Continuous phase transitions with a convex dip in the microcanonical entropy

Hans Behringer

Fakultät für Physik, Universität Bielefeld, D-33615 Bielefeld, Germany

Michel Pleimling

Institut für Theoretische Physik I, Universität Erlangen-Nürnberg, D-91058 Erlangen, Germany

The appearance of a convex dip in the microcanonical entropy of finite systems usually signals a first order transition. However, a convex dip also shows up in some systems with a continuous transition as, for example, in the Baxter-Wu model and in the four-state Potts model in two dimensions. We demonstrate that the appearance of a convex dip in those cases can be traced back to a finite-size effect. The properties of the dip are markedly different from those associated with a first order transition and can be understood within a microcanonical finite-size scaling theory for continuous phase transitions. Results obtained from numerical simulations corroborate the predictions of the scaling theory.

I. INTRODUCTION

The microcanonical analysis of phase transitions has gained growing interest in recent years due to the inequivalence of the canonical and the microcanonical descriptions of finite systems with short-range interactions as well as of systems with long-range interactions [1–17]. Whereas the discrimination of the order of a phase transition from finite-size data can be a difficult task in the canonical ensemble, microcanonical quantities usually yield clear signatures which reveal the continuous or the discontinuous character of a phase transition [2]. In small microcanonical systems which exhibit a continuous transition in the thermodynamic limit the character of the transition is signaled by typical features of symmetry breaking, as, e.g., the abrupt onset of a nonzero order parameter when a pseudocritical point is approached from above. These features are accompanied by singular physical quantities [18–27]. The associated singularities, however, are not the consequence of a nonanalytic microcanonical entropy and can therefore be characterized by classical critical exponents [19,22]. Similarly, intriguing features are also revealed in the microcanonical entropy of small systems with a discontinuous transition in the infinite volume limit [5,28–33]. A typical back-bending of the microcanonical caloric curve is observed, leading to a negative heat capacity. This property, which has also been observed in recent experiments [34,35], has been used as a tool for the determination of the first order character of phase transitions in microcanonical systems. In the canonical context the first order character is then signaled by a double-peak structure in certain histograms (e.g. [36–38]).

However, some systems (as, for example, the Baxter-Wu model [39,40]), with a continuous phase transition in the thermodynamic limit, have been reported to show a similar double-peak structure in canonical histograms or, equivalently, a negative microcanonical specific heat [41,42]. It follows from this observation that the mere existence of a convex dip in the entropy is not sufficient for the identification of a discontinuous transition [43].

In this work we examine more closely the finite-size behavior of the microcanonical specific heat and of the convex dip in the entropy function of this kind of systems, thereby taking the Baxter-Wu model and the four-state Potts model in two dimensions as examples. In particular we demonstrate that the microcanonical finite-size scaling theory presented in Ref. [26] for continuous phase transitions relates the appearance of these features to a peculiar finite-size effect. In addition we deduce properties of the dip in the microcanonical entropy which we test in numerical simulations of both the Baxter-Wu and the four-state Potts model.

The rest of the paper is organized as follows. In Sec. II a brief introduction to the microcanonical analysis of physical systems is given. We particularly discuss the properties of the microcanonical specific heat both for systems with continuous and discontinuous phase transitions in the infinite volume limit. The microcanonical finite-size scaling theory of Ref. [26] is used in Sec. III to deduce the scaling properties of the convex intruder in the microcanonical specific heat of systems undergoing a continuous phase transition in the thermodynamic limit. In Sec. IV we present numerical results both for the Baxter-Wu and for the two-dimensional four-state Potts model which belong to the same universality class. These numerical results corroborate the findings obtained from the finite-size scaling theory as the properties of the convex dip are consistent with the theoretical predictions. Finally, Sec. V summarizes our results.

II. SIGNATURES OF PHASE TRANSITIONS IN THE MICROCANONICAL SPECIFIC HEAT

In finite systems the thermostatic quantities of a system undergoing a phase transition in the thermodynamic limit show characteristic features. The canonical specific heat of finite systems, for example, is a regular function that exhibits a maximum at a certain temperature. The continuous or discontinuous character of the phase transition is revealed by the size-dependence of the increase of the specific heat maximum which is well-understood within canonical finite-size scaling theory [44,45]. In the case of a continuous phase transition the increase of the specific heat maximum $c_{\max}$ with the system size L is given by $c_{\max} \sim L^{\alpha/\nu}$ where α de-

scribes the divergence of the specific heat of the infinite system when approaching the critical temperature (here and in the following we only consider the case $\alpha > 0$), whereas ν is the usual correlation length critical exponent. For a discontinuous phase transition, however, one finds $c_{max} \sim L^d$ [46] where d is the dimensionality of the system.

The thermodynamic behavior can also be investigated in the microcanonical ensemble which describes systems which are isolated from any environment [1,2]. The starting point in the microcanonical analysis is the density of states Ω which, for a discrete spin system, measures the degeneracy of the macrostate (E), i.e., $\Omega(E)$ is the number of configurations (or microstates) with energy E. For a d-dimensional system with linear extension L physical quantities are then calculated from the microcanonical entropy density

$$s(e, L^{-1}) := \frac{1}{L^d} \ln \Omega(L^d e, L^{-1}) \tag{1}$$

which depends on the energy density $e := E/L^d$ and the system size L. In the following the dependence on the system size is indicated by the inverse system size $l := L^{-1}$. Note that the specific entropy also depends on the boundary conditions which have to be specified for finite systems. This dependence, however, is not indicated in the notation here. The inverse microcanonical temperature β_μ shows up as the conjugate variable to the natural variable energy e and is defined by

$$\beta_\mu(e, l) := \frac{d}{de} s(e, l). \tag{2}$$

The corresponding microcanonical specific heat is given by

$$c(e, l) = -[\beta_\mu(e, l)]^2 \left(\frac{d\beta_\mu(e, l)}{de} \right)^{-1}. \tag{3}$$

