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Finite-Size Scaling for First-Order Transitions: Potts Model

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The finite-size scaling algorithm based on bulk and surface renormalization of de Oliveira is tested on q-state Potts models in dimensions $D=2$ and 3. Our Monte Carlo data clearly distinguish between first- and second-order phase transitions. Continuous-q analytic calculations performed for small lattices show a clear tendency of the magnetic exponent $\mathscr{Y} = D - \beta/\nu$ to reach a plateau for increasing values of q, which is consistent with the first-order transition value $\mathscr{Y} = D$. Monte Carlo data confirm this trend.

KEY WORDS: Potts model; renormalization; surface effects.

1. INTRODUCTION

A new type of renormalization or finite-size scaling algorithm was proposed some time ago[1] and tested on a variety of models.[2] For spin-1/2 Ising models, it is based on a majority rule for either all spins of the system or the spins on two opposite-surfaces of the finite system under consideration. Basically, the surface criterion tests whether the two opposite surfaces have predominantly the same magnetization or are mostly uncorrelated. In this way one finds out whether the system is in a single-domain state or is divided into many domains with different signs of the magnetization.

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In the q-state Potts model[3] each spin can be in one of q different states, $q=2$ corresponding to the usual Ising model. Accordingly, we now check, for the two opposite surfaces of the lattice, which spin state dominates one surface and which the other one. If both surfaces are dominated by the same state, a counter is increased by 1; if they are dominated by two different states, this counter is decreased by $1/(q-1)$. If there is no correlation between the two surfaces, the average value of this counter thus stays at zero, whereas for well-correlated surfaces due to long-range ferromagnetic order, the counter is increased by one unit each time it is measured. At the end, we normalize the counter by the number of measurements, denoting the result by $\mathscr{T}$; in the thermodynamic limit, $\mathscr{T}$ is unity for well-correlated surfaces (temperature $T<T_c$) and zero for uncorrelated ones ($T>T_c$), i.e., a step function of $T-T_c$. We start with a random distribution of spins, wait until equilibrium has been established at the given temperature $T>T_c$, then decrease the temperature slightly for a new equilibrium situation, and so-on until $T<T_c$ is reached.

In this form this criterion holds for second-order transitions where the correlation length diverges. At a first-order transition, however, the correlation length remains finite, and thus a multidomain state is possible also below the phase transition temperature, if all coexisting states have the same energy. This is the case for the q-state Potts model in two dimensions if q is larger than 4, and in three dimensions if q is at least 3. We thus expect in a simulation below the transition temperature that for a second-order transition the normalized counter is close to one for all samples, whereas for a first-order transition it is close to zero in some samples and close to one in others, for lattice sizes not larger than the correlation length.

The complications inherent to the first-order transition can be avoided if, instead of cooling down slowly from a random initial configuration, we heat up slowly an initially ordered configuration where all spins are the same. Then, below the transition temperature the normalized counter should stay near unity, and should jump to zero if we heat above the transition temperature.

We have written a C-language program which stores eight lattices in 32-bit words, allowing $0<q<16$. We ran it on PC's for testing in two dimensions, and on IBM Powerstations for runs with up to 658×658 and $106\times106\times106$ spins. Sites were updated regularly; for each Monte Carlo updating a new direction for the spin was selected randomly and accepted with the usual thermal probability of the Metropolis technique. As we adopted periodic boundary conditions, the above-mentioned two opposing surfaces of an $L\times L\times L$ cubic lattice correspond to two parallel planes $L/2$ lattice parameters apart from each other. In order to improve the statistics,

after each whole lattice sweep (WLS), we average correlations between planes i and $i+L/2$ for $i=1, 2,..., L/2$ along all three directions, corresponding to a total of $3L/2$ distinct averaged values.

2. QUALITATIVE RESULTS

In three dimensions, our data qualitatively confirm our two-dimensional conclusions to be presented in the next paragraph: for $q=2$ (Ising model), the transition was found near $J=0.22$ (in units of $k_B T$), and for $q=4$ near $J=0.15$. In the Ising case, at low temperatures the normalized counter was unity in all eight simulated lattices. The same applied for $q=4$ only if we started with an ordered phase and low temperatures and heated the system up. If instead we cooled down an initially random configuration, then some lattices had the normalized counter at or near unity, and the others near zero.

