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Microcanonical Finite-Size Scaling

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In the microcanonical ensemble, suitably defined observables show nonanalyticities and power-law behavior even for finite systems. For these observables, a microcanonical finite-size scaling theory is established and combined with the experimentally observed power-law behavior. Scaling laws are obtained which relate exponents of the finite system and critical exponents of the infinite system to the system-size dependence of the affiliated microcanonical observables.

KEY WORDS: Phase transitions; microcanonical ensemble; finite-size scaling; critical exponents.

1. INTRODUCTION

Numerical studies of phase transitions are restricted to finite systems. This automatically leads to a confrontation with the peculiarities of the statistical physics of finite systems and with the difficulties of an extrapolation to the thermodynamic limit. Here we are concerned with two of these aspects:

• The equivalence of statistical ensembles, valid for systems in the thermodynamic limit for a wide class of the physically relevant interaction potentials,[(1)] does not hold for finite systems. For example, microcanonical and canonical quantities differ in general, though both of them converge towards the corresponding infinite system value with increasing system size. However, the use of one of the statistical ensembles might be advantageous if the convergence towards the thermodynamic limit value is faster, or more expedient, than in the other ensemble.

• Properties of the infinite system have to be deduced from finite system data, for which finite-size scaling can be the method of choice. As introduced by Fisher and Barber,[(2)] finite-size scaling relations are derived

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for observables of the canonical ensemble, and will therefore be referred to as canonical finite-size scaling. These relations enable the determination of critical exponents of the infinite system from the system-size dependence of finite-system data. In this paper, features of microcanonical observables as sketched in Section 2 are combined with the method of finite-size scaling, to lead to an alternative tool for the analysis of finite-system data.

Note: This paper is not about microcanonical simulation techniques. The way that the data are produced is irrelevant for all that follows. As the microcanonical and the canonical ensemble are connected via Laplace transforms, from a suitable set of simulation data, both microcanonical and canonical observables can be computed. This paper is concerned with such microcanonical observables and their system size dependence.[2]

2. MICROCANONICAL DESCRIPTION OF FINITE SYSTEMS

By definition, the microcanonical entropy is the logarithm of the microcanonical partition function (density of states) Ω,

$$s(\varepsilon, m, L^{-1}) = L^{-d} \ln \Omega(\varepsilon, m, L^{-1}) \tag{2.1}$$

where L is the linear size, d is the spatial dimension of the system, m is the specific magnetization and ε the specific interaction energy. In a microcanonical description of finite systems, the zero-field magnetization and the isothermal magnetic susceptibility[3] can be defined in terms of the microcanonical entropy $s(\varepsilon, m, L^{-1})$. The zero-field magnetization $m_{h=0}$ follows from[(4, 5)]

$$\lim_{h \searrow 0} \{\max_m [s(\varepsilon, m, L^{-1}) + hm]\} = s(\varepsilon, m, L^{-1})\,|_{m = m_{h=0}(\varepsilon, L^{-1})} \tag{2.2}$$

The zero-field isothermal magnetic susceptibility (see ref. 6 for the straightforward but somewhat arduous derivation) reads

$$\chi_{T;\,h=0}(\varepsilon, L^{-1}) := \left.\frac{\partial m}{\partial h}\right|_{T;\,h=0} (\varepsilon, L^{-1})$$
$$= \left\{ \left[\frac{\partial s}{\partial \varepsilon} \left[\left(\frac{\partial^2 s}{\partial \varepsilon\, \partial m} \right)^2 \Big/ \frac{\partial^2 s}{\partial \varepsilon^2} - \frac{\partial^2 s}{\partial m^2} \right]^{-1} \right] (\varepsilon, m, L^{-1}) \right\}_{m = m_{h=0}(\varepsilon, L^{-1})} \tag{2.3}$$

[2] Reference 3 presents finite-size scaling of microcanonical quantities. The natural variables of a microcanonical potential of an Ising system are ε and m. In that sense the calculations in ref. 3 are not truly microcanonical.

[3] In this paper, results are presented for the zero-field magnetization and the isothermal magnetic susceptibility. An extension to other observables, e.g., the specific heat, can be done in a straightforward manner.