Similar to the canonical case the finite-size behavior of the microcanonical specific heat shows also certain characteristics if the system has a phase transition in the infinite lattice. In the case of a continuous transition the entropy density is concave everywhere. The microcanonical specific heat [Eq. (3)] is thus positive and displays a maximum whose value increases with growing system size L [23,26]. As the derivative of $\beta_\mu(e, l)$ is the second order derivative of the entropy, it measures the curvature of the entropy density. This curvature is negative and has a maximum at a certain energy which can be identified as the pseudocritical energy e_{pc} of the finite system. The value of the derivative of β_μ at this pseudocritical energy scales like

$$\beta_\mu'(e_{pc}, l) := \frac{d}{de} \beta_\mu(e, l)|_{e=e_{pc}} = \frac{d^2}{de^2} s(e, l)|_{e=e_{pc}} \sim l^{\alpha_\varepsilon/\nu_\varepsilon} \tag{4}$$

in the regime $l \to 0$. The microcanonical critical exponent α_ε is thereby related to the canonical critical exponent α by $\alpha_\varepsilon = \alpha/(1-\alpha)$ [18,19]. Generally, a canonical critical exponent κ translates to the microcanonical exponent $\kappa_\varepsilon = \kappa/(1-\alpha)$ if α is positive, whereas for nonpositive α the critical exponents of the microcanonical description are identical to the canonical ones [47]. Relation (4) is obtained from
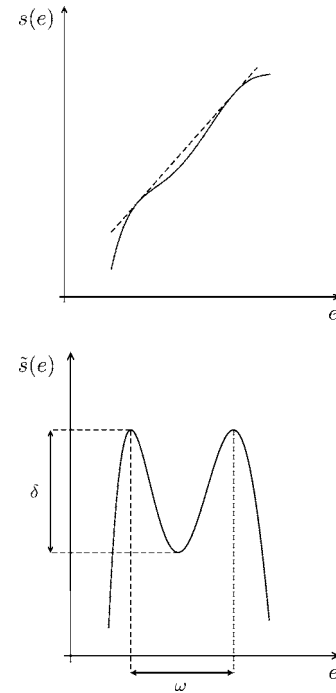

FIG. 1. Schematic depiction of the convex dip in the entropy of a finite system whose corresponding infinite system undergoes a discontinuous phase transition. The double-tangent with slope β_t is indicated by a dashed line (top). For the function $\tilde{s} = s - \beta_t e$ the definitions of the width ω and of the depth δ of the dip are shown (bottom).

a decomposition of the microcanonical entropy into a regular part and a singular part which obeys a certain homogeneity relation in the vicinity of the pseudocritical point. Note that the size-dependence of the increase of the specific heat maximum allows the determination of the corresponding microcanonical critical exponent of the specific heat of the infinite system. For more details see Sec. III and in particular Ref. [26]. Note also that other microcanonical quantities like the spontaneous magnetization and the susceptibility also exhibit typical features of continuous phase transitions in finite systems [19–22,25,27]. These aspects are, however, not studied in the present work.

The behavior of the specific heat is completely different if the system undergoes a discontinuous phase transition. In this case the microcanonical entropy density of a finite system has a convex dip which leads to a negative microcanonical specific heat for a certain energy interval [5,28–33]. This is different in the canonical ensemble where the specific heat, which is related to the variance of the energy, is always positive for any finite system. Of course in the thermodynamic limit the convex dip in the microcanonical entropy density disappears in systems with finite-range interactions and the specific heat is positive everywhere. The curvature properties of the entropy density of a finite system allow the determination of an inverse pseudotransition temperature β_t by the double-tangent (or Maxwell) construction. This is depicted schematically in Fig. 1. The discontinuous character of the transition is revealed by a certain scaling behavior of the convex dip. Defining the auxiliary function
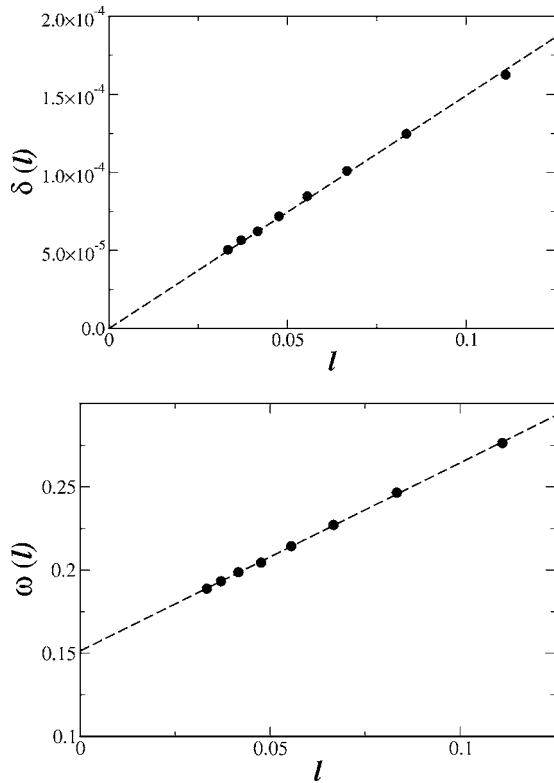
FIG. 2. The depth $\delta(l)$ and width $\omega(l)$ of the convex dip in the microcanonical entropy of the three-state Potts model in three dimensions as a function of the inverse system size. The dashed lines are linear fits to the data. Error bars are comparable to the size of the symbols.

