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LETTER TO THE EDITOR

Resolving the order of phase transitions in Monte Carlo simulations

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Abstract. We made a Monte Carlo simulation of the two-dimensional Potts model with $q=3$, 4 and 5 to examine the question whether numerical methods can distinguish the order of a phase transition for the subtle cases that this model exemplifies. We found that the finite-size scaling test for susceptibilities has sufficient power for this purpose, whereas the simple method of detecting metastability signals often fails.

Determination of the order of phase transitions presents the first basic step in the analysis of statistical systems. There are only a few cases where this problem can be solved analytically, and for most physically interesting systems one has to rely on numerical simulation techniques to determine the order. This method, though quite powerful [1], has an inherent limitation of a finite lattice size and finite statistics, determined by computing resources available. This sometimes leads to a controversy on the order. A recent instance is the deconfining phase transition of the pure SU(3) gauge theory [2]. Fortunately, this system has a first-order transition strong enough so that a relatively small effort was sufficient to elucidate its nature [3]. In general problems arise when a first-order transition is so weak that the correlation length at the transition point is large, exceeding the dimension of the system practically feasible in the simulation. Also a subtle situation is encountered for a system close to a multicritical point [4, 5]. There is then a general practical problem of what quantities best serve as indicators for the order of a phase transition, and to what extent the method conventionally used leads to a decisive answer on the order in Monte Carlo simulations.

In this letter we consider this problem, taking as an example the q-state Potts model in two dimensions defined by

$$Z=\sum \exp\left(\beta \sum_{\langle ij\rangle} \delta_{s_i s_j}\right) \tag{1}$$

with s_i taking q possible values¶. We choose the model because it provides one of the most subtle cases so far known, and yet the nature of its phase transition is well understood; the system has a second-order transition for the number of spin states

¶ A Monte Carlo simulation of this model was previously made by Binder [6]. This work, however, did not actively examine the points addressed here.

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$q \leq 4$ [7] with the critical indices explicitly known [8, 9]. The transition for $q > 4$ is first order [7], but close to $q = 4$ the correlation length at the transition point is quite large, e.g. O(100) for the $q = 5$ model [10]. (For reviews, see Wu [11] and Barber [12].)

The most popularly used indicator for a first-order phase transition in Monte Carlo simulations is a metastability signal between the low and high temperature states and the associated double peak structure of observable histograms; our belief is that the histogram should be singly peaked for a second-order transition. However, it has been reported [5] that the $q = 4$ model with a second-order transition exhibits a doubly peaked histogram in the energy and an order parameter. A similar result has been known for a tricritical $q = 2$ model [4].

In order to examine whether this is a real effect, and not due to insufficient statistics, we have studied the $q = 3$, 4 and 5 Potts models on a $L \times L$ square lattice making two million sweeps per β by the standard heat-bath algorithm for $L = 32$, 64, and 128 and ten million sweeps for $L = 196$ and 256 with the periodic boundary condition. Two definitions of the order parameter were used:

$$\Phi_1 = \max\{p_n | n = 1, \ldots, q\} \tag{2}$$

$$\Phi_2 = \left(\sum_{n=1}^{q} p_n^2 - \frac{2}{q-1} \sum_{n>m} p_n p_m \right)^{1/2} \tag{3}$$

with

$$p_n = \frac{1}{L^2} \sum_{i=1}^{L^2} \delta_{n,s_i} \tag{4}$$

the number of spins in the nth state. The first is the maximum population definition usually used in the literature. The second represents a generalisation of $|p_1 - p_2|$ for the Ising case ($q = 2$), taking values between 0 (completely disordered) and 1 (completely ordered).

In figure 1 we show the histogram for $L = 256$ for the order parameter Φ_1 (the results for Φ_2 are similar) and the energy E per bond close to β_c. A clear double peak is seen in both quantities for $q = 5$ as expected for the first-order transition of the

