analytical expression $\eta=2-\sigma$ expected to hold also in the whole nonclassical regime. *b* indicates the values obtained from the scaling relation involving both exponents, $\nu=\gamma+2\beta$. The quoted results of Ref. [5] are the ones obtained by expansion in $\Delta\sigma=\sigma-0.5$ up to the second order. The expansion in $(1-\sigma)$ [6] is not quoted in the table. It holds very close to $\sigma=1$ and we may quote only the value for $\sigma=0.9$ which is equal to $\nu^{-1}=0.447$. The results of Ref. [5] are also expected to be more reliable closer to $\sigma=0.5$. Other approaches cover the whole range of σ evenly, but their results are rather different and their accuracy as well. Our MC results agree the best with the FRS results.

In Ref. [10], which deals with the Potts model with an arbitrary number of states q, we found intriguing the conjecture that the exponent ν would remain the same for other values of q (when the transition is of the second order), which is in contrast to earlier results of FRS [9]. A MC approach can thus be used to provide an independent calculation. (It also has an advantage over both used approaches in that it is able to distinguish a first- from a second-order transition [28,16].) Our first calculations [29], performed along the same lines as above, give for the case $q=3$, $\sigma=0.9$ the value $1/\nu=0.48\pm0.01$, which would rather be in favor of the FRS results.

In conclusion, we have applied MC simulations to the two-state Potts model with LR interactions on chains of up to

TABLE II. Results for ν^{-1} compared with earlier results of Nagle and Bonner [4], Fisher *et al.* [5], Monroe *et al.* [8], FRS [9], and Cannas and Magalhães [10]. For the meaning of labels *a* and *b*, see the text.

	This work	[4]		[5]	[8]		[9]	[10]
σ		*a*	*b*		*a*	*b*		
0.6	0.50 ± 0.02	0.504	0.540	0.5098	0.441	0.471	0.501	
0.7	0.51 ± 0.02	0.542	0.552	0.4856	0.478	0.461	0.518	0.376
0.8	0.47 ± 0.02	0.533	0.538	0.4461	0.505	0.446	0.483	
0.9	0.40 ± 0.01	0.529	0.526	0.4032	0.542	0.421	0.405	0.256

20 000 sites by using the Swendsen-Wang algorithm to calculate the cluster statistics, in particular the size distribution of the largest cluster. The approach was used as an alternative calculation of the critical behavior in this model in the nonclassical regime $0.5<\sigma<1$. We have shown that the scaling analysis of Binder's fourth-order cumulant ratio of the largest-cluster size gives the critical temperature and the critical exponent ν with reasonable accuracy (better then 0.2% and 4%, respectively). Although the overlapping fit is not expected to be very precise, nor were the simulations pushed to their extreme, the estimated errors are significantly smaller than the differences between the results obtained by different approaches. The results obtained, presented in Tables I and II, are closest to the values obtained earlier by FRS. While the present work deals only with Binder's fourth-order cumulant ratio, a wider analysis, which includes other quantities that may be derived from the cluster statistics, should be performed in future. We believe that the approach through cluster statistics might be useful to study other cases of the Potts model and other models with discrete symmetries, where in the case of LR interactions the alternative methods are very restricted.

[1] F. J. Dyson, Commun. Math. Phys. **12**, 91 (1969).

[2] Rigorous proof for the transition at finite T_c in the most important case $\sigma=1$, characterized by a defect-mediated critical behavior and related to the Kondo problem [P. W. Anderson and G. Yuval, Phys. Rev. B **1**, 1522 (1970)] was given much later [J. Fröhlich and T. Spencer, Commun. Math. Phys. **84**, 87 (1982)], long after the Thouless result [D. J. Thouless, Phys. Rev. **187**, 732 (1969)] on the discontinuous nature of the order parameter in this case.

[3] F. Y. Wu, Rev. Mod. Phys. **54**, 235 (1982).

[4] J. F. Nagle and J. C. Bonner, J. Phys. C **3**, 359 (1970).

[5] M. E. Fisher, S. K. Ma, and B. G. Nickel, Phys. Rev. Lett. **29**, 917 (1972).

[6] J. M. Kosterlitz, Phys. Rev. Lett. **37**, 1577 (1976).

[7] Z. Glumac and K. Uzelac, J. Phys. A **22**, 4439 (1989).

[8] J. L. Monroe, R. Lucente, and J. P. Hourlland, J. Phys. A **23**, 2555 (1990).

[9] Z. Glumac and K. Uzelac, J. Phys. A **26**, 5267 (1993).

[10] S. A. Cannas and A. C. N. de Magalhães, J. Phys. A **30**, 3345 (1997).

[11] E. Luijten and H. W. J. Blöte, Int. J. Mod. Phys. C **6**, 359 (1995).

[12] U. Wolff, Phys. Rev. Lett. **62**, 361 (1989).

[13] E. Luijten and H. W. J. Blöte, Phys. Rev. B **56**, 8945 (1997).

[14] E. Luijten and H. W. J. Blöte, Phys. Rev. Lett. **76**, 1557 (1996).

[15] E. Luijten, Phys. Rev. E **60**, 7558 (1999).

[16] M. Kretch and E. Luijten, Phys. Rev. E **61**, 2058 (2000).

[17] R. H. Swendsen and J.-S. Wang, Phys. Rev. Lett. **58**, 86 (1987).

[18] D. Stauffer, Phys. Rep. **54**, 1 (1979).

[19] P. W. Kasteleyn and C. M. Fortuin, J. Phys. Soc. Jpn. Suppl. **26**, 11 (1969); C. M. Fortuin and P. W. Kasteleyn, Physica (Amsterdam) **57**, 536 (1972).

[20] A. Coniglio and W. Klein, J. Phys. A **13**, 2775 (1980).

[21] M. D'Onorio Meo, D. W. Heermann, and K. Binder, J. Stat. Phys. **60**, 585 (1990).

[22] J. Machta, Y. S. Choi, A. Lucke, T. Schweizer, and L. M. Chayes, Phys. Rev. Lett. **75**, 2492 (1995); Phys. Rev. E **54**, 1332 (1996).

[23] M. Z. Bazant, Phys. Rev. E **62**, 1660 (2000).

[24] K. Binder, Phys. Rev. Lett. **47**, 693 (1981).

[25] A. Margolina and H. J. Herrmann, Phys. Lett. **104A**, 295 (1984).

[26] J. L. Monroe, J. Phys. A **32**, 7083 (1999).

[27] M. E. Fisher and M. N. Barber, Phys. Rev. Lett. **28**, 1516 (1972).

[28] Z. Glumac and K. Uzelac, Phys. Rev. E **58**, 4372 (1998).

[29] K. Uzelac and Z. Glumac (unpublished).