$\tilde{s}(e,l) := s(e,l) - \beta_t(l)e$, a size-dependent width $\omega(l)$ and depth $\delta(l)$ of the dip can be measured, as shown in Fig. 1. With increasing system size, i.e., for the regime $l \to 0$, the depth scales like $\delta(l) \sim l$ and the width like $\omega(l) - \omega_\infty \sim l$ [48–50]. Here ω_∞ is the length of the linear section of the function $\tilde{s}$ of the infinite system and is in fact the latent heat of the transition. The asymptotic behavior linear in l and the appearance of a nonzero latent heat ω_∞ signal the discontinuous character of the transition in the infinite system. This can be illustrated by investigating the three-state Potts model in three dimensions. The general q-state Potts model is defined by the Hamiltonian

$$\mathcal{H}(\sigma) = -\sum_{\langle ij \rangle} \delta_{\sigma_i, \sigma_j}, \qquad (5)$$

where the sum runs over nearest-neighbor sites of the lattice and the spins σ_i can take on the values $\sigma_i = 1, \ldots, q$ [40,51,52]. The coupling constant is set to unity. The three-state model in three dimensions undergoes a (relatively weak) first order transition and therefore one expects that the characteristic quantities of the convex dip evolve linearly in the inverse system size (compare [53] for a canonical and [29] for a microcanonical investigation of the model). This is indeed confirmed by numerical data as shown in Fig. 2.

III. MICROCANONICAL FINITE-SIZE SCALING THEORY

In this section the implications of the microcanonical finite-size scaling theory [26] are investigated for systems with a continuous phase transition where $\alpha_\varepsilon \geq \nu_\varepsilon$ (canonically $\alpha \geq \nu$). Note that the condition $\alpha_\varepsilon \geq \nu_\varepsilon$ corresponds to a rather restricted class of model systems. Nevertheless important spin models like the Baxter-Wu and the four-state Potts model in two dimensions have critical exponents $\alpha_\varepsilon = \nu_\varepsilon$ and therefore belong to this class. These models are more closely studied in the next section. Other models are reported in the literature to have exponents satisfying $\alpha_\varepsilon > \nu_\varepsilon$ [54,55].

Consider the entropy density $s(e,l)$ of a finite d-dimensional microcanonical system near the pseudocritical energy e_{pc}. Recall that e_{pc} is defined by the maximum of the second derivative of s. The microcanonical finite-size scaling theory for a system with a continuous transition [26] assumes that the entropy can be split up into two parts, namely into a so-called regular part s_r and into a part s_s which is called singular as it becomes nonanalytic in the infinite volume limit. This is in contrast to the regular part which is analytic also in the infinite system. The singular part has to satisfy the scaling relation

$$s_s(\varepsilon,l) = l^d \phi(l^{-1/\nu_\varepsilon}\varepsilon) \qquad (6)$$

with $\varepsilon := e - e_{pc}$ and ϕ being a scaling function with no further explicit size-dependence. This decomposition $s(\varepsilon,l) = s_r(\varepsilon,l) + s_s(\varepsilon,l)$ is only valid for asymptotically large system sizes and in the regime $l^{-1/\nu_\varepsilon}\varepsilon \to 0$, in particular for energies close to the pseudocritical one. Note that the singular part and thus the function ϕ in relation (6) is also analytic for finite systems and must fulfill the required scaling property which states that it is a homogeneous function. Due to the analyticity of the microcanonical entropy the decomposition together with the required scaling relation for the singular part states that the entropy is of the form

$$s(\varepsilon,l) = s_0(l) + \beta_{pc}(l)\varepsilon + \frac{1}{2}A_2(l)\varepsilon^2 + \frac{1}{4}A_4(l)\varepsilon^4 + \cdots \quad (7)$$

for small ε [26]. Here $\beta_{pc}(l) = \beta_\mu(e_{pc}, l)$. The coefficients of the second and fourth order terms are of the form

$$A_2(l) = B_2 l^{\alpha_\varepsilon/\nu_\varepsilon} + C_2(l) \qquad (8)$$

and

$$A_4(l) = B_4 l^{(\alpha_\varepsilon-2)/\nu_\varepsilon} + C_4(l) \qquad (9)$$

in terms of the critical exponents of the microcanonical system. The coefficient A_4 has to be negative, otherwise higher order terms in the energy deviation ε have to be taken into account. The size-dependence contained in the coefficients C_2 and C_4 stems from the regular part s_r of the entropy density whereas the dependencies involving the critical exponents α_ε and ν_ε have their origin in the singular part s_s [or equivalently in the scaling function ϕ in relation (6)] of the entropy. In particular, the coefficient B_2 has to be negative in the case of a continuous transition and, due to the regularity of s_r, the coefficient C_2 is of the form

$$C_2(l) = v_1 l + v_2 l^2 + \cdots \qquad (10)$$

for small l whereas the coefficient C_4 has the expansion $C_4(l) = z_0 + z_1 l + \cdots$ in the inverse system size (see Ref. [26] for further details). Note that α_ε has to satisfy $\alpha_\varepsilon \leq 2$ for C_4 to be the subdominant term in the coefficient A_4. This is assumed in the following considerations.

