OBSERVATION OF FSS FOR A FIRST ORDER PHASE TRANSITION

A. Billoire
Service de Physique Théorique de Saclay*
91191 Gif-sur-Yvette Cedex, France
T. Neuhaus
Universität Bielefeld
Fakultät für Physik, Universität Bielefeld,
D-W 4800 Bielefeld, FRG
and B. Berg
Wissenschaftskolleg zu Berlin†
Wallotstr. 19, D-1000 Berlin 33, FRG

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We present the results of a multicanonical simulation of the $q=20$ 2-
d Potts model in the transition region. This is a very strong first order
phase transition. We observe, for the first time, the asymptotic finite size
scaling behavior predicted by Borgs and Kotecký close to a first order phase
transition point.

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*Laboratoire de la Direction des Sciences de la Matière du CEA.
†On sabbatical from the Florida State University.
1 INTRODUCTION

This paper addresses the question of lattice sizes needed in practical applications in order to fulfil the asymptotic scaling behaviour predicted by Borgs and Kotecký [1, 2], close to a first order phase transition point.

• Very strong first order transitions are easy to detect. The system behavior is very close to the infinite volume behavior. Ergodicity is broken. Thermodynamical quantities are discontinuous at the transition point, with metastable branches. A starting configuration half ordered, half disordered will relax to very different states on both sides of the transition.

• In less clear cases, one must simulate systems of increasing volumes $L^d$ and try to convince oneself that the above described very large volume behavior is approached. Let us use the language of energy driven transitions in what follows, and introduce the energy probability distribution $P_L(E)$. In the transition region, it has two peaks of heights $P^o_L$ (ordered phase) and $P^d_L$ (disordered phase), separated by a minimum of height $P^\text{min}_L$. For a first order transition, at fixed $P^o_L/P^d_L$, $P^\text{min}_L/P^o_L$ decreases as $L$ grows. This has been proposed by Lee and Kosterlitz [3] as an indicator of first order phase transitions (for a microcanical version see [4, 5]). One can also plainly look at a plot of $P_L(E)$ and decide “by eye” whether it looks more and more like two delta functions as $L$ grows. Another class of indicators are moments of the distribution $P_L(E)$, that go to zero in the large volume limit, for all temperatures, but at a first order transition point. An example is the energy fluctuation $CV/L^d = \beta^2(<E^2>-<E>^2)$, another is Binder’s cumulant $BL = \frac{1}{\beta}(1-<E^4>/<E^2>^2)$.

• The most sophisticated (and trustworthy) method is finite size scaling. One insists in seeing the finite size behavior as predicted by the theory in the vicinity of a first order phase transition. In that case only one can be pretty sure that the trend observed for lattices of increasing size does continue up to the thermodynamical limit. One insists on seeing

$$\frac{1}{L^d} \ln \frac{P^\text{min}_L(L)}{P^o_L(L)} \sim A/L$$

$$CV^\text{max}_L/L^d \sim CV^{(1)} + CV^{(2)}/L^d$$

$$BL^\text{min}_L \sim BL^{(1)} + BL^{(2)}/L^d$$
where $CV_{\text{max}}$ is the maximum of the specific heat, and $BL_{\text{min}}$ is the minimum of $BL$.

The above described large volume behavior has never really been observed in a numerical simulation. The results of all high precision simulations show strong curvatures in e.g. the curve representing $BL_{\text{min}}$ as a function of $1/L^d$. This is the case of the 3-d $Z(3)$ Potts model with antiferromagnetic admixture on lattices up to $48^3$. This is also the case of the 5 states 2-d Potts model on lattices up to $256^2$. In the later case, the exact asymptotic limit is $BL_{\text{min}} \sim -0.44 \ 10^{-3}$ whereas the data presented would suggest a much lower value ($\sim -1.2 \ 10^{-3}$). This shows that the $BL_{\text{min}}$ indicator is not a trustworthy indicator of first order phase transitions on lattices up to $256^2$ when the correlation length is equal to a few thousands lattice spacings.

