A New Method to Determine First-Order Transition Points from Finite-Size Data

Christian Borgs and Wolfhard Janke*
Institut für Theoretische Physik
Freie Universität Berlin
Arnimallee 14, 1000 Berlin 33, Germany

FUB-HEP 6/91

Abstract

We consider a temperature driven first-order phase transition describing the coexistence of q ordered low-temperature phases and one disordered high-temperature phase at the infinite volume transition temperature T_0. Analysing the exponential corrections to the usual heuristic formula of the periodic partition function in a box of volume V, $Z_{per} = \sum_m \exp(-\beta f_m V)$, where $\beta = 1/k_B T$ and f_m is the (metastable) free energy of the phase m, we propose several definitions of a finite volume transition temperature $T_0(V)$ which involve only exponential corrections with respect to T_0. We test our propositions in the $d = 2$ Potts model for $q = 5, 8$ and 10 by means of Monte Carlo simulations, using the single cluster update procedure.

PACS numbers: 05.50. +q, 64.60. Pi, 75.10. Hk

*Present address: HLRZ, Forschungszentrum Jülich, 5170 Jülich, Germany

In the idealized infinite volume limit, first-order phase transitions are characterized by discontinuities in the first derivative of the free energy, i. e. , by discontinuities of an order parameter like the internal energy or the magnetization. As a consequence, the specific heat or the susceptibility show δ-function singularities at the transition. In a finite volume V, however, the singularities are smoothed out and the derivative of the order parameter has a finite peak near the infinite volume transition point.

If the volume is cubic or nearly cubic, the width of the peak is proportional to $1/V$, and the maximum of this peak is shifted by an amount $O(V^{-\alpha})$ with respect to the actual infinite volume transition, where $\alpha > 0$ depends on the model and the type of boundary conditions in consideration [1]-[6].

Another definition of a finite volume transition point involves the Binder parameter [7], $B_V = 1 - \langle E^4 \rangle_V / 3 \langle E^2 \rangle_V^2$, where $\langle \cdot \rangle_V$ denotes expectations in the volume V and E is the energy. In the infinite volume limit, B has a discrete minimum $B_{min} < 2/3$ at the transition point, while $B = 2/3$ away from the transition. In a finite volume the location of the minimum is again shifted by an amount proportional to $V^{-\alpha}$ if the volume is approximately cubic [8]. For models describing the coexistence of finitely many phases at the transition point [9], these shifts are typically of the order $O(V^{-1})$ if one consideres periodic boundary conditions. Finite-size scaling using different volumes may improve the error, but it always is proportional $O(V^{-\alpha})$ for some $\alpha < \infty$. But a precise knowledge of the transition point is often desirable since many quantities of physical interest are just defined at the a priory unknown) transition point. It therefore seems desirable to find definitions of a finite volume transition point which involve no power-law corrections at all.

In fact, such a definition has already been given in ref. [10] and [11], see also ref. [12]. It starts from the observation that the periodic partition function of a model describing the coexistence of $q+1$ phases is given by

$$Z_{per}(V,\beta) = \left(\sum_{m=0}^{q} e^{-\beta f_m(\beta) V}\right)\left(1 + O\left(V e^{-L/L_0}\right)\right), \tag{1}$$

where $L_0 < \infty$ is a constant, L is the diameter of V, and $f_m(\beta)$ is some sort of meta-stable free energy of the phase m. It is equal to the free energy $f(\beta)$ if m is stable and strictly larger than $f(\beta)$ if m is unstable. As a consequence

$$N(\beta) := \lim_{V\to\infty} Z_{per}(V,\beta) e^{\beta f(\beta) V} \tag{2}$$

is equal to the number of stable phases at the inverse temperature β [13]. Since $N(\beta)$ has a discrete maximum at the transition point, it seems natural to define a finite volume transition point $\beta_{V/V}$ as the point where a suitable finite-size approximation to $N(\beta)$, say

$$N(V_1, V_2, \beta) = \left[\frac{Z_{per}(V_1,\beta)^{\alpha}}{Z_{per}(V_2,\beta)}\right]^{\frac{1}{\alpha-1}} \tag{3}$$

is maximal. Here $\alpha = V_2/V_1$. Due to the bound (1) (and similar bounds for derivatives, see ref. [10] and [11] for details) this definition leads only to *exponentially* small shifts with respect to the infinite volume transition point.

The theoretical methods of ref. [10] and [11] do not allow, however, to calculate the constants in the above asymptotic bound (1). It is therefore not clear a priory if the above criterion is of any practical use in the numerical determination of the transition point [14]. The goal of this paper is to test the above criterion in the two-dimensional q states Potts model [15], which shows a (temperature driven) first-order transition for $q > 4$. We will also discuss other definitions of finite-size transition points which involve only exponentially small systematic corrections.