In certain model systems the critical exponents satisfy the relation $\alpha_\varepsilon = \nu_\varepsilon$. Examples include the Baxter-Wu model and the four-state Potts model in two dimensions. In this situation the leading behavior of the coefficient $A_2(l)$ in relation (7) is the linear term in the inverse system size, i.e., $A_2(l) \sim al$ for $l \to 0$ where the amplitude a is the sum $B_2 + v_1$. If the amplitude a is positive, i.e., v_1 is positive and large enough compared to the modulus of the negative amplitude B_2, the entropy density develops a convex dip for all finite system sizes. Note that the corresponding condition $A_2(l) > 0$ is a necessary condition for the appearance of a convex dip in the microcanonical entropy. Thus in the framework of the microcanonical finite-size scaling theory a convex dip can appear even so the transition in the infinite system is continuous. Furthermore, from expression (7) one can then deduce scaling relations for the width and the depth of the convex dip in such a case. Applying the double-tangent construction to the entropy (7) with $\alpha_\varepsilon = \nu_\varepsilon$ and a positive A_2 one finds that

$$\omega(l) = 2\sqrt{\frac{A_2(l)}{|A_4(l)|}} \overset{l \to 0}{\sim} l^{1/\alpha_\varepsilon} \qquad (11)$$

and

$$\delta(l) = \frac{[A_2(l)]^2}{|A_4(l)|} \overset{l \to 0}{\sim} l^{1+2/\alpha_\varepsilon} \qquad (12)$$

for small l. This scaling behavior of the convex dip in the microcanonical entropy is therefore different from the linear behavior in the inverse system size encountered for discontinuous transitions and discussed in Sec. II [54,55]. For a negative amplitude a, on the other hand, the signatures of a continuous transition with the scaling behavior $\beta'_\mu(e_{pc}, l) \sim A_2(l) \sim l (= l^{\alpha_\varepsilon/\nu_\varepsilon})$ are observed. Whether the predicted convex dip really appears or whether one encounters typical features of continuous transitions thus depends on the sign and relative size of the amplitudes entering the scaling form (7) of the entropy near the pseudocritical energy.

Let us end this section by considering the situation where α_ε is strictly larger than ν_ε. In this case the leading behavior of the coefficient A_2 is still linear in l provided the amplitude v_1 is nonzero. For positive v_1 one then has again a convex dip with the scaling relations $\omega(l) \sim l^{1/2 - (\alpha_\varepsilon - 2)/(2\nu_\varepsilon)}$ and $\delta(l) \sim l^{2 - (\alpha_\varepsilon - 2)/\nu_\varepsilon}$ for its characteristic extensions. For negative v_1 instead one observes features of a continuous transition with the asymptotic behavior $\beta'_\mu(e_{pc}, l) \sim l$, which does not allow one to uncover the actual critical exponents from the leading size-dependence of the evolution of the microcanonical specific heat, in contrast to the corresponding situation for $\alpha_\varepsilon \leq \nu_\varepsilon$.

In conclusion, a convex dip in the microcanonical entropy is in general possible for systems with a continuous phase transition if the critical exponents satisfy $\alpha_\varepsilon \geq \nu_\varepsilon$. For systems with $\alpha_\varepsilon > \nu_\varepsilon$ such a dip shows up if the amplitude v_1 of the linear term in the expansion of C_2 in Eq. (10) is positive. In a situation with $\alpha_\varepsilon = \nu_\varepsilon$ the amplitude v_1 has to satisfy the additional requirement that $v_1 > |B_2|$. In both cases we end up with the necessary condition $A_2(l) > 0$, see Eq. (8).

IV. MICROCANONICAL SPECIFIC HEAT OF THE BAXTER-WU AND OF THE FOUR-STATE POTTS MODEL

A. The Baxter-Wu model

The Baxter-Wu model is a classical spin model whose free energy can be calculated exactly in zero magnetic field [39,40]. The model is defined on a two-dimensional triangular lattice, with the Hamiltonian

$$\mathcal{H}(\sigma) = -\sum_{\langle ijk \rangle} \sigma_i \sigma_j \sigma_k \qquad (13)$$

where the strength of the coupling constant has been set to unity. The spins σ_i are Ising spins with the possible values $\sigma_i = \pm 1$. The sum in Eq. (13) extends over all triangles of the triangular lattice (here denoted by $\langle ijk \rangle$ with i, j, and k specifying the vertices of the triangles). The system has a continuous phase transition in the infinite system at the critical temperature $T_c = 2/\ln(1 + \sqrt{2})$. The critical exponents which characterize the singular behavior of physical quantities near the critical point are known exactly. For the specific heat and the correlation length one has, for example, $\alpha = \nu = 2/3$ or $\alpha_\varepsilon = \nu_\varepsilon = 2$ microcanonically. In this section the microcanonical specific heat of the Baxter-Wu model is investigated numerically [56]. To this end the microcanonical entropies of systems with linear sizes ranging from 16 to 96 are calculated using the very efficient transition observable method [20,27] for both open and periodic boundary conditions.

As the Baxter-Wu model exhibits a continuous phase transition in the infinite lattice, one expects at first sight that the microcanonical specific heat shows a maximum with the associated increase for increasing system sizes. For finite systems with *open* boundary conditions this is indeed the case. The derivative $\beta'_\mu(e_{pc}, l)$ of the microcanonical temperature at its maximum value, i.e., at the pseudocritical energy, is negative and its modulus decreases, leading to an increasing specific heat maximum when the system size is increased. For the Baxter-Wu model the critical exponents α_ε and ν_ε are equal and therefore one expects from Eq. (4) and the discussion in Sec. III to observe the scaling relation $\beta'_\mu(e_{pc}, l) \sim l$ for small l. This expectation is indeed confirmed by the data shown in Fig. 3.

The situation is different for finite Baxter-Wu systems with *periodic* boundary conditions. In Fig. 4 the function $\tilde{s}$ is shown for a finite system with linear extension $L = 60$. A convex dip is clearly visible. This observation apparently suggests at first sight that the model seems to undergo a *discontinuous* transition in contradiction to the known *continuous* character of the phase transition. Note that recently a double-peak structure in canonical histograms of the energy was reported in the literature [42].

