ELSEVIER

Nuclear Physics B (Proc. Suppl.) 63A-C (1998) 631–633

NUCLEAR PHYSICS B
PROCEEDINGS
SUPPLEMENTS

Canonical versus microcanonical analysis of first-order phase transitions

Wolfhard Janke[a]*

[a]Institut für Physik, Johannes Gutenberg-Universität Mainz, Staudinger Weg 7, 55099 Mainz, Germany

I discuss the relation between canonical and microcanonical analyses of first-order phase transitions. In particular it is shown that the microcanonical Maxwell construction is equivalent to the equal-peak-height criterion often employed in canonical simulations. As a consequence the microcanonical finite-size estimators for the transition point, latent heat and interface tension are identical to standard estimators in the canonical ensemble. Special emphasis is placed on various ways for estimating interface tensions. The theoretical considerations are illustrated with numerical data for the two-dimensional 10-state Potts model.

1. INTRODUCTION

First-order phase transitions [1] play an important role in the statistical mechanics of many physical phenomena ranging from the evolution of the early universe over fragmentation processes in nuclear physics to applications in condensed matter physics and material science. In the past few years considerable effort has been spent to develop refined analytical [2] and numerical [3–5] methods for their description. Most of this work starts from the *canonical* ensemble whose properties are governed by the partition function

$$Z_L(\beta) = \sum_{\{\sigma_i\}} e^{-\beta H} = \sum_E \Omega_L(E) e^{-\beta E}, \qquad (1)$$

where H is the Hamiltonian of the system, $\{\sigma_i\}$ denotes the degrees of freedom, $\beta = 1/k_B T$ is the inverse (canonical) temperature in natural units, and the subscript L indicates the system size. Alternatively one could also start directly from the density of states,

$$\Omega_L(E) = \sum_{\{\sigma_i\}} \delta_{H(\{\sigma_i\}),E}, \qquad (2)$$

which is the characteristic function of the *microcanonical* ensemble [6,7].

In the thermodynamic limit $L \longrightarrow \infty$ both approaches are known to be equivalent. In this note I will consider small systems and focus on a comparison of finite-size scaling (FSS) studies in the two ensembles.

*The author thanks the DFG for a Heisenberg fellowship.

2. CANONICAL AND MICROCANONICAL OBSERVABLES

From (2) the *microcanonical* entropy density and the inverse temperature can be defined as,

$$s_L(e) = \frac{1}{V} \ln \Omega_L(E), \quad \beta_{\mathrm{micro},L}(e) = \frac{\partial s_L(e)}{\partial e}, \qquad (3)$$

where V is the volume of the system and $e = E/V$. In simulations of the canonical ensemble it is straightforward to measure the energy distribution,

$$P_{\beta,L}(E) = c_1 \Omega_L(E) e^{-\beta E}, \qquad (4)$$

at a given inverse temperature β. Here c_1 is a constant *independent* of E which will be unimportant in the following. Together with (3) this yields immediately the microcanonical entropy,

$$\frac{1}{V} \ln(P_{\beta,L}(E)) = s_L(e) - \beta e + c_2, \qquad (5)$$

up to a constant and an additional linear term in e, which, however, is also added in a purely microcanonical setting when visualizing the anomaly of $s_L(e)$ at a first-order phase transition (cp., e.g., Fig. 1(a) of Ref. [7]). The microcanonical inverse temperature (3), on the other hand, is completely determined by the canonical data since the constant drops out and the canonical β acts just as a known constant offset,

$$\beta_{\mathrm{micro},L}(e) = \frac{\partial}{\partial e}\left[\frac{1}{V} \ln(P_{\beta,L}(E))\right] + \beta. \qquad (6)$$

For an illustration see Fig. 1(b).

PII S0920-5632(97)00854-2

The microcanonical pseudo-transition point $\beta_{t,L}$ is defined in a Maxwell construction by requiring that the line $\beta_{\text{micro},L}(e) = \beta_{t,L}$ divides the s-shaped curve of $\beta_{\text{micro},L}(e)$ into two equal areas, $\mathcal{A}_- = \mathcal{A}_+$ (see Fig. 1(b)) [6,7]. This also yields a finite-size estimator for the latent heat,

$$\Delta E_{\text{micro},L} = E_d - E_o, \tag{7}$$

and the interfacial entropy,

$$\Delta s^{\text{surf}}_{\text{micro},L} = \mathcal{A}_- = \mathcal{A}_+. \tag{8}$$