Results of a simulation of the $q = 10$ 2-d Potts model on lattices as large as $50^2$ can be found in Ref. [8]. This is a model with a strong, obvious, first order transition, with an exactly known [9] correlation length $\xi(\beta - t) = 10^{.56}$. The results for the extrema of $CV/L^d$, $BL$ and $U_4$

\[
U_4 = \frac{\langle (E - <E>)^4 \rangle}{\langle (E - <E>)^2 \rangle^2}
\]  

(4)

and for the value $CV(\beta_t)/L^d$ are compared with the large volume predictions, namely the extrema behave like $X^{(1)} + X^{(2)}/L^d + \mathcal{O}(1/L^{2d})$, and $CV(\beta_t)/L^d$ behaves like $X^{(1)} + X^{(2)}/L^d + \mathcal{O}(e^{-bL})$ for some $b > 0$. The four different constants $\{X^{(1)}\}$ are exactly known. One single unknown parameter, e.g. the ordered specific heat at the transition point $C_o$, determines the four $X^{(2)}$'s. The precision of the data is very good, and in all cases strong deviations from the $X^{(1)} + X^{(2)}/L^d$ limiting behavior are seen. These corrections do not seem to behave simply as function of $L$, and are definitely not under control. Not surprisingly, the values for the four slopes $\{X^{(2)}\}$ one would infer from the data give inconsistent estimates of $C_o$. Furthermore, the data do not substantiate the prediction that $CV(\beta_t)$ is asymptotic earlier than $CV_{\text{max}}$.

\footnote{The correlation length of the 2-d Potts model at the transition point can be computed exactly using the 6-vertex representation. The result is interpreted as the disordered phase correlation length in the limit $\beta \rightarrow \beta^-$. The ordered phase correlation length is smaller. Duality does not relate these two correlation lengths.}

\footnote{Due to a systematic typing error, every times a numerical value for $C_d$ is given in Ref. [8] (e.g. in Table 1), the value for the ordered phase $C_o$ is meant. In particular, the $q = 10$ curves are drawn using the estimate of $C_o = 12.7 \pm .3$, not $C_d = 12.7 \pm .3$.}
In conclusion, the FSS behavior is not observed even for a transition as strong as the 2-d $q = 10$ Potts model transition, on lattices as large as $50^2$. Three possible explanations come to the mind: i) Eqs.2,3 are only proven in the large $q$ limit, they may not hold down to $q = 10$. ii) Much larger lattices may be needed in order to extract the true asymptotic behavior, even though on the largest lattices simulated $P_L(E)$ has a textbook first order shape. iii) A programming error may be possible. We are however in the position to compare high precision results for the $q = 10$ Potts model, which were obtained in two completely independent simulations [8, 10], e.g. using different random number sequences. Results for thermodynamic quantities agree on same lattice sizes to high precision, making the existence of a programming error unlikely.

2 Exact Results

Those have been obtained [1] for models that can be represented by a contour expansion with small activities, like [2] the q states Potts model for large $q$. In such a case, the partition function for a $L^d$ lattice with periodic boundary conditions can be written as

$$Z(\beta, L) = e^{-L^d\beta f_d(\beta)} + q e^{-L^d\beta f_o(\beta)} + O(e^{-bL})e^{-\beta f(\beta)L^d}; \ b > 0 \quad (5)$$

where $f_o(\beta)$ and $f_d(\beta)$ are smooth $L$ independent functions. The free energy is $f(\beta) = \min\{f_o(\beta), f_d(\beta)\}$. The phenomenological two gaussian peak model of the energy probability distribution $P_L(E)$ introduced by Binder and Landau [11, 12] follows through inverse Laplace transform. The above exact result fixes the relative weights of the two peaks: At the infinite volume limit transition point, $\beta = \beta_t$, the ordered and disordered peak weights are exactly in the ratio $q$ to one.