In the previous section III we have shown that the microcanonical finite-size scaling theory permits the appearance of
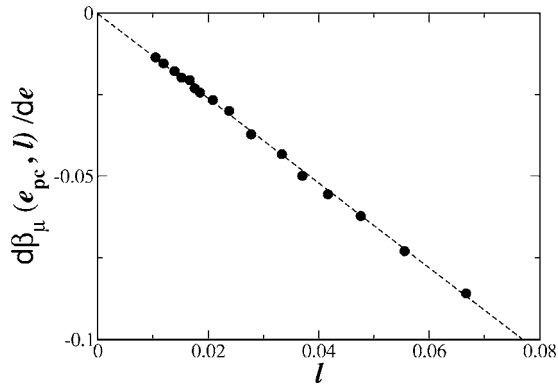
FIG. 3. The derivative $\beta'_\mu(e_{\rm pc},l)=d\beta_\mu(e_{\rm pc},l)/de$ of the Baxter-Wu model as a function of the inverse system size l for open boundary conditions. The errors are approximately as large as the symbol size. The dashed line shows a linear fit. The data extrapolate to zero in the limit $l \to 0$, corresponding to a divergent specific heat in the infinite system.

such a convex dip for the case $\alpha_\varepsilon = \nu_\varepsilon$. With the relations (12) and (11) and the known value $\alpha_\varepsilon = 2$ for the Baxter-Wu model we expect to observe the scaling behavior $\omega(l) \sim \sqrt{l}$ for the width and $\delta(l) \sim l^2$ for the depth of the convex dip. These predictions are indeed confirmed by our numerical data obtained for the Baxter-Wu model as shown in Fig. 5. The full lines are fitted functions containing the expected asymptotic behavior in the inverse system size l. For the dashed lines the leading correction term coming from the regular part $s_{\rm r}$ of the microcanonical entropy (which is proportional to l^3 for the depth and to $l^{3/2}$ for the width) has been included. In agreement with the continuous character of the phase transition the dip scales away in the macroscopic limit $l \to 0$. The size-dependences of both the depth and the width of the convex dip follow the theoretical predictions. This is especially clear from the inset of Fig. 5 where we compare $\omega(l)$ with the expected behavior in a double-logarithmic plot. This agreement gives strong evidence to the general scaling theory presented in the previous section III.
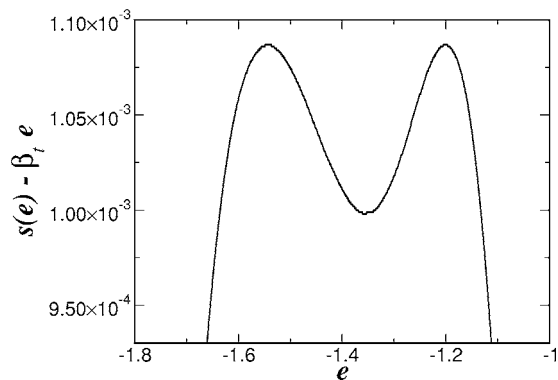

FIG. 4. The function $\tilde{s}$ for the finite Baxter-Wu system with $L=60$ and periodic boundary conditions (here $\beta_{\rm t}=0.43945$). Note that $\tilde{s}$ is only obtained from a numerical simulation up to an additive constant. The data show a double-peak structure typical of finite systems with a discontinuous transition in the macroscopic limit.
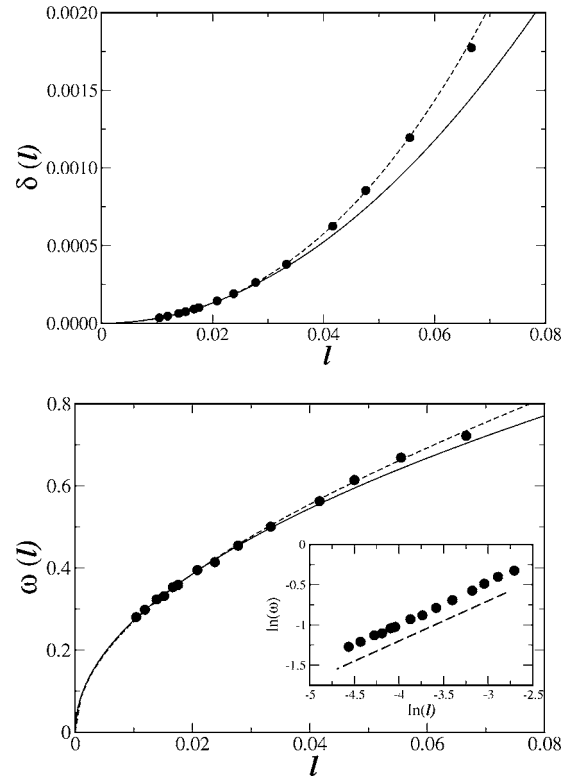

FIG. 5. The depth $\delta(l)$ and width $\omega(l)$ as functions of the inverse system size l for Baxter-Wu systems with periodic boundary conditions. The errors are of the order of the symbol size. The full lines show fits to the theoretically predicted behavior [Eqs. (11) and (12)] using the six largest system sizes. The dashed lines include in addition the first correction term coming from the regular part $s_{\rm r}$ of the microcanonical entropy. The inset shows a double-logarithmic plot of the width together with a straight line of slope 1/2. From the six largest systems one gets a slope of 0.481(3).

It should be stressed again that the different behavior of the microcanonical entropy of the Baxter-Wu model for different boundary conditions is related to different properties of the expansion coefficients in Eq. (7). In particular the coefficient A_2 seems to be deeply affected by the boundary conditions. A microscopic explanation of this observation is, however, still lacking.