How are these quantities related to observables usually considered in the canonical ensemble? We will now prove that, for any system size L, $\beta_{t,L}$ is identical to $\beta_{\text{eqh},L}$, the inverse temperature at which the two peaks of the canonical energy distribution are of equal height (see Fig. 1(a)). Let us denote the location of the two maxima by E_o and E_d, and that of the minimum by E_{min}. At these extrema we obviously have $\partial P_{\beta,L}/\partial E = 0$, and thus by (6) $\beta_{\text{micro},L}(e_i) = \beta_{\text{eqh},L}$, $i = o, d, \text{min}$. To convince ourselves that $\beta_{\text{eqh},L}$ is equal to the microcanonically defined $\beta_{t,L}$ we have now to show that $\mathcal{A}_- = \mathcal{A}_+$. By using (3) we obtain $\mathcal{A}_- = \beta_{\text{eqh},L}(e_{\text{min}} - e_o) - (s_L(e_{\text{min}}) - s_L(e_o))$, and inserting (5) we arrive at

$$\mathcal{A}_- = \frac{1}{V} \ln \frac{P_{\beta,L}(E_o)}{P_{\beta,L}(E_{\text{min}})} = \frac{2\sigma_{od,L}}{L}, \tag{9}$$

with $\beta = \beta_{\text{eqh},L}$. Similarly we derive

$$\mathcal{A}_+ = \frac{1}{V} \ln \frac{P_{\beta,L}(E_d)}{P_{\beta,L}(E_{\text{min}})} = \frac{2\sigma_{od,L}}{L}. \tag{10}$$

Since $P_{\beta,L}(E_o) = P_{\beta,L}(E_d)$ at $\beta = \beta_{\text{eqh},L}$ we find as anticipated that $\mathcal{A}_- = \mathcal{A}_+$, and therefore that $\beta_{t,L} = \beta_{\text{eqh},L}$.

Moreover, Eqs. (9) and (10) also show that the definition (8) of $\Delta s^{\text{surf}}_{\text{micro},L}$ coincides with the common canonical definition of the interface tension $\sigma_{od,L}$ evaluated from equal-height energy distributions. Finally it is now trivial that the microcanonical definition (7) of $\Delta E_{\text{micro},L}$ is identical to the distance of the peaks of $P_{\beta,L}(E)$ at $\beta = \beta_{\text{eqh},L}$. In summary we have shown that microcanonical and canonical definitions of pseudo-transition points, latent heat, and interface tension are identical for all system sizes L. Therefore their FSS behaviour must trivially be the same.

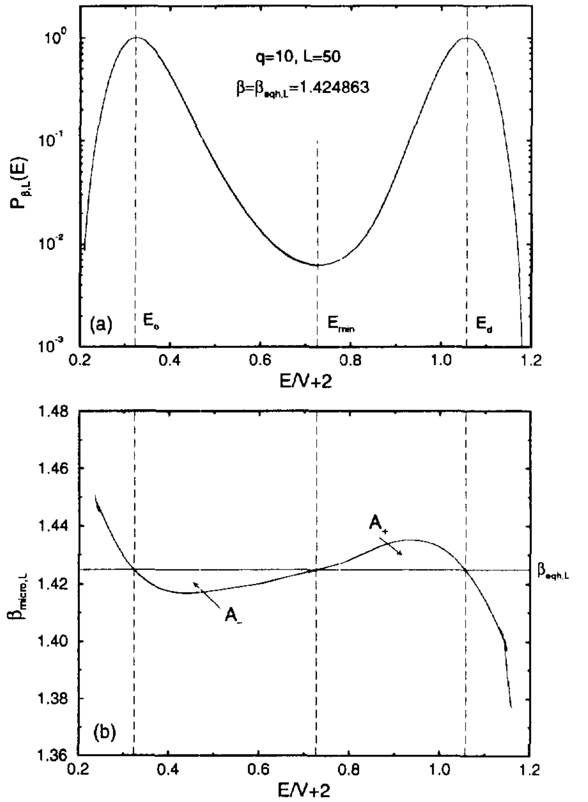

Figure 1. (a) Canonical energy distribution for $L=50$ reweighted to $\beta_{\text{eqh},L}$ on a logarithmic scale. (b) The microcanonical inverse temperature (6) derived from the energy distribution in (a).

3. NUMERICAL RESULTS

To illustrate these results we now consider the two-dimensional q-state Potts model Hamiltonian

$$H = -\sum_{\langle ij \rangle} \delta_{\sigma_i \sigma_j}, \tag{11}$$

with spins $\sigma_i = 1, \ldots, q$ living on square lattices of size $V = L \times L$ with periodic boundary conditions. Our canonical data for $L = 12$, 16, 20, 26, 34, and 50 are a combination from (unpublished) high-statistics simulations with the heat-bath and Metropolis algorithm and more recent multicanonical and multibondic simulations [5]. The canonical energy distribution reweighted to $\beta_{\text{eqh},L}$ for $L = 50$, and the resulting s-shaped curve for $\beta_{\text{micro},L}$ are shown in Fig. 1. In Fig. 2

the estimates of the interface tension according to the microcanonical definition (8) (i.e., (9) or (10) at $\beta_{t,L} = \beta_{\text{eqh},L}$) are plotted against $1/L$. As noticed previously [7], these finite-size estimates are closer to the infinite-volume limit than those obtained by evaluating (9) or (10) at the exactly known transition point $\beta_t = \ln(1+\sqrt{q})$ [8]. As we have shown above, however, this observation has nothing to do with the difference between microcanonical and canonical analyses. Rather, it is only caused by choosing two different β-sequences ($\beta_{t,L} = \beta_{\text{eqh},L}$ or β_t).