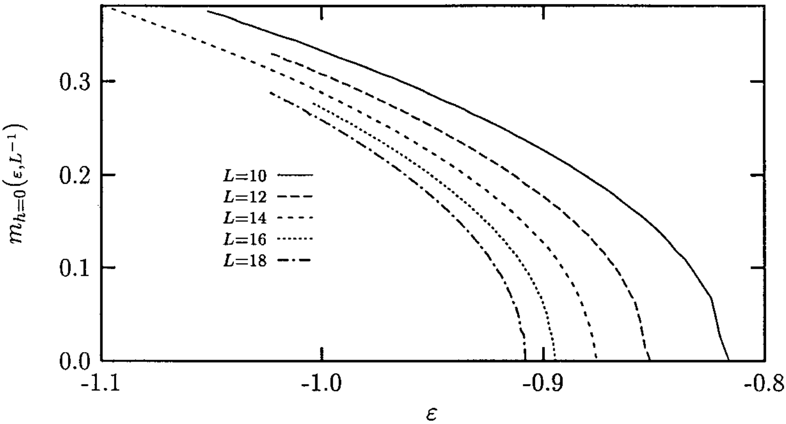

Fig. 1. Microcanonical zero-field magnetizations of finite 3*d*-Ising systems. As a guide to the eye, the data points are connected by straight lines.

Here, h is the magnetic field and, for notational convenience, the zero-field limit is denoted by $h = 0$.

The zero-field magnetization (Fig. 1) and the zero-field magnetic susceptibility (Fig. 2) are plotted for various system sizes of the 3*d*-Ising system with nearest-neighbour interaction and periodic boundary conditions on a cubic lattice.[4] The zero-field magnetization shows an instantaneous set-in as in the infinite system, and the zero-field susceptibility of the finite system is not rounded! The finite-system transition interaction energy, denoted by $\varepsilon_{TR}(L)$, is determined by the location of certain "transition features" like the peak of the susceptibility, and is obviously dependent on system-size. In Figs. 3 and 4, magnetizations and susceptibilities are plotted as functions of the finite-system reduced interaction energy

$$\tilde{\varepsilon} := \frac{\varepsilon - \varepsilon_{TR}(L)}{|\varepsilon_{TR}(L)|} \tag{2.4}$$

on a log–log–scale. The plots suggest power-law behavior and therefore the introduction of finite-system exponents $\beta_{\varepsilon, L}$ and $\gamma_{\varepsilon, L}$ defined by

$$m_{h=0}(\varepsilon, L^{-1}) \sim |\tilde{\varepsilon}|^{\beta_{\varepsilon, L}} \Theta(-\tilde{\varepsilon}) \qquad \text{and} \qquad \chi_{T;\, h=0}(\varepsilon, L^{-1}) \sim |\tilde{\varepsilon}|^{-\gamma_{\varepsilon, L}} \tag{2.5}$$

where Θ is Heavyside's step function.

In Figs. 5 and 6, magnetizations and susceptibilities are plotted as functions of the finite-system reduced interaction energy again. Data

[4] The data were generated by means of Monte Carlo-simulations. Due to the discreteness of the Ising system, the derivatives in (2.3) are substituted by ratios of differences.

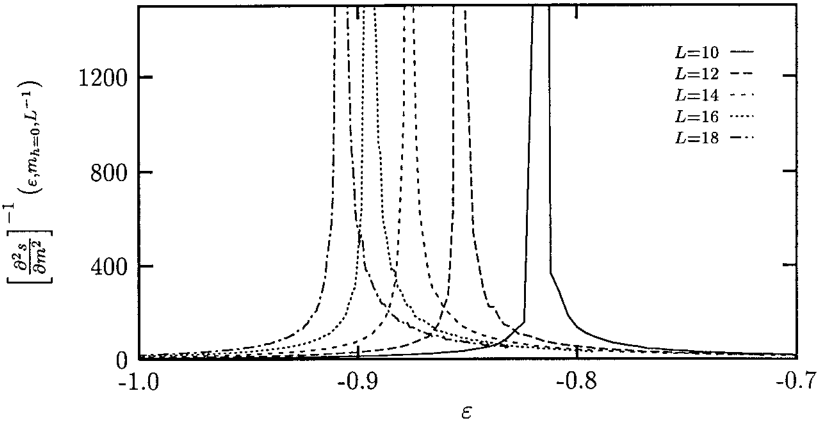

Fig. 2. Microcanonical zero-field isothermal magnetic susceptibilities of finite 3d-Ising systems. For numerical convenience, $[(\partial^2 s)/(\partial m^2)]^{-1}$ is plotted instead of $\chi_{T;\,h=0}$, as both quantities show the same microcanonical finite-size scaling behavior and—in the thermodynamic limit—the same critical behavior. Again, as a guide to the eye, the data points are connected by straight lines.