For the convenience of the reader we start with a heuristic derivation of the bound (1) in the context of a temperature driven transition describing the coexistence of q ordered low-temperature and one disordered high-temperature phase at the infinite volume transition temperature $T_0 = 1/k_B\beta_0$, assuming that all string tensions are non zero and that all phases have a finite correlation length at T_0.

A typical configuration contributing to Z_{per} then consists of regions $V_m,\ m = 0,\ \ldots, q$, corresponding to small perturbations of the disordered ($m = 0$) or ordered phases ($m = 1, \ldots q$), and "domain walls" separating these regions. We distinguish two types of configurations: those with domain walls which wind around the torus (the corresponding sum will be denoted by $Z_{tunnel}(V, \beta)$), and those which do not contain such domain walls. The sum over the second type of configurations may then be written as a sum of $q + 1$ terms $Z_m(V, \beta)$, each describing a gas of excitations immersed in the m'th phase, and

$$Z_{per}(V, \beta) = Z_{tunnel}(V, \beta) + \sum_{m=0}^{q} Z_m(V, \beta). \tag{4}$$

Assuming that domain walls W of size $|W|$ are suppressed like $e^{-c|W|}$ (which is plausible as long as all string tensions are non zero) one may bound Z_{tunnel} by $e^{-\beta f(\beta)V} O(Ve^{-cL})$, where L is the diameter of V and the preexponential factor V in the above bound counts for the different possibilities to locate a domain wall in V.

In order to define $f_m(\beta)$ we follow an idea originally appearing in ref. [16] and introduce truncated partition functions $Z_m^{trunc}(V, \beta)$ where all configurations containing domain walls with diameter larger than the size, $L_c^{(m)}(\beta)$, of a critical droplett in the corresponding droplett model are supressed. Since

$L_c^{(m)}(\beta) = \infty$ if m is stable, while $L_c^{(m)}(\beta) \sim |\beta - \beta_0|^{-1}$ if m is unstable, the corresponding free energies, $f_m(\beta)$, are equal to $f(\beta)$ if m is stable and strictly larger than $f(\beta)$ if m is unstable.

Let us now assume that $|\beta - \beta_0|$ is so small that the diameter L of V is smaller than $L_c^{(m)}(\beta)$ for all phases m (in the context considered here, where $|\beta - \beta_0| \leq O(V^{-1}) \ll L^{-1}$ this is no restriction at all, since $L_c(\beta) \sim |\beta - \beta_0|^{-1}$). Then *all* phases of the model behave as if they were stable (in the sense that large domain walls are suppressed), and $Z_m(V, \beta) = Z_m^{trunc}(V, \beta)$. Since Z_m is defined on a torus, and since a torus has neither corners, nor edges or boundaries, $\log Z_m(V, \beta)$ contains no surface corrections and $|\log Z_m(V, \beta) + \beta f_m(\beta) V|$ may be bounded by $O\left(V e^{-L/L^{(m)}}\right)$, where $L^{(m)}$ is of the order of the correlation length of the phase m. Combining this bound with the above bound for Z_{tunnel} we get (1), provided $|\beta - \beta_0| L < 1$ (actually, the bound (1) remains true for $|\beta - \beta_0| L > 1$ as well, see ref. [10] for details).

At this point we want to stress that the bound (1) is only a bound and does not imply that the exponential corrections do actually behave like $V e^{-L/L_0}$. As an illustration we consider the leading configurations contributing to Z_{tunnel} in $d = 2$. They consist of two parallel domain walls in one of the coordinate directions, both closed by periodicity. If we neglect the interaction between them, each of them should behave like a closed random walk, leading to an effective weight $\left(L \times L^{-1/2} e^{-cL}\right)^2 \sim L e^{-2cL}$, where the factor L counts for the translation invariance perpendicular to the chosen coordinate direction.

Unfortunately, the numerical determination of $\beta_{V/V}$ requires simulations on two different lattices. We therefore looked for another definition of a

finite-size transition point which requires data from one lattice only. It is based on the fact that the partition function of a statistical system may be written as

$$Z = \sum_{configurations} e^{-\beta E} = \sum_{E} N(E) e^{-\beta E}, \tag{5}$$

where $N(E)$ is the number of configurations with the energy E. In practice, by recording energy histograms, one measures the closely related probability distribution $P_\beta(E) = Z^{-1} N(E) e^{-\beta E}$, which, around a first-order transition, has the typical double-peak form displayed for three characteristic temperatures in fig. 1. At the infinite volume transition point all free energies $f_m(\beta)$ are equal, so that

$$\sum_{m=1}^{q} Z_m(V, \beta) = q Z_0(V, \beta), \tag{6}$$

apart from exponentially small corrections. A natural definition of a finite volume transition point β_W is thus the point where the ratio of the total weight of the ordered phases to the weight of the disordered phase approaches q,

$$R(V, \beta) \equiv \sum_{E<E_0} P_\beta(E) / \sum_{E \geq E_0} P_\beta(E) \equiv W_o / W_d \stackrel{\beta=\beta_W}{=} q. \tag{7}$$