In two dimensions, Fig. 1 shows this behavior for $q=5$ on an $L\times L$ lattice with $L=32$: we simulated 16 samples, starting from 16 distinct random spin configurations at high temperatures (low values of the coupling constant J in the plot). After 1000 transient and 10,000 averaging WLSs for each fixed temperature, we decrease T by a small finite amount and perform another set of $1000+10,000$ WLSs. Below the critical point, we observe that 10 among these 16 samples have become ordered, and the average value of the counter is $\mathscr{T}=1$ for them. The other 6 samples remain disordered, the averaged value of the counter being $\mathscr{T}\sim 0$ for them. Taking separate averages for these two sets of samples, we get the two curves shown in Fig. 1. They collapse onto each other near the known transition temperature corresponding to $J_c=0.234872$, both staying at zero for higher temperatures (disordered phase). We have not observed any metastability effect for both first- and second-order transitions. For instance, we have observed no trace of hysteresis by heating or cooling (in this case choosing only ordered low-temperature samples) the same system.

As explained above, the behavior observed in Fig. 1 is expected for first-order transitions. Nevertheless, it is dangerous to adopt this criterion in order to determine whether a given phase transition is first or second order. For instance, we get the same qualitative behavior for $q=3$ and 4 in two dimensions, for which the transition is known to be continuous, by using the same parameters. In the latter case, this is only a transient-time and finite-size effect, and one can get all samples ordered at low temperatures simply by taking longer transient times and larger lattice sizes. However, the computer power actually needed to draw such a distinction may become prohibitively high. Thus, our criterion to determine the character (continuous or first-order) for a given phase transition is another

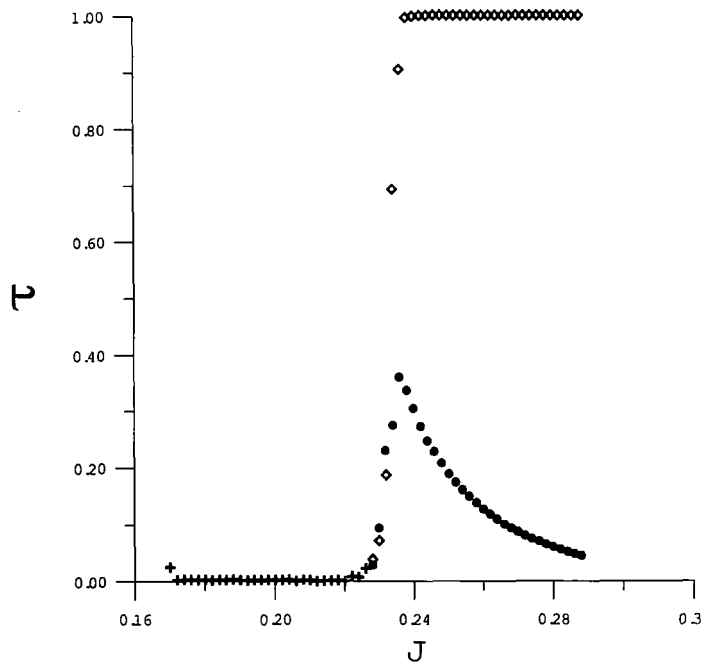

Fig. 1. Surface correlation $\mathcal{T}$ versus coupling constant J for 32×32 lattice and $q = 5$. Simulations start from 16 distinct random spin configurations (samples) at a temperature well above the critical point (at left on the J axis). Diamonds correspond to the average over 10 samples which showed $\mathcal{T} = 1$ below the critical temperature, while bullets correspond to the remaining 6 samples which present $\mathcal{T} \sim 0$. For these, the observed peak comes from the large value (although finite) of the correlation length near the transition point. Both curves collapse near and above the critical temperature (crosses).

quantitative one, based on the magnetic critical exponent $\mathcal{Y}$ to be explained below.

3. THE METHOD

The surface correlation function $\mathcal{T}$ has already been defined. The bulk quantity $\mathcal{Q}$ is defined as the average of another counter, as follows. First, one must adopt a privileged state among the q possible spin orientations (this corresponds simply to choosing a particular orientation of an external magnetic field). For a given lattice spin configuration we determine whether the majority of spins are in this privileged state (setting the counter equal to 1) or in any other state [setting the counter equal to $-1/(q-1)$ instead]. We define $\mathcal{Q}$ as the average of this counter. For $q = 2$,

this corresponds to taking the average of the sign of the sum of the Ising spins ± 1, according to the original definition.[1,2]