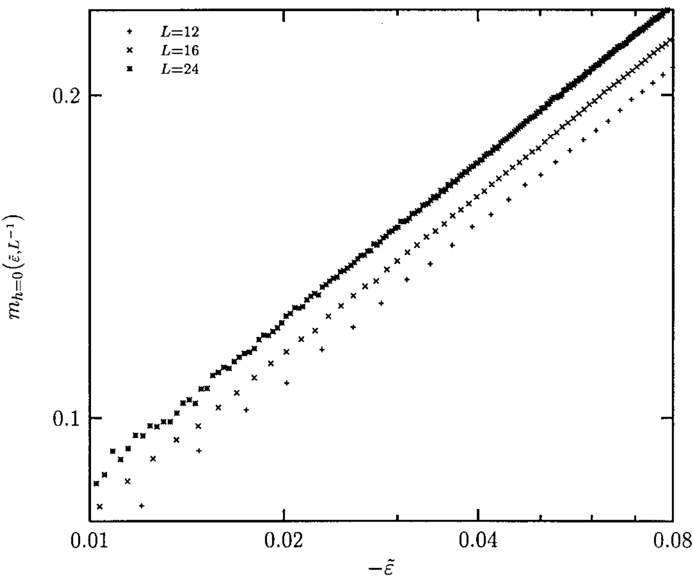

Fig. 3. Log–log–plot of the microcanonical zero-field magnetizations of finite 3d-Ising systems versus the finite-system reduced interaction energy $\tilde{\varepsilon}$. The behavior of $m_{h=0}$ suggests power-law behavior and the introduction of a finite-system exponent $\beta_{\varepsilon,\,L}$ which appears to be independent of the system-size.

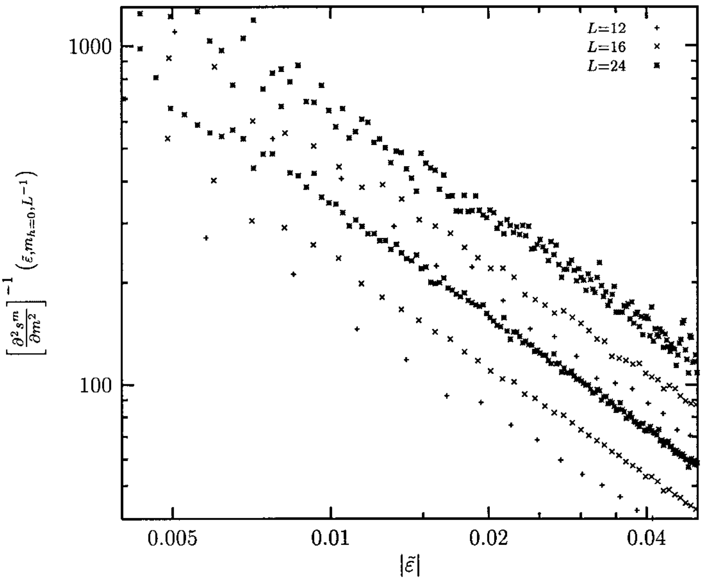

Fig. 4. Log–log–plot of the microcanonical zero-field isothermal magnetic susceptibilities of finite $3d$-Ising systems versus $|\tilde{\varepsilon}|$. For numerical convenience, $[(\partial^2 s)/(\partial m^2)]^{-1}$ is plotted instead of $\chi_{T;\,h=0}$, as both quantities show the same microcanonical finite-size scaling behavior and—in the thermodynamic limit—the same critical behavior. The behavior of $[(\partial^2 s)/(\partial m^2)]^{-1}$ suggests power-law behavior and the introduction of a finite-system exponent $\gamma_{\varepsilon,\,L}$ which appears to be independent of the system-size.