Here E_0 is defined as the energy at the minimum between the two peaks at the temperature where both peaks of $P_\beta(E)$ have equal height. Clearly, also other definitions of E_0 would be reasonable as well, as for example the internal energy at the temperature where the specific heat is maximal. Since it is expected that the relativ height of the minimum between the two peaks decreases like $e^{-2cL^{d-1}}$ as $L \to \infty$, all these definitions do in fact only differ by exponentially small errors. It is therefore a matter of practical convenience

to choose E_0. Note that in (7) we have assumed that the number of ordered phases, q, is known by general arguments. If this is not the case, one may use the crossing points $\beta_{W/W}$ satisfying $R\left(V_1, \beta_{W/W}\right) = R\left(V_2, \beta_{W/W}\right)$ as estimates for β_0. This, of course, requires again the simulation on two lattices.

Clearly, all these considerations apply to field driven first-order transitions as well. The point $\beta_{V/V}$, e. g. should then be replaced by the position $h_{V/V}$ of the maximum of the ratio (3) as a function of the field h. And instead of energy histograms one should use magnetization histograms.

We have tested our propositions by Monte Carlo simulations of the two-dimensional q-state Potts model with $q = 5, 8$, and 10 [15] on square lattices with the periodic boundary condition. The Potts models for $q > 4$ are exactly known [17, 15] to show a temperature driven first-order phase transition at $\beta_0 = \log\left(1 + \sqrt{q}\right)$. To update the spin configurations we have used the cluster algorithm [18] in its single-cluster variant [19] which is very successful in reducing critical slowing down near continuous phase transitions. At the first-order transitions considered here, however, the overall gain in CPU time as compared to the standard Metropolis algorithm turned out to be only quite modest [20].

For each q and lattice size, we have first performed one relatively short simulation at some $\hat{\beta}$ near the transition point [21] and recorded the energy histogram $P_{\hat{\beta}}(E)$. Using the relation

$$P_\beta(E) = e^{-\left(\beta-\hat{\beta}\right)E} P_{\hat{\beta}}(E) / \sum_E e^{-\left(\beta-\hat{\beta}\right)E} P_{\hat{\beta}}(E) \tag{8}$$

this allows in principle to calculate the energy distribution and hence expectation values at any inverse temperature β [22]. In practice statistical errors limit the actual range of β to $|\beta - \hat{\beta}|E = \mathcal{O}(1)$, but this is still wide

enough to get an estimate of the specific-heat maximum, β_{Cmax}, and the Binder-parameter minimum, β_{Bmin}. We have then performed three rather long simulations at β_0, β_{Cmax}, and β_{Bmin}, and recorded again the energy histograms. Their typical shapes can be inspected in Fig. 1 for the case $q = 8$ and $V = 57 \times 57$. For non-trivial models with unknown β_0 one can use eq. (7) to get a first rough estimate of the transition point from the short run. The run-time t_{run} of the long simulations is of the order $(3-5) \times 10^6$, where t_{run} is defined (in units comparable to Metropolis sweeps) as $(\langle C \rangle / V) \times$ number of cluster steps, with $\langle C \rangle$ denoting the average cluster size. Finally, basically applying eq. (8), we have combined the three histograms at fixed q and V to a single, optimized histogram [23], which was then used for all further analyses.

In Fig. 2 (a) - (c) we plot the positions of the specific-heat maximum and Binder-parameter minimum for $q = 5, 8$, and 10 and various lattice sizes. Also shown are the infinite volume transition points and the leading $1/V$ corrections, which are both exactly known for $2D$ Potts models. In non-trivial models the infinite volume transition point would have to be estimated from linear extrapolations in $1/V$. As can be seen in Fig. 2, in particular for weak first-order phase transitions (small q) this can be quite misleading. Note that the next correction term $\propto (1/V)^2$ is extremely small (at least for $2D$ Potts models) and does not improve the agreement with the data. Rather, it even goes in the wrong direction. In view of our earlier discussion of exponential corrections this is not surprising at all. In fact, allowing also terms $\propto e^{-L/L_0}$ besides the $1/V$ corrections, and performing fits to the data, we find the interpolating dashed curves in Fig. 2.