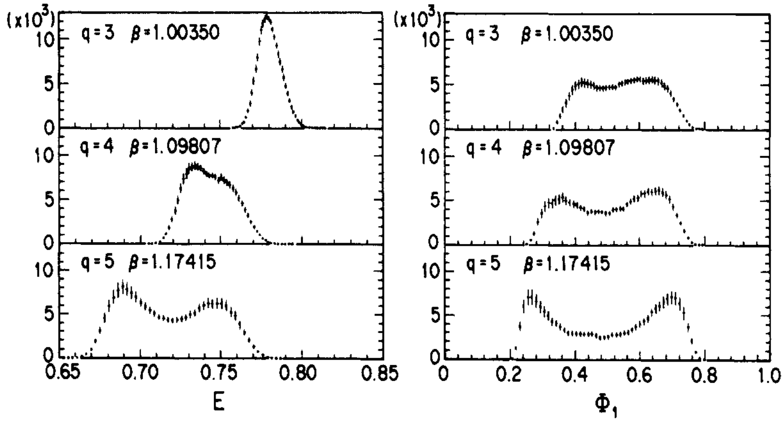

Figure 1. Histograms of the energy E and the susceptibility Φ_1 for $L = 256$ constructed with the aid of the spectral density method from simulations made at $\beta = 1.0042$ for $q = 3$, $\beta = 1.09825$ for $q = 4$ and $\beta = 1.1741$ for $q = 5$.

system. We did not detect any signal for the spurious states as reported by Katznelson and Lauwers [13] with our statistics 30 times that of their longest run. A double peak, though less pronounced, is also clearly observed in Φ_1 for the $q=4$ model, as reported in [5], while that in E is less clear. It is our suprise to find in Φ_1 a wide plateau, suggestive of a double peak with a shallow valley, even for $q=3$, not so close to the critical value $q=4$. We found that these structures for $q=3$ and 4 change little with the lattice size. The time history of Φ_1 fluctuates irregularly. Nevertheless, it is not impossible to take the fluctuating pattern as evidence for metastability. With only these data one might mistakenly conclude a first-order transition.

The double peak for $q=4$ and 3 is expected to merge into a single peak as $L\rightarrow\infty$. Our runs show, however, that the approach is very slow, and observing a single peak does not seem feasible in practice. These examples warn that determining the order of phase transition from a double peak structure in the histogram could sometimes be rather subtle.

We then studied whether the finite-size scaling analysis [12, 14] can disentangle this subtle situation. We examined the behaviour of the susceptibilities,

$$\chi_i = L^2(\langle\Phi_i^2\rangle - \langle\Phi_i\rangle^2) \qquad i=1,2 \tag{5}$$

drawing curves for χ_i as a continuous function of β with the spectral density method [15, 16]. The height $\chi_{1,\max}$ of the peak of the susceptibility χ_1 is plotted in figure 2 as a function of L^2, and full curves represent the finite-size scaling prediction $\chi_{\max}\propto L^{\gamma/\nu}$ with $\gamma/\nu=26/15$ ($q=3$), $7/4$ ($q=4$) [7] and $\chi_{\max}\propto L^2$ ($q=5$) (see below for the $q=4$ case for more detail). In order to check the agreement more closely, we fitted $\chi_{i,\max}$ with a power form

$$\chi_{i,\max} = A_i L^{p_i} \qquad i=1,2. \tag{6}$$

The resulting index p_i using the lattice sizes $L=32-256$ is tabulated in table 1 together with the chi-square (χ^2) of the fit obtained by the jack-knife error as input. The result $p_1=1.742(11)$ and $p_2=1.744(11)$ for $q=3$ are quite close to the exact value $p=\gamma/\nu$ which takes $26/15=1.733$. For $q=5$, the fitted powers $p_1=1.893(10)$, $p_2=1.915(10)$ are a little smaller than the first-order index $p=2$. They, however, are constrained

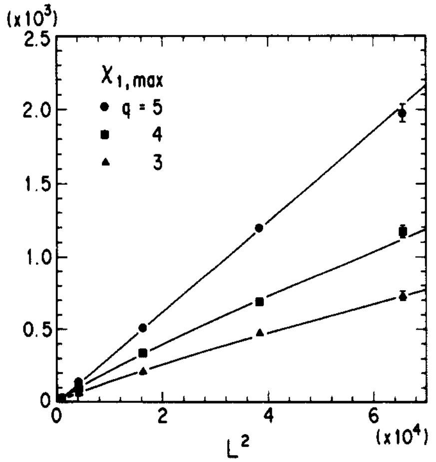

Figure 2. Peak height of the susceptibility χ_1 as a function of the volume L^2. Curves shown are the prediction with the finite-size scaling formula with the exactly known indices.