collapse has been achieved by the use of L-dependent scale factors $A(L^{-1})$ for $m_{h=0}$ and $B(L^{-1})$ for $\chi_{T;\,h=0}$ on the vertical axes. Therefore, it seems to be evident that the finite-system exponents are independent of the system-size (i.e., take on the same value $\forall L^{-1} \neq 0$), and for the $3d$-Ising system we obtain $\beta_{\varepsilon,\,L} \approx 0.5$ and $\gamma_{\varepsilon,\,L} \approx 1$ for all L considered. Note that these values differ from those expected in the thermodynamic limit, $\beta_\varepsilon = \beta/(1-\alpha) \approx 0.37$ and $\gamma_\varepsilon = \gamma/(1-\alpha) \approx 1.38$ (see Section 3 for the definitions of these exponents). At first sight this seems to be alarming. In Remark (d) of Section 3, however, a proposal will be made how to resolve this problem. The finite-system exponents $\beta_{\varepsilon,\,L}$ and $\gamma_{\varepsilon,\,L}$ are found to show approximately mean-field[5] values. Regrettably, we cannot give a sound explanation for this observation. A connection between the mean-field values and the analyticity properties of the microcanonical entropy is established in Remark (f) of Section 3.

[5] Not only for $3d$-Ising systems with periodic boundary conditions as investigated in this paper. The same values have been found for $3d$-Ising systems with open boundary conditions and for $2d$-Ising systems with periodic boundary conditions.

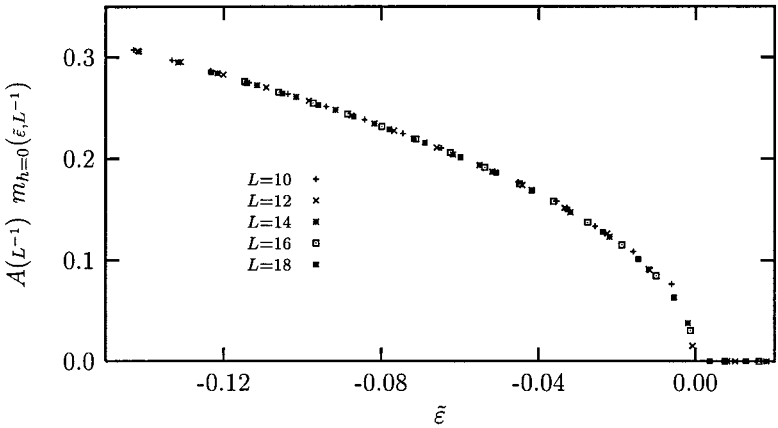

Fig. 5. Scaling plot of the microcanonical zero-field magnetization. Multiplication of $m_{h=0}$ by suitable scaling factors $A(L^{-1})$ and plotting the thus obtained results against $\tilde{\varepsilon}$ yields data collapse. This observation gives rise to the assumption that the finite-system exponent $\beta_{\varepsilon,L}$ shows no system-size dependence. For convenience, only some of the data points are shown.

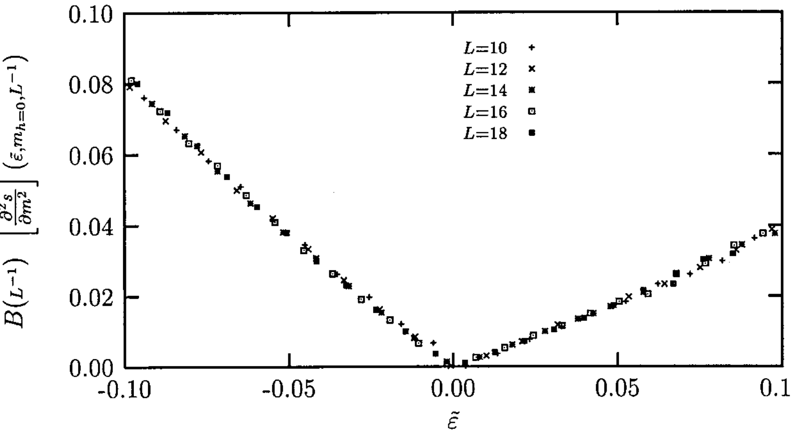

Fig. 6. Scaling plot of the microcanonical zero-field isothermal magnetic susceptibility. Multiplication of $[(\partial^2 s)/(\partial m^2)]^{-1}$ by suitable scaling factors $B(L^{-1})$ and plotting the thus obtained results against $\tilde{\varepsilon}$ yields data collapse. This observation gives rise to the assumption that the finite-system exponent $\gamma_{\varepsilon,L}$ shows no system-size dependence. Again, for convenience, only some of the data points are shown.