Our method is based on these two thermodynamic quantities $\mathscr{T}$ and $\mathscr{Q}$ which are shown[1,2] to scale as L^0 at the critical temperature and in the thermodynamic limit, where L is the linear size of the system. So, they behave like Binder's fourth-order cumulant[4] or the Nightingale ratio (correlation length over strip width),[5] or yet the Ziff percolation spanning probability,[6] being step functions of the temperature T, in the thermodynamic limit. Concerning the phenomenological RG,[5] it has been shown[7] to be a particular case of our method if one computes $\mathscr{T}$ using lattices with the same strip geometry. However, these functions $\mathscr{T}$ and Q have the further advantage of also describing correctly the critical behavior around $T=0$ and $T\to\infty$, including the effects of an external magnetic field H as well. For instance, according to the definition of Q, one can obtain exactly the low-temperature scaling behavior $H\sim l^D$ for ferromagnets, the first-order character signature of the reversing field transition below the

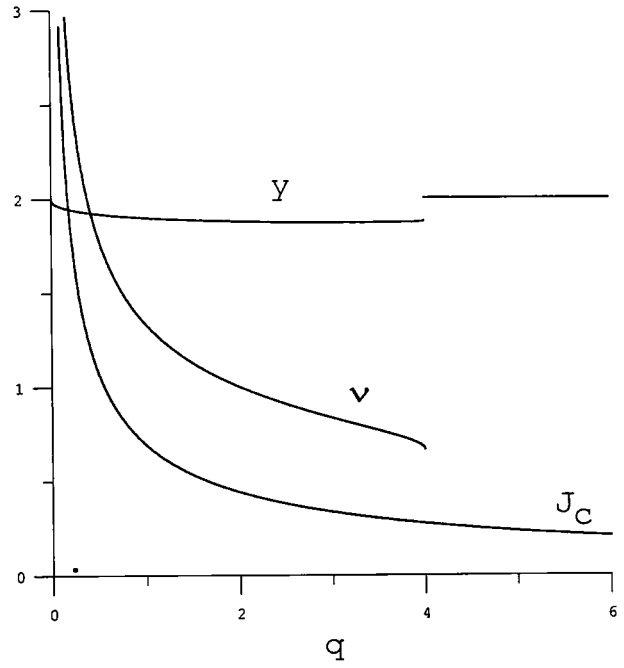

Fig. 2. Exactly known values of the critical coupling J_c and thermal and magnetic exponents ν and $\mathscr{Y}$ as functions of q, for the two-dimensional Potts model. For $q>4$, one gets $\mathscr{Y}=D=2$ according to the first-order character of the transition.

critical temperature, where l is the RG length scaling factor. Also, one obtains $H \sim l^{D/2}$ at high temperatures, the signature of the lack of long-range order above the critical temperature. On the other hand, in zero field, the function $\mathscr{T}$ gives the correct scaling behavior $J \sim l^{D-1}$ at low temperatures. The function $\mathscr{Q}$ is based on a bulk measure of the majority of spins, whereas $\mathscr{T}$ measures the correlation between two opposite surfaces of the system.

The magnetic exponent $\mathscr{Y}$ is obtained through the finite-size scaling relation $M \sim L^{\mathscr{Y}}$, valid at the critical temperature, where M is the bulk magnetization. For the Ising model, M is simply the average of the absolute value of the sum of all spins.[1,2] For general q on a finite lattice with N spins, one must first determine the state of the majority of the spins for the current configuration and count the number m of these majority spins. Then, the value of M will be the average of $m-(N-m)/(q-1)$.