To the order in $1/L^d$ which we consider, all quantities are expressed in terms of $\beta_t$ and of the energies and specific heats of the two coexisting phases. The transition temperature, $E_o$, $E_d$ and the difference $C_o - C_d$ are known exactly for the 2-d Potts models [13]. Values for the $q = 10$ and $q = 20$ cases can be found in Tab.3. It follows from Eq.5 that the specific heat

$$CV = \beta^2 L^d(<E^2> - <E>^2) \quad (6)$$
has a maximum at

$$\beta(CV_{\text{max}}) = \beta_t - \frac{\ln q}{E_d - E_o} \frac{1}{L^d} + \frac{\beta_{CV}^{(2)}}{L^{2d}} + O(1/L^{3d}). \quad (7)$$

The height of this maximum increases linearly with $L^d$

$$CV_{\text{max}} = L^d \frac{\beta_t^2}{4} (E_o - E_d)^2 + CV^{(2)} + O(1/L^d). \quad (8)$$

whereas for fixed $\beta \neq \beta_t$, $CV(\beta)$ goes to a constant, as $L$ goes to infinity. One finds that $BL$ reaches a minimum equal to \[14, \, 1, \, 15\]

$$BL_{\text{min}} = -\frac{(E_o^2 - E_d^2)^2}{12(E_oE_d)^2} + \frac{BL^{(2)}}{L^d} + O(1/L^{2d}) \quad (9)$$

at the point

$$\beta(BL_{\text{min}}) = \beta_t - \frac{\ln(q(E_o/E_d)^2)}{E_d - E_o} \frac{1}{L^d} + \frac{\beta_{BL}^{(2)}}{L^{2d}} + O(1/L^{3d}). \quad (10)$$

Expressions of the coefficients $\beta_{BL}^{(2)}$, $BL^{(2)}$, $\beta_{CV}^{(2)}$ and $CV^{(2)}$ as functions of the $E_i$’s and $C_i$’s can be found in \[13\]. $U_4$ reaches a minimum \[8\]

$$U_{4\text{min}} = 1 + \frac{8(C_o + C_d)}{L^d \beta_t^2 (E_o - E_d)^2} + O(1/L^{2d}). \quad (11)$$

at the point

$$\beta(U_{4\text{min}}) = \beta_t - \frac{\ln q}{E_d - E_o} \frac{1}{L^d} + \frac{(C_o - C_d)(\ln q - 8)}{L^{2d} 2 \beta_t^2 (E_o - E_d)^3} + O(1/L^{3d}). \quad (12)$$

The above formulae for the extrema $CV_{\text{max}}$, $BL_{\text{min}}$, $U_{4\text{min}}$ and the corresponding effective $\beta$’s have higher power law corrections that may hide the asymptotic behavior on lattices that can be simulated. In contrast, the expressions for bulk averages evaluated at the (infinite volume limit) transition point $\beta = \beta_t$ do not have power law corrections, as a consequence of Eq.\[5\], e.g. the specific heat behaves like

$$CV(\beta_t) = \frac{C_d + C_o q}{1 + q} + \frac{L^d q}{(1 + q)^2} (E_o - E_d)^2 \beta_t^2 + O(e^{-bL}) \quad (13)$$
3 Simulation of the $q=20$ model using the Multicanonical Algorithm

We have decided to simulate the $q = 20$ Potts model, as an example of a model with much stronger phase transition than the $q = 10$ model (see Tab.1). The conventional Metropolis (and Swendsen-Wang [16]) algorithm suffers from exponential slowing down close to a strong first order point, namely the probability to jump from one phase to another goes like $P_{o,d} \sim e^{-2A_{o,d}L^d-1}$, where $A^{o,d}$ is the order-disorder surface tension. This makes simulation of a $\approx 50^2$ lattice with such algorithms impossible even with vastly more powerful computers than available now.