In this paper, a microcanonical finite-size scaling theory is developed, taking into account the following constraints (partly justified above):

(i) consistence with the canonical finite-size scaling theory

(ii) power-law behavior of the finite-system magnetization and susceptibility

(iii) finite-system exponents which do not depend on the system-size and which are not necessarily identical to the critical exponents of the infinite system.

Any case other than power-law behavior will be disregarded in this paper.

3. MICROCANONICAL FINITE-SIZE SCALING

In the vicinity of a critical point ($t, h \approx 0$ or $\varepsilon^*, m \approx 0$), the standard separation of thermodynamic potentials[7, 8] into a singular part (subscript *sing*) which describes the non-analytic behavior of the observables under investigation, and a regular part (subscript *reg*) containing all other terms, can be performed. For the free energy density and the specific entropy this reads

$$g(t, h) = g_{sing}(t, h) + g_{reg}(t, h) \tag{3.1}$$

$$s(\varepsilon^*, m) = s_{sing}(\varepsilon^*, m) + s_{reg}(\varepsilon^*, m) \tag{3.2}$$

where $t := (T - T_c)/T_c$ is the reduced temperature, T_c the critical temperature, $\varepsilon^* = \tilde{\varepsilon}(L^{-1} \to 0) = (\varepsilon - \varepsilon_c)/|\varepsilon_c|$ is the reduced interaction energy and ε_c the critical interaction energy. It can be shown (see e.g., ref. 9 and references therein) that in the thermodynamic limit the singular parts of the various potentials are homogeneous functions. In terms of the free energy density and the specific entropy, this reads

$$g_{sing}(t, h) = \lambda^{-1} g_{sing}(\lambda^{a_t} t, \lambda^{a_h} h) \tag{3.3}$$

and

$$s_{sing}(\varepsilon^*, m) = \lambda^{-1} s_{sing}(\lambda^{a_\varepsilon} \varepsilon^*, \lambda^{a_m} m) \tag{3.4}$$

The critical exponents are implicitly defined by the power laws

$$c_{h=0}(T) \sim |t|^{-\alpha_t} \qquad c_{h=0}(\varepsilon) \sim |\varepsilon^*|^{-\alpha_\varepsilon} \tag{3.5}$$

$$m_{h=0}(T) \sim |t|^{\beta_t}\, \Theta(-t) \qquad m_{h=0}(\varepsilon) \sim |\varepsilon^*|^{\beta_\varepsilon}\, \Theta(-\varepsilon^*) \tag{3.6}$$

$$\chi_{T;\,h=0}(T) \sim |t|^{-\gamma_t} \qquad \chi_{\beta;\,h=0}(\varepsilon) \sim |\varepsilon^*|^{-\gamma_\varepsilon} \tag{3.7}$$

$$m_{t=0}(h) \sim |h|^{1/\delta_h}\,\mathrm{sgn}(h) \qquad h_{\varepsilon^*=0}(m) \sim |m|^{1/\delta_m}\,\mathrm{sgn}(m) \tag{3.8}$$

where the exponents α_t, β_t, γ_t, δ_h are the "traditional" critical exponents (α, β, γ, δ) and sgn denotes the sign function. The critical exponents can be expressed in terms of the degrees of homogeneity (a_t, a_h) or (a_ε, a_m) of Eqs. (3.3) and (3.4):

$$\alpha_t = \frac{2a_t - 1}{a_t} \qquad \alpha_\varepsilon = \frac{1 - 2a_\varepsilon}{a_\varepsilon} = \frac{\alpha_t}{1 - \alpha_t} \tag{3.9}$$

$$\beta_t = \frac{1 - a_h}{a_t} \qquad \beta_\varepsilon = \frac{a_m}{a_\varepsilon} = \frac{\beta_t}{1 - \alpha_t} \tag{3.10}$$

$$\gamma_t = \frac{2a_h - 1}{a_t} \qquad \gamma_\varepsilon = \frac{1 - 2a_m}{a_\varepsilon} = \frac{\gamma_t}{1 - \alpha_t} \tag{3.11}$$

$$\delta_h = \frac{a_h}{1 - a_h} \qquad \delta_m = \frac{a_m}{1 - a_m} = \frac{1}{\delta_h} \tag{3.12}$$

The degrees of homogeneity of (3.3) and (3.4) are connected via the relations $a_t = 1 - a_\varepsilon$ and $a_h = 1 - a_m$.