The findings of this section have direct implications for the behavior of canonical energy histograms, which have been discussed for the Baxter-Wu model in Ref. [42]. The energy histograms are directly related to the canonical distribution function $P_\beta(e)$ which is the probability of finding a microstate with energy density e at the inverse canonical temperature β. In terms of the microcanonical entropy this distribution function is basically given by $P_\beta(e) \sim \exp(\beta L^d e - L^d s(e,l))$. Thus for the inverse pseudo-transition temperature $\beta_{\rm t}$ obtained from the Maxwell construction applied to the microcanonical entropy the canonical energy histogram exhibits two peaks at equal height with the peaks appearing at the same energies as the peaks in $\tilde{s}=s-\beta_{\rm t}e$. It follows that in the canonical histograms the peaks at the energies e_1 and e_2 approach each other according to the scaling law $|e_1-e_2| \sim \sqrt{l}$.

An important quantity which influences the kinetics of first order phase transitions is the interface tension Σ defined by

$$2\beta_t\Sigma = \frac{1}{L^{d-1}} \ln \frac{P_{\beta_t}(e_{max})}{P_{\beta_t}(e_{min})}, \tag{14}$$

where the double-peaked distribution P_{β_t} has one of the two peaks of equal height at energy e_{max} whereas the minimum between the two peaks appears at the energy e_{min} [57]. From the above discussion one gets $\Sigma \sim \delta(l)/l \sim l$ and thus the interface tension vanishes in the limit of asymptotically large systems. Consequently a coexistence between an ordered phase and a disordered phase at temperature β_t is hardly detectable in this case although the canonical distribution function P_{β_t} exhibits a double-peak structure. For moderately small systems, however, the dip still represents a considerable barrier between the order phase and the disordered one. In some sense one can speak of a phase coexistence for not too large finite systems.

B. The four-state Potts model

The four-state Potts model in two dimensions belongs to the same universality class as the Baxter-Wu model. The character of the phase transition of the q-state Potts model in two dimensions changes exactly at $q=4$ from continuous for low values of q to discontinuous for large q. This makes the four-state Potts model particularly interesting. Due to the presence of marginal scaling fields for $q=4$ the singular behavior of the four-state Potts model is not simply described by pure power laws, but physical quantities like the specific heat or the susceptibility acquire additional logarithmic factors [58,59]. Logarithmic corrections then also show up in the finite-size scaling form of the specific heat [44]. This is in contrast to the Baxter-Wu model where these marginality effects are absent and the singular behavior of the specific heat does not exhibit logarithmic corrections [58,60].

Using the same numerical technique as for the Baxter-Wu model, we have computed the microcanonical entropy density of the four-state Potts model on a square lattice with open and periodic boundary conditions. For open boundary conditions system sizes ranging from $L=12$ to 80 have been considered, whereas for periodic boundary conditions system sizes from $L=14$ to 50 have been simulated.

As shown in Fig. 6 the derivative $\beta'_\mu(e_{pc},l)$ of the microcanonical temperature evaluated at the pseudocritical energy is found to be negative for open boundary conditions. As its modulus decreases as a function of the inverse system size, the resulting specific heat maximum increases when the system size is increased, thus yielding the typical finite-size features of a continuous transition in the thermodynamic limit. The critical exponents α_ε and ν_ε being equal for the four-state Potts model, one expects [see Eq. (4)] the scaling relation $\beta'_\mu(e_{pc},l) \sim l$ for small l. However, as Fig. 6 demonstrates, this asymptotic regime is not yet fully reached for the system sizes considered here. Presumably, this has its origin in the presence of logarithmic correction terms. Nevertheless, the data are consistent with the expectation of a leading
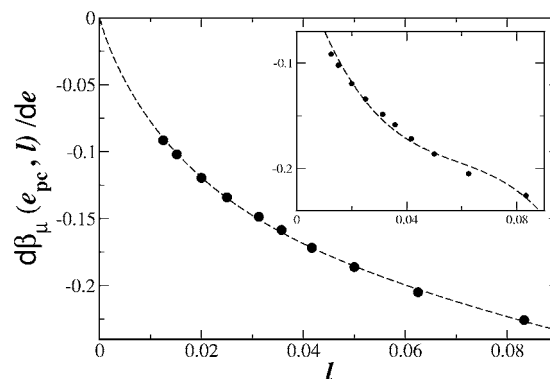

FIG. 6. The derivative $\beta'_\mu(e_{pc},l)=d\beta_\mu(e_{pc},l)/de$ of the four-state Potts model as a function of the inverse system size l for open boundary conditions. The errors are approximately of the order of the symbol size. The dashed line shows a fit with an asymptotic linear term and corrections including a logarithmic term. The data extrapolate to zero for the limit $l \to 0$, yielding a divergent specific heat in the infinite system. The inset shows a fit without the logarithmic correction term (see main text for further details).

linear dependence in the inverse system size in the asymptotic limit $l \to 0$. To demonstrate this a function of the form $[\beta'_\mu(e_{pc},l)]_{fit}=al+bl/\ln(l)+cl^2$ has been fitted to the data (dashed line in Fig. 6). To get a rough impression of the presence of a logarithmic correction, a fit function with correction terms $b_1l^2+c_1l^3$, i.e., without a logarithmic term but with the same number of fit parameters, has also been fitted to the numerical data, yielding a much poorer result (see inset of Fig. 6).

For the Potts model with periodic boundary conditions our findings are in qualitative agreement with the considerations of Sec. III and with the results obtained for the Baxter-Wu model with periodic boundaries. The microcanonical entropy displays the same convex dip for finite systems. Note that a double-peak structure in energy histograms obtained from canonical Monte Carlo simulations was already reported in the literature for this model [41]. The scaling behaviors of the depth and the width of this dip are again consistent with the predicted scaling relations (11) and (12) as depicted in Fig. 7, even so we were forced to include a logarithmic correction term in addition to the leading correction term coming from the regular part.