$$\begin{array}{lccccc}
q & C_o & E_d - E_o & C_d - C_o & \xi_{\beta_c} & (C_o/(E_o - E_d)^2)^{1/d} \\
10 & 12.7 \pm .3 & 0.69605 & .44763 & 10.56 & 5.12 \pm .06 \\
20 & 5.2 \pm .2 & 1.19416 & .77139 & 2.70 & 1.91 \pm .04 \\
\end{array}$$

Table 1: The $q = 10$ and $q = 20$ 2-d Potts model: Estimated values of $C_o$, exact values for $E_d - E_o$, $C_d - C_o$, and correlation length $\xi(\beta \rightarrow \beta^-)$. A transition is strongly first order, on $L^d$ lattice when $L \gg \xi, L^d \gg C_o/(E_d - E_o)^2$

Such a simulation became possible with the invention of the “multicanonical ensemble” [10]. It amounts to perform the simulation with a weight factors designed in such a way that $P_L(E)$ is smooth between $E_o$ and $E_d$, and to “reweight” the events when computing expectation values. The multicanonical algorithm has only polynomial slowing down.

The multicanonical algorithm is only partially vectorizable. On a $38^2$ lattice, our program takes 7.7 micro-sec to update a spin on a CRAY X-MP, 27.8 micro-sec on a RS6000-550 and 35.0 micro-sec on a DEC 6000-510. We have made runs on lattices indicated in Tab.3. Most runs were performed on workstations, using the pseudo random number sequence $I_i = I_{i-147} \otimes I_{i-250}$, where $\otimes$ is the logical exclusive OR. Run #4 at $L = 24$, and run #1 at $L = 38$ were performed on a CRAY X-MP, using the congruential pseudo random number generator RANF(). Statistical analysis was performed using Jackknife technique, with first order bias correction. In many cases, we
performed several simulations for a given lattice size, using more or less optimized weights. Each run gave us results for e.g. $CV_{max}$. Those were averaged using weighted averages. In some cases, we obtained $\chi^2$ as bad as $\approx 2\ p.d.f$. We believe this would disappear with higher statistics.

Our results for $CV_{max}/L^d$, $BL_{min}$ and $U_{4_{min}}$ can be found in Figs.1, 2 and 3 together with the theoretical estimate using the value $C_o = 5.2 \pm .2$. In all cases the predicted $X^{(0)} + X^{(1)}/L^d$ behavior is approached on the largest lattices, furthermore the values of the three slopes $\{X^{(2)}\}$ one infer from our data give consistent estimates of $C_o$. This was not true in case of the $q = 10$ simulation on similar size lattices. Our results for $\beta(CV_{max})$ and $\beta(BL_{min})$ can be found in Fig.4. Perfect agreement is found with the theoretical predictions. The effect of the $1/L^{2d}$ correction is not visible, and the data for $\beta(U_{4_{min}})$ (not plotted) are not distinguishable from those for $\beta(CV_{max})$. The behavior of $CV(\beta_t)$ is shown in Fig.5. No deviation is seen from the predicted $X^{(0)} + X^{(1)}/L^d$ behavior. This agrees with the prediction that corrections are $O(e^{-bL})$.

In conclusion our data for the $q = 20$ Potts model are in excellent agreement with Finite Size Scaling predictions. In particular the data for $CV(\beta_t)$ agree with FSS for all lattices considered. This indicates that the disagreement between FSS and data for the 2-d $q = 10$ Potts model were small system effects. It means however than the asymptotic behavior predicted by Binder, and later proven by Borgs and Kotecký, only sets in for very large lattices. The lattice size must fulfil the conditions $L >> \xi$, $L^{d-1} >> 1/A^{ad}$ (If Widom’s relation \cite{widom} holds this condition is equivalent to the first one), and $L^d >> C_o/(E_o - E_d)^2$, $L^d >> C_d/(E_o - E_d)^2$, where $>>$ means five to ten times larger. It is unfortunate that for such large systems, the transition is already blatantly first order.