The concept of thermodynamic potentials can be carried over to finite systems. However, since the equivalence of ensembles is valid only in the thermodynamic limit, thermodynamic potentials of finite systems have to be classified as **c**anonical (superscript c) or **m**icrocanonical (superscript m) quantities. Starting point for canonical finite-size scaling (CFSS) is the

CFSS Assumption.

$$g^c_{sing}(t, h, L^{-1}) = \lambda^{-1} g^c_{sing}(\lambda^{a_t} t, \lambda^{a_h} h, \lambda^{1/d} L^{-1}) \tag{3.13}$$

i.e., for large but finite systems, $g^c_{sing}(t, h, L^{-1})$ is a homogeneous function.[2] Starting point for microcanonical finite-size scaling (MFSS) is the

MFSS Assumption.

$$s^m_{sing}(\varepsilon^*, m, L^{-1}) = \lambda^{-1} s^m_{sing}(\lambda^{a_\varepsilon} \varepsilon^*, \lambda^{a_m} m, \lambda^{1/d} L^{-1}) \tag{3.14}$$

i.e., for large but finite systems, $s^m_{sing}(\varepsilon^*, m, L^{-1})$ is a homogeneous function.

In the rest of this paper, the consequences of the microcanonical finite-size scaling assumption are discussed. The structure of this assumption looks extremely similar to that of the canonical one. Nevertheless, in connection with some additional knowledge about microcanonical observables,

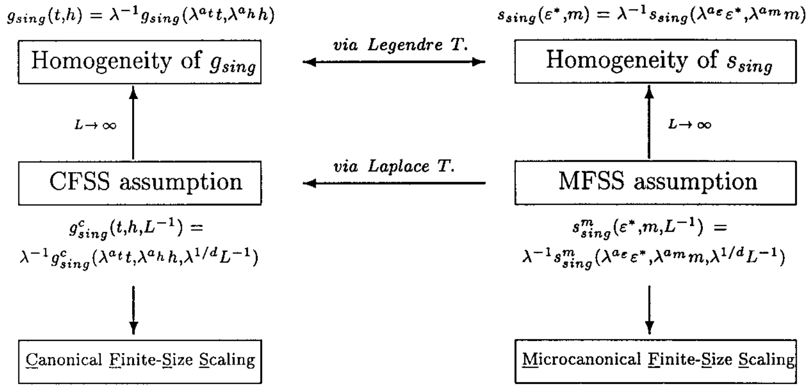

Fig. 7. Homogeneity relations for the singular parts of the free energy density and the specific entropy for finite (Eqs. (3.13), (3.14)) as well as infinite systems (Eqs. (3.3), (3.4)). In the thermodynamic limit, a Legendre transform connects the homogeneity of g_{sing} to the homogeneity of s_{sing} (see ref. 7), whereas for finite systems it can be shown that the canonical finite-size scaling (CFSS) assumption is a consequence of the microcanonical finite-size scaling (MFSS) assumption, i.e., MFSS is consistent with CFSS.[6]

it leads to remarkable consequences—stated in the remarks at the end of this section—beyond those familiar to canonical finite-size scaling.

We have shown elsewhere[6] that the microcanonical finite-size scaling assumption (3.14) entails the canonical one (3.13), and thus complies with the demanded property (i) of Section 2. The interrelation between the various homogeneity relations and their connection to the finite-size scaling formalisms is sketched in Fig. 7.