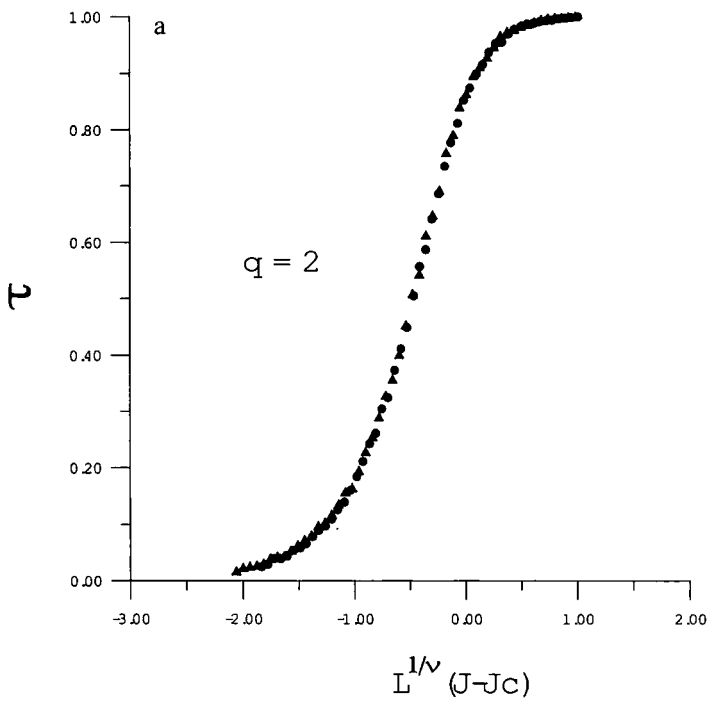

Fig. 3. Data collapsing plots of $\mathscr{T}$ versus $L^{1/\nu}(J-J_c)$, taken for (a) $q=2$ and (b) $q=6$ on two-dimensional lattices of linear sizes $L=26$ (triangles) and 34 (circles). The error bars are smaller than the symbols.

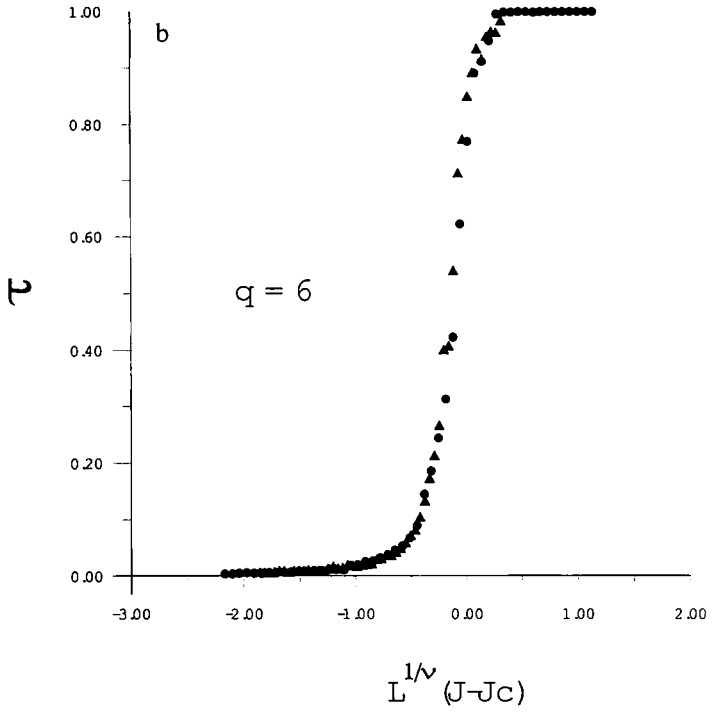

Fig. 3 (*continued*)

For a first-order transition, this quantity M clearly scales as L^D, where D is the geometrical dimension of the system. Thus, one can extend the definition of the magnetic critical exponent $\mathscr{Y}$ even to first-order transitions. On the other hand, the thermal critical exponent ν which governs the divergence of the correlation length cannot be defined in those cases. Figure 2 shows the q-dependence of the critical coupling J_c and the exponents $\mathscr{Y}$ and ν, known for the two-dimensional Potts model.[3] We performed continuous-q analytic calculations, for small lattices, which showed a clear tendency of the magnetic exponent $\mathscr{Y}$ to reach a plateau for increasing values of q, mimicking the correct behavior of Fig. 2, but without the jump at $q=4$. These preliminary results motivated us to simulate larger lattices.

The critical coupling J_c and the thermal exponent ν can be obtained by plotting the function $\mathscr{T}$ against $L^{1/\nu}(J-J_c)$ for different linear lattice sizes L in zero field. The parameters J_c and ν must be adjusted in order to collapse all data onto the same curve. The result is shown for the two-

dimensional Ising model in Fig. 3a. One can note the good accuracy obtained with a small computational effort. Values obtained for larger lattices also collapse onto this same curve, but we decided to plot only data corresponding to the two smallest lattice sizes simulated, in order to show that one has no need of much computer power. We have chosen the correct known value $\nu = 1$ and adjusted $J_c = 0.4407$, also coincident with the correct known value. Any deviation on the fourth decimal clearly gives a poorer collapse. Similar accuracy is also obtained for $q = 3$, 4, 5, and 6 in two dimensions, with the same modest computational effort. In the cases of $q = 5$ and 6, the curves present an almost vertical jump near the transition point, and one can extract J_c without resorting to data collapsing. Nevertheless, we obtain also a good collapse for these cases where the thermal exponent is not defined, adopting the value $\nu = 2/3$ corresponding to $q = 4$ (the collapse is not much sensitive to this artificial value). The case for $q = 6$ is shown in Fig. 3b.