Knowing the (optimized) probability distributions $P_\beta(E)$, also the posi-

tions $\beta_{V/V}$ of the maxima of $N\,(V_1,\ V_2,\ \beta)$ in eq. (3) are readily determined. We have chosen V_1 and V_2 to ensure that $\alpha = V_2/V_1$ is roughly constant (≈ 1.6). As is demonstrated in Fig. 2, the resulting points $\beta_{V/V}$ approach β_0 quite rapidly from below, thus confirming the theoretical expectations.

Our second criterion in eq. (7) is only little more laborious to implement. First, using relation (8) we vary the temperature until both peaks have equal height and determine the energy E_0 at the minimum between them. A good starting point for this procedure is β_{Cmax} (see Fig. 1). Using again (8), we finally adjust β until $R(V,\ \beta_W) = q$. In Fig. 2 we see that the transition points β_W are even closer to β_0 then the corresponding points $\beta_{V/V}$. Notice that on the larger lattices, in order to disentangle the small systematic deviations of the order $|\beta_W - \beta_0| \approx 10^{-4}$ from statistical errors, we would need much higher statistics.

In summary, we have proposed and successfully tested two simple criterions for locating first-order transition points in Monte Carlo simulations on finite periodic lattices that have only exponentially small corrections with respect to the infinite volume limit.

References

[1] M. E. Fischer, A.N. Berker, Phys. Rev. **B26** (1982) 2507.

[2] V. Privman, M.E. Fischer, J. Stat. Phys. **33** (1983) 385.

[3] K. Binder, D.P. Landau, Phys. Rev. **B30** (1984) 1477.

[4] M.S.S. Challa, D.P. Landau, K. Binder, Phys. Rev. **B34** (1986) 1841.

[5] V. Privman, J. Rudnik, J. Stat. Phys. **60** (1990) 551.

[6] For a recent review, see V. Privman in "Finite size scaling and numerical simulations of Statistical Physics", V. Privman (ed.) World Scientific, Singapore 1990.

[7] K. Binder, Z. Phys. **B43** (1981) 119.

[8] Long cylinders show a different finite size scaling, see e. g. ref. [2], or C. Borgs, J. Imbrie, Commun. Math. Phys. in print.

[9] A priory, this does not exclude continuous spin models (an example is the scalar ϕ^4 model in an external field), but it does exclude models like the field driven Heisenberg model at low temperatures where the transition is related to the breaking of a continuous symmetry.

[10] C. Borgs, R. Kotecký, Journ. Stat. Phys. **61** (1990) 79.

[11] C. Borgs, R. Kotecký, S. Miracle-Solé, Journ. Stat. Phys. **62**(1991) 529.

[12] C. Borgs, R. Kotecký, Finite-size effects at asymmetric first-order transitions, to appear in Phys. Rev. Lett.

[13] This fact was already observed in C. Borgs, J. Imbrie, Commun. Math. Phys. **123**(1989) 305.

[14] As a first guess, one could hope that our criterion is useful whenever it is possible to make the system larger than the infinite volume correlation length at the transition point.

[15] For a general review of the Potts model, see e. g. F. Y. Wu, Rev. Mod. Phys. **54** (1982) 235.

[16] M. Zahradniḱ, Commun. Math. Phys. **93** (1984) 559.

[17] R. J. Baxter, J. Phys. **C6** (1973) L445.

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

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

[20] More precise statements depend in quite a complicated way on the strength of the first-order transition, the lattice size and the temperature at which the simulation is performed. These dynamical aspects of the single-cluster algorithm at first-order transitions are discussed in W. Janke, preprint in preparation.

[21] Since for the two-dimensional Potts models β_0 is exactly known the natural choice is $\hat{\beta} = \beta_0$, but this is inessential.

[22] A. Ferrenberg, R. H. Swendsen, Phys. Rev. Lett. **61** (1988) 2635.

[23] A. Ferrenberg, R. H. Swendsen, Phys. Rev. Lett. **63** (1989) 1195.

Figure Headings

Fig. 1 The typical double-peak form of the probability distribution $P_\beta(E)$ at (a) β_0, (b) β_{Cmax}, and (c) β_{Bmin}.

Fig. 2 The finite volume transition points $\beta_{V/V}(\triangle)$ and $\beta_W(\Box)$, resulting from the new criterions proposed in this note. For comparison, we also show β_{Cmax} ($\bullet$) and β_{Bmin} ($\circ$). The solid straight lines are the exactly known $1/V$ corrections corresponding to $\bullet$ and $\circ$, and the dashed, almost interpolating curves show exponential fits to the data. The long dashed horizontal lines indicate the exact transition point β_0.