Table 1. Power indices of the height of the peak in susceptibilities.

q	p_1	χ^2	p_2	χ^2	p_{exact}
3	1.742 (11)	3.2	1.744 (11)	4.3	26/15 = 1.733
4	1.775 (10)	5.9	1.789 (10)	6.6	7/4 = 1.75
5	1.893 (10)	1.4	1.915 (10)	1.1	2

particularly by the small size data of $L = 32$ and 64, and slowly increase with the size; e.g. $p_1 = 1.88(2)$ for $L = 32-128$ and 1.95(7) for $L = 128-256$. This slow variation may be ascribed to the large correlation length of O(100) at the transition point for $q = 5$ [10]. This analysis allows us to conclude that the phase transition of the Potts model with $q = 3$ is definitely second order, and that for $q = 5$ is consistent with first order within our lattice size and statistics.

For the critical case $q = 4$ the indices from the pure power fit (6) ($p_1 = 1.775(10)$, $p_2 = 1.789(10)$) are slightly smaller than the exact value 7/4. For this case with a marginal operator we expect logarithmic corrections in the finite-size scaling formula [17]. Following the treatment of [17], we can easily derive the susceptibility scaling as

$$\chi \sim L^{7/4}(a + b \log L)^{-1/8}. \tag{7}$$

We attempted to fit the data with this form. We could not confirm the logarithmic correction with a small power, however, as the constant a dominates over the log L term for our lattice size.

We conclude that the finite-size scaling analysis of the susceptibility is capable of distinguishing between a first- and a second-order transition even for the most subtle case examined here, where a simple method of detecting metastability fails.

We have also made an analysis for the specific heat $C = \partial E/\partial \beta$ (see figure 3). Assuming

$$C_{\max} = AL^r + B \tag{8}$$

for the height of the specific-heat peak, we obtained $r = 0.44(7)$ for $q = 3$ using $L = 32-256$ (exact solution predicts it to be 2/5). For $q = 4$ this simple form underestimates

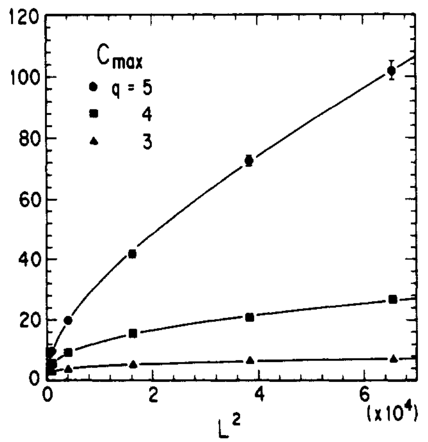

Figure 3. Peak height of the specific heat as a function of the volume L^2. Curves are obtained with the fitting functions discussed in the text.

the index ($r=0.75(5)$ for $L=32-256$ as compared with the exact value $r=1$; for discussion on this point, see [12] and references therein). The logarithmic correction, however, is quite significant here and the theoretical prediction $C_{\max}\sim L(A+B\log L)^{-3/2}$ [17] indeed fits the data well ($\chi^2=3.3$). With (8) the first-order index ($r=2$) is not obtained for $q=5$ (we find $r=1.2(4)$). However an excellent fit is achieved ($\chi^2=1.1$), if the form suggested by Ferrenberg and Swendsen [16]

$$C_{\max}(L)=\alpha L^2+B+C\exp(-L/L_0) \tag{9}$$

is adopted with $\alpha=\Delta E^2$ and the latent heat ΔE fixed to the theoretical value 0.0265 [7], as shown in figure 3. The parameter L_0 turns out to be large, ~500. This may not be unreasonable since the correlation length is O(100) at $\beta=\beta_c$. Therefore, we can conclude that our data for the specific heat also nicely agree with the expected behaviour for all cases. On the other hand, the need for terms additional to the pure power in L diminishes the merit of using $C_{\max}$ for the order determination when we do not know the nature of the finite-size behaviour *a priori.*

Finally we studied the reduced cumulant proposed by Challa, Landau and Binder (CLB) [18] as an indicator of the order of phase transitions

$$V_L=1-\frac{\langle E^4\rangle}{3\langle E^2\rangle^2}. \tag{10}$$

Figure 4 shows the minimum value of this quantity $V_{L,\min}$ as a function of L^{-2}. We observe that $V_{L,\min}$ for $q=3$ and 4 converges to 2/3 within statistical accuracy as L increases. On the other hand, $V_{L,\min}$ for $q=5$ does not seem to approach 2/3. It is interesting to remember that the distribution of energy for the $q=4$ case exhibits a double-peak like structure even at the largest lattice that we worked with (see figure 1). This indicates the effectiveness of the CLB indicator even for this marginal case.