V. CONCLUSIONS

The determination of the order of a phase transition presents a basic issue in the statistical analysis of physical systems. As there are only a few model systems that can be tackled analytically this question is usually addressed through numerical simulations. A widely used indicator of a first order transition is the metastability between two coexisting phases [36,37,41]. This leads to a convex dip in the microcanonical entropy and thus to a negative microcanonical specific heat in the transition region. In the canonical ensemble the convex dip corresponds to a double-peak structure in histograms of suitable observables. However, the appearance of a double-peak structure in canonical histograms
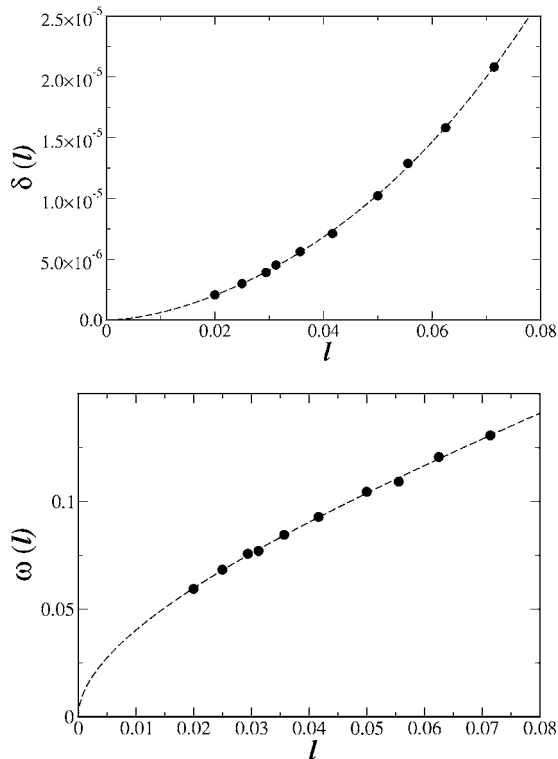
FIG. 7. The depth $\delta(l)$ and width $\omega(l)$ as functions of the inverse system size l for four-state Potts systems with periodic boundary conditions. The errors are approximately as large as the symbol size. The dashed lines show fits of the expected scaling relations (11) and (12) to the data with a logarithmic correction term.

or a convex dip in the microcanonical entropy is not sufficient to identify a first order transition as such features have been reported in the literature for certain model systems that are known to undergo a continuous transition in the thermodynamic limit. To identify the first order character additional scaling properties of the convex dip in the microcanonical entropy (or the double-peak structure in canonical histograms [36,37]) have to be satisfied.

In this work we analyzed the Baxter-Wu model and the two-dimensional four-state Potts model, which are known to have continuous transitions in the thermodynamic limit, but for which double-peak structures in canonical histograms are observed [41,42]. Using a recently developed phenomenological finite-size scaling theory for systems with continuous phase transitions [26] the possible properties of the microcanonical entropy of models where $\alpha \gtrsim \nu$ have been investigated. It turns out that finite-size effects may indeed lead to a convex dip in the entropy of any finite system although the models show continuous transitions. The finite-size scaling relations for the microcanonical entropy predict in this case certain scaling properties of the convex dip that are different from those encountered at a first order transition. The numerical studies of the Baxter-Wu system and the four-state Potts model with periodic boundary conditions indeed reveal an entropy with a convex dip. The properties of the convex dip are in agreement with the expected scaling relations deduced from the microcanonical finite-size scaling theory. This gives strong support to the validity of the scaling theory proposed in [26] for finite microcanonical systems. The systems with open boundaries on the other hand do not show a convex dip in the corresponding entropy. For this case too, the computed specific heat satisfies the scaling relation of the microcanonical scaling theory. The different behavior for different boundary conditions could be traced back to the qualitatively different properties of the expansion coefficient A_2 in Eq. (7). Future studies have to clarify in more detail the influence of different boundary conditions on the finite-size behavior of the microcanonical entropy function.

Even so the appearance of a convex dip in the microcanonical entropy usually signals a first order transition, it may also show up in systems with a continuous transition. We have shown in this work that its appearance in those cases (and therefore also the related appearance of a double-peak structure in canonical histograms) can be traced back to a finite-size effect and that the properties of the dip, which are markedly different from those associated with a first order transition, can be understood within a scaling theory developed for the description of continuous phase transitions in the microcanonical ensemble.

Note added in proof: The same phenomenology of discontinuous-like finite-size signatures at a continuous phase transition is also observed in the collapsing of lattice polymers in high spatial dimensions [61]. We thank Thomas Prellberg for bringing this to our attention.

[1] D. H. E. Gross, *Microcanonical Thermodynamics: Phase Transitions in "Small" Systems (Lecture Notes in Physic 66)* (World Scientific, Singapore, 2001).

[2] M. Pleimling and H. Behringer, Phase Transitions **78**, 787 (2005).

[3] W. Thirring, Z. Phys. **235**, 339 (1970).

[4] M. Bixon and J. Jortner, J. Chem. Phys. **91**, 1631 (1989).

[5] A. Hüller, Z. Phys. B: Condens. Matter **93**, 401 (1994).

[6] R. S. Ellis, K. Haven, and B. Turkington, J. Stat. Phys. **101**, 999 (2000).

[7] T. Dauxois, P. Holdsworth, and S. Ruffo, Eur. Phys. J. B **16**, 659 (2000).

[8] D. H. E. Gross and E. V. Votyakov, Eur. Phys. J. B **15**, 115 (2000).

[9] M. Pleimling and A. Hüller, J. Stat. Phys. **104**, 971 (2001).

[10] J. Barré, D. Mukamel, and S. Ruffo, Phys. Rev. Lett. **87**, 030601 (2001).

[11] I. Ispolatov and E. G. D. Cohen, Physica A **295**, 475 (2001).