The magnetic exponent $\mathscr{Y}$ is obtained by further simulations at J_c, measuring the value of M for different linear lattice sizes L. Figure 4 shows the results for $q = 5$ in two dimensions. The straight line confirms the expected scaling relation $M \sim L^{\mathscr{Y}}$, with $\mathscr{Y} = 1.997$ in this case, corresponding to an error less than 0.2% relative to the first-order value $\mathscr{Y} = D = 2$. For $q = 6$, we obtained $\mathscr{Y} = 2.010$. Two-dimensional Potts model simulations are normally used as tests for methods conceived to determine whether a given transition is first or second order, and we are aware of this kind of work (see, for instance, ref. 8) for at least $q = 7$ and upward where the first-order character is already well defined. The good results we obtained for $q = 5$ and 6 give confidence in the present method. Another very good test is the three-dimensional Potts model for $q = 3$, known to suffer a weak first-order transition, staying very near the borderline from second order. From our simulations we get $\mathscr{Y} = 2.97$, with a similar modest computational effort to that employed in two dimensions.

The second-order transitions for $q = 2$, 3, and 4 in two dimensions seem to need more computational effort in order to yield the same degree of accuracy in determining $\mathscr{Y}$. We get $\mathscr{Y} = 1.86$ for $q = 2$ (statistical errors are always in the last displayed digit), to be compared with the known value $\mathscr{Y} = 1.875$. For $q = 3$, our value $\mathscr{Y} = 1.93$ must be compared with $\mathscr{Y} = 1.867$. Even with this poorer accuracy, our data are safe enough to guarantee that $\mathscr{Y} < D$ in both cases, confirming the continuous character of these transitions. For the borderline case $q = 4$, we get $\mathscr{Y} = 1.997$, to be compared with $\mathscr{Y} = 1.875$. The $q = 4$ case is indeed problematic, not only for the present method, but for all other numerical methods, because it is known to present very strong logarithmic corrections to the simple scaling power laws. Moreover, in Fig. 2 one can note the gap between $\mathscr{Y} = 1.875$

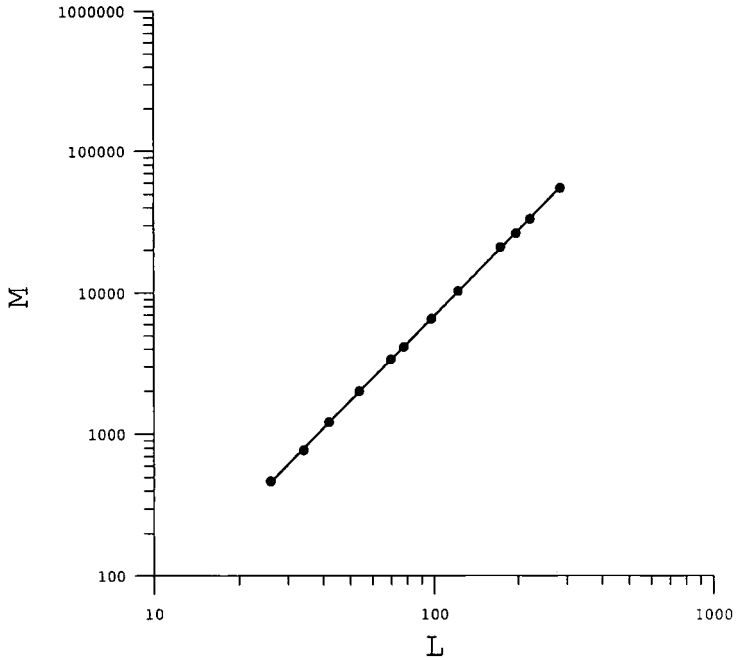

Fig. 4. Plot of the bulk magnetization M versus linear lattice size L, measured at the critical temperature, for $q=5$ in two dimensions. The slope of the straight line is the magnetic exponent $\mathscr{Y}$.

and $\mathscr{Y}=2$ occurring just at this borderline $q=4$. Our result for $q=4$ reproduces very well the correct one for $q=4+\varepsilon$.[9]

In conclusion, the algorithm of ref. 1 seems to work also for first-order transitions, being very accurate also in these cases.

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