In this letter we have seen that the conventionally adopted indicator of detecting metastability signals for a first-order transition may fail for some cases, and particular care is necessary when the separation of two states is not clear. We have demonstrated

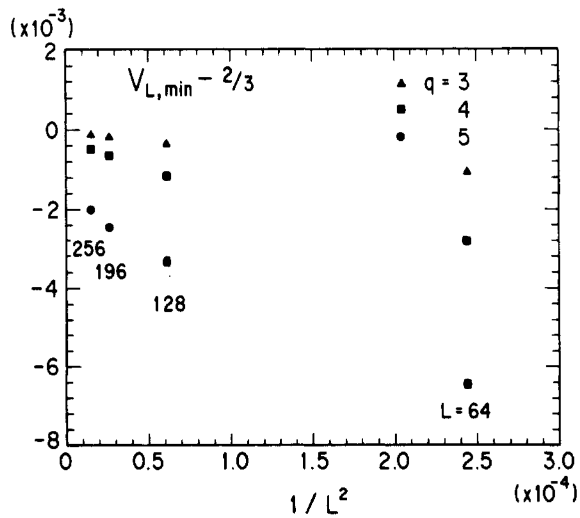

Figure 4. The minimum of the CLB cumulant (a constant 2/3 subtracted) as a function of L^{-2}.

that the finite-size scaling test reveals its power even for the most subtle cases. In our example, we could conclude solely from numerical simulations that the $q = 4$ Potts model has a second-order transition and the $q = 5$ model has a first-order transition.

References

[1] Binder K 1984 *Application of the Monte Carlo Method in Statistical Physics* (Berlin: Springer)
[2] Brown F R *et al* 1988 *Phys. Rev. Lett.* **61** 2058
Bacilieri P *et al* 1988 *Phys. Rev. Lett.* **61** 1545
[3] Fukugita M, Okawa M and Ukawa A 1989 *Phys. Rev. Lett.* **63** 1768; 1990 *Nucl. Phys.* B in press
[4] Landau D P and Swendsen R H 1981 *Phys. Rev. Lett.* **46** 1437
[5] McCarthy J F 1989 *Preprint* IUHET164 Indiana University
[6] Binder K 1981 *J. Stat. Phys.* **24** 69
[7] Baxter R J 1973 *J. Phys. C: Solid State Phys.* **6** L445
[8] den Nijs M P M 1979 *J. Phys. A: Math. Gen.* **12** 1857
Nienhuis B, Riedel E K and Schick M 1980 *J. Phys. A: Math. Gen.* **13** L189
Pearson R B 1980 *Phys. Rev.* B **22** 2579
[9] Blöte H W J and Nightingale M P 1982 *Physica* **112A** 405
[10] Hamer C J 1981 *J. Phys. A: Math. Gen.* **14** 2981
[11] Wu F Y 1982 *Rev. Mod. Phys.* **54** 235
[12] Barber M N 1983 *Phase Transitions and Critical Phenomena* vol 8, ed C Domb and J L Lebowitz (New York: Academic)
[13] Katznelson E and Lauwers P G 1987 *Phys. Lett.* **186B** 385
[14] Fisher M E 1971 Critical Phenomena *Proc. 51st Enrico Fermi Summer School, Varenna* (New York: Academic)
[15] McDonald I R and Singer K 1967 *Discuss. Faraday Soc.* **43** 40
[16] Ferrenberg A M and Swendsen R 1988 *Phys. Rev. Lett.* **61** 2635
[17] Nauenberg M and Scalapino D J 1980 *Phys. Rev. Lett.* **44** 837
Cardy J L, Nauenberg M and Scalapino D J 1980 *Phys. Rev.* B **22** 2560
[18] Challa M S S, Landau D P and Binder K 1986 *Phys. Rev.* **34** 1841