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[17] See e.g. D. B. Abraham in “Phase Transitions and Critical Phenomena”, Vol 10.
| $L$ | M sweeps | bins |
|-----|----------|------|
| 16  | 3.7      | 8    |
| 16  | 10.2     | 20   |
| 16  | 90.5     | 180  |
| 18  | 10.0     | 20   |
| 18  | 10.0     | 20   |
| 18  | 10.0     | 20   |
| 18  | 30.0     | 60   |
| 20  | 60.0     | 120  |
| 24  | 7.7      | 15   |
| 24  | 10.2     | 20   |
| 24  | 50.5     | 100  |
| 24  | 20.2     | 40   |
| 24  | 40.5     | 80   |
| 30  | 10.2     | 20   |
| 30  | 10.0     | 20   |
| 30  | 50.5     | 100  |
| 32  | 40.5     | 80   |
| 34  | 7.2      | 14   |
| 34  | 29.7     | 59   |
| 38  | 40.0     | 80   |
| 38  | 10.0     | 20   |
| 38  | 10.0     | 20   |

Table 2: $q = 20$ 2-d Potts model: Simulated lattices. Lattice sizes, number of mega sweeps performed and number of bins used to perform the analysis. The first bin may contain a different number of sweeps that the others. It has always been discarded for thermalization.
Table 3: $q = 20$ 2-d Potts model: Results for $CV_{\text{max}}/L^2$, $BL_{\text{min}}$, $U_{4\text{min}}$ and $CV(\beta_t)/L^2$. 

| L  | $CV_{\text{max}}/L^2$       | $BL_{\text{min}}$   | $U_{4\text{min}}$ | $CV(\beta_t)/L^2$ |
|----|----------------------------|---------------------|-------------------|-------------------|
| 16 | 1.03647 (15)               | -0.59302 (15)       | 1.07660 (6)       | 0.2066 (12)       |
| 18 | 1.03598 (17)               | -0.58489 (17)       | 1.06186 (5)       | 0.2010 (16)       |
| 20 | 1.03582 (19)               | -0.57878 (18)       | 1.05080 (5)       | 0.1988 (22)       |
| 24 | 1.03482 (10)               | -0.57013 (10)       | 1.03602 (2)       | 0.1924 (17)       |
| 30 | 1.03360 (13)               | -0.56230 (14)       | 1.02352 (2)       | 0.1952 (34)       |
| 32 | 1.03317 (22)               | -0.56058 (24)       | 1.02080 (3)       | 0.1923 (58)       |
| 34 | 1.03286 (18)               | -0.55911 (17)       | 1.01851 (4)       | 0.1837 (55)       |
| 38 | 1.03218 (12)               | -0.55653 (12)       | 1.01492 (2)       | 0.1941 (56)       |
Figure 1: \( CV_{\text{max}}/L^2 \) as a function of \( 1/L^2 \) for the 2-d q=20 Potts model. The three curves are drawn using the central value and the one standard estimates for \( C_o \).
Figure 2: $BL_{\text{min}}$ as a function of $1/L^2$ for the 2-d q=20 Potts model. The three curves are drawn using the central value and the one standard estimates for $C_o$. 
Figure 3: $U_{4\text{min}}$ as a function of $1/L^2$ for the 2-d q=20 Potts model. The three curves are drawn using the central value and the one standard estimates for $C_o$. 
Figure 4: $\beta(CV_{\text{max}})$ and $\beta(BL_{\text{min}})$ as a function of $1/L^2$ for the 2-d $q=20$ Potts model. The curves are drawn using the central value for $C_o$. The effect of the uncertainty on $C_o$ would not be visible.
Figure 5: $CV(\beta_t)/L^2$ as a function of $1/L^2$ for the 2-d $q=20$ Potts model. The three curves are drawn using the central value and the one standard estimates for $C_o$. 