Moreover, even though the data according to the microcanonical definition are apparently closer to the infinite-volume limit, they are much more difficult to extrapolate. In fact, by using our data up to $L = 50$, we would clearly overestimate σ_{od}. This is even true for the data of Ref. [3] up to $L = 100$ and also most other earlier studies employing the equal-peak-height criterion. On the other hand, a least-squares fit to the FSS ansatz $\sigma_{od,L} = \sigma_{od} + c/L$ of our data at β_t yields $2\sigma_{od} = 0.09498(31)$ (with $Q = 0.27$), in excellent agreement with the exact result $2\sigma_{od} = 0.094701\dots$ [9] and the numerical estimate $2\sigma_{od} = 0.0950(5)$ at β_t of Ref. [8]. Of course, in general β_t is not known exactly. We have therefore evaluated (9), (10) also at the points $\beta_{w,L}$ (ratio-of-weights method) as defined in Ref. [4], which exhibit only exponentially small deviations from β_t. Here the FSS extrapolation yields $2\sigma_{od} = 0.09434(40)$ (with $Q = 0.63$), again in very good agreement with the exact result.

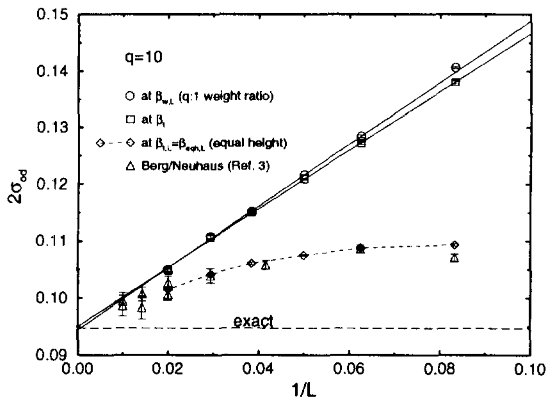

Figure 2. FSS of the interface tension.

4. CONCLUSIONS

We have explicitly demonstrated that the microcanonical Maxwell construction at first-order phase transitions is equivalent to the equal-peak-height criterion often employed in canonical simulations. This implies that the microcanonical and canonical pseudo-transition points $\beta_{t,L}$ and $\beta_{\text{eqh},L}$ coincide for all system sizes L. Consequently also the finite-size definitions of the latent heat and the interface tension are identical in the two ensembles. Furthermore it is shown that, contrary to a recent claim in the literature, FSS extrapolations of interface tensions at β_t or $\beta_{w,L}$ (ratio-of-weights method) are more reliable than those at $\beta_{t,L} = \beta_{\text{eqh},L}$.

REFERENCES

1. J.D. Gunton, M.S. Miguel, and P.S. Sahni, in *Phase Transitions and Critical Phenomena*, Vol. 8, eds. C. Domb and J.L. Lebowitz (Academic Press, New York, 1983); K. Binder, Rep. Prog. Phys. 50 (1987) 783; H.J. Herrmann, W. Janke, and F. Karsch (eds.) *Dynamics of First Order Phase Transitions* (World Scientific, Singapore, 1992).
2. C. Borgs and R. Kotecký, J. Stat. Phys. 61 (1990) 79; Phys. Rev. Lett. 68 (1992) 1734; C. Borgs, R. Kotecký, and S. Miracle-Solé, J. Stat. Phys. 62 (1991) 529.
3. B.A. Berg and T. Neuhaus, Phys. Lett. B267 (1991) 249; Phys. Rev. Lett. 68 (1992) 9.
4. C. Borgs and W. Janke, Phys. Rev. Lett. 68 (1992) 1738; W. Janke, Phys. Rev. B47 (1993) 14757.
5. W. Janke and S. Kappler, Phys. Rev. Lett. 74 (1995) 212.
6. A. Hüller, Z. Phys. B88 (1992) 79; B93 (1994) 401; B95 (1994) 63; R.W. Gerling and A. Hüller, Z. Phys. B90 (1993) 207.
7. D.H.E. Gross, A. Ecker, and X.Z. Zhang, Ann. Physik 5 (1996) 446.
8. A. Billoire, T. Neuhaus, and B.A. Berg, Nucl. Phys. B413 (1994) 795.
9. C. Borgs and W. Janke, J. Phys. I France 2 (1992) 2011.