[12] F. Gulminelli and Ph. Chomaz, Phys. Rev. E **66**, 046108 (2002).

[13] F. Leyvraz and S. Ruffo, J. Phys. A **35**, 285 (2002).

[14] F. Bouchet and J. Barré, J. Stat. Phys. **118**, 1073 (2005).

[15] M. Costeniuc, R. S. Ellis, H. Touchette, and B. Turkington, J. Stat. Phys. **119**, 1283 (2005).

[16] M. Costeniuc, R. S. Ellis, H. Touchette, and B. Turkington, Phys. Rev. E **73**, 026105 (2006).

[17] M. Kastner, Physica A **359**, 447 (2006).

[18] M. Promberger and A. Hüller, Z. Phys. B: Condens. Matter **97**, 341 (1995).

[19] M. Kastner, M. Promberger, and A. Hüller, J. Stat. Phys. **99**, 1251 (2000).

[20] A. Hüller and M. Pleimling, Int. J. Mod. Phys. C **13**, 947 (2002).

[21] H. Behringer, J. Phys. A **36**, 8739 (2003).

[22] H. Behringer, J. Phys. A **37**, 1443 (2004).

[23] J. Hove, Phys. Rev. E **70**, 056707 (2004).

[24] J. Naudts, Europhys. Lett. **69**, 719 (2005).

[25] M. Pleimling, H. Behringer, and A. Hüller, Phys. Lett. A **328**, 432 (2004).

[26] H. Behringer, M. Pleimling, and A. Hüller, J. Phys. A **38**, 973 (2005).

[27] A. Richter, M. Pleimling, and A. Hüller, Phys. Rev. E **71**, 056705 (2005).

[28] F. R. Brown and A. Yegulalp, Phys. Lett. A **155**, 252 (1991).

[29] M. Schmidt, Z. Phys. B: Condens. Matter **95**, 327 (1994).

[30] D. J. Wales and R. S. Berry, Phys. Rev. Lett. **73**, 2875 (1994).

[31] D. H. E. Gross, A. Ecker, and X. Z. Zhang, Ann. Phys. **5**, 446 (1996).

[32] M. Deserno, Phys. Rev. E **56**, 5204 (1997).

[33] S. B. Ota and S. Ota, J. Phys.: Condens. Matter **12**, 2233 (2000).

[34] M. D'Agostino, F. Gulminelli, Ph. Chomaz, M. Bruno, F. Cannata, R. Bougault, F. Gramegna, I. Iori, N. Le Neindre, G. V. Margagliotti, A. Moroni, and G. Vannini, Phys. Lett. B **473**, 219 (2000).

[35] M. Schmidt, R. Kusche, T. Hippler, J. Donges, W. Kronmüller, B. von Issendorff, and H. Haberland, Phys. Rev. Lett. **86**, 1191 (2001).

[36] J. Lee and J. M. Kosterlitz, Phys. Rev. Lett. **65**, 137 (1990).

[37] J. Lee and J. M. Kosterlitz, Phys. Rev. B **43**, 3265 (1991).

[38] W. Janke, Nucl. Phys. B (Proc. Suppl.) **63A-C**, 631 (1998).

[39] R. J. Baxter and F. Y. Wu, Phys. Rev. Lett. **31**, 1294 (1973).

[40] R. J. Baxter, *Exactly Solved Models in Statistical Mechanics* (Academic Press, London, 1982).

[41] M. Fukugita, H. Mino, M. Okawa, and A. Ukawa, J. Phys. A **23**, L561 (1990).

[42] N. Schreiber and J. Adler, J. Phys. A **38**, 7253 (2005).

[43] A. Stemmer and A. Hüller, Phys. Rev. B **58**, 887 (1998).

[44] M. N. Barber, in *Phase Transition and Critical Phenomena*, Vol. 8, edited by C. Domb and J. L. Lebowitz (Academic Press, London, 1983).

[45] V. Privman, *Finite Size Scaling and Numerical Simulation of Statistical Systems* (World Scientific, Singapore, 1990).

[46] M. S. S. Challa, D. P. Landau, and K. Binder, Phys. Rev. B **34**, 1841 (1986).

[47] H. Behringer, J. Stat. Mech.: Theory Exp. (2005) 06014.

[48] C. Borgs and R. Kotecký, J. Stat. Phys. **61**, 79 (1990).

[49] C. Borgs and R. Kotecký, Phys. Rev. Lett. **68**, 1734 (1992).

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

[51] R. B. Potts, Proc. Cambridge Philos. Soc. **48**, 106 (1952).

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

[53] W. Janke and R. Villanova, Nucl. Phys. B **489**, 679 (1997).

[54] R. Badke, P. Reinicke, and V. Rittenberg, J. Phys. A **18**, 73 (1985).

[55] R. Badke, P. Reinicke, and V. Rittenberg, J. Phys. A **18**, 653 (1985).

[56] S. S. Martinos, A. Malakis, and I. Hadjiagapiou, Physica A **352**, 447 (2005), in this work the density of states of the Baxter-Wu model has been determined in an approximate way and has then been used in a standard canonical analysis.

[57] K. Binder, Rep. Prog. Phys. **50**, 783 (1987).

[58] M. Nauenberg and D. J. Scalapino, Phys. Rev. Lett. **44**, 837 (1980).

[59] J. Salas and A. D. Sokal, J. Stat. Phys. **88**, 567 (1997).

[60] M. A. Novotny, D. P. Landau, and R. H. Swendsen, Phys. Rev. B **26**, 330 (1982).

[61] A. L. Owczarek and T. Prellberg, Europhys. Lett. **51**, 602 (2000); T. Prellberg and A. L. Owczarek, Phys. Rev. E **62**, 3780 (2000).