From the microcanonical finite-size scaling assumption (3.14) and Eqs. (2.2) and (2.3), the microcanonical finite-size scaling relations of the magnetization and the susceptibility are easily derived:[5]

$$m^*_{h=0}(\varepsilon^*, L^{-1}) = \lambda^{-a_m} m^*_{h=0}(\lambda^{a_\varepsilon} \varepsilon^*, \lambda^{1/d} L^{-1}) \stackrel{\lambda = L^d}{=} L^{-d a_m} \Phi_{m^*}(L^{d a_\varepsilon} \varepsilon^*) \tag{3.15}$$

$$\chi^*_{T;\, h=0}(\varepsilon^*, L^{-1}) = \lambda^{1-2a_m} \chi^*_{T;\, h=0}(\lambda^{a_\varepsilon} \varepsilon^*, \lambda^{1/d} L^{-1}) \stackrel{\lambda = L^d}{=} L^{d(1-2a_m)} \Phi_{\chi^*}(L^{d a_\varepsilon} \varepsilon^*) \tag{3.16}$$

where the Φ_i are so-called microcanonical finite-size scaling functions which describe the behavior of the magnetization and the susceptibility of finite systems in the vicinity of the critical point ε_c of the infinite system.

Microcanonical finite-size scaling of the transition point: The scaling behavior of the finite-system transition interaction energy ε_{TR} can be deduced from either one of the functions Φ_{m^*} or Φ_{χ^*}: Let x_{TR} be the value of x for which $\Phi_{m*}(x)$ or $\Phi_{\chi*}(x)$ show a certain "transition feature." Then the associated finite-system transition interaction energy can be defined implicitly by

$$x_{TR} = L^{da_\varepsilon} \varepsilon^* |_{\varepsilon = \varepsilon_{TR}(L)} = L^{da_\varepsilon} \frac{\varepsilon - \varepsilon_c}{|\varepsilon_c|} \bigg|_{\varepsilon = \varepsilon_{TR}(L)} \tag{3.17}$$

With $D := x_{TR} |\varepsilon_c|$, the finite-size scaling relation

$$\varepsilon_{TR}(L) = \varepsilon_c + D L^{-da_\varepsilon} \tag{3.18}$$

is obtained.

Remarks. (a) A further quantity $\tilde{s}^m_{sing}$ can be introduced, which is defined as the singular part of the entropy, written in terms of the finite-system reduced interaction energy (2.4). Using (3.18), the thus defined entropy $\tilde{s}^m_{sing}$ can be shown to possess the same degrees of homogeneity as s^m_{sing}:

$$\tilde{s}^m_{sing}(\tilde{\varepsilon}, m, L^{-1}) = \lambda^{-1} \tilde{s}^m_{sing}(\lambda^{a_\varepsilon} \tilde{\varepsilon}, \lambda^{a_m} m, \lambda^{1/d} L^{-1}) \tag{3.19}$$

where

$$\tilde{s}^m_{sing}(\tilde{\varepsilon}, m, L^{-1}) := s^m_{sing}\left(\varepsilon^* = \tilde{\varepsilon} \frac{\varepsilon_{TR}(L)}{\varepsilon_c} + x_{TR} L^{-da_\varepsilon}, m, L^{-1}\right) \tag{3.20}$$

Starting from (3.19), microcanonical finite-size scaling relations can be derived for the magnetization and the susceptibility. They illustrate the system-size dependence of the behavior of $m_{h=0}$ and $\chi_{T;\,h=0}$ in the vicinity of the transition point $\varepsilon_{TR}(L)$ of the finite system:

$$\tilde{m}_{h=0}(\tilde{\varepsilon}, L^{-1}) = \lambda^{-a_m} \tilde{m}_{h=0}(\lambda^{a_\varepsilon} \tilde{\varepsilon}, \lambda^{1/d} L^{-1}) \overset{\lambda = L^d}{=} L^{-da_m} \Phi_{\tilde{m}}(L^{da_\varepsilon} \tilde{\varepsilon}) \tag{3.21}$$

$$\tilde{\chi}_{T;\,h=0}(\tilde{\varepsilon}, L^{-1}) = \lambda^{1-2a_m} \tilde{\chi}_{T;\,h=0}(\lambda^{a_\varepsilon} \tilde{\varepsilon}, \lambda^{1/d} L^{-1}) \overset{\lambda = L^d}{=} L^{d(1-2a_m)} \Phi_{\tilde{\chi}}(L^{da_\varepsilon} \tilde{\varepsilon}) \tag{3.22}$$

(b) Numerical data suggest power-law behavior for both the magnetization and the susceptibility of finite systems. Then, the microcanonical finite-size scaling functions $\Phi_{\tilde{m}}$ and $\Phi_{\tilde{\chi}}$ have to be power laws, governed by the respective finite-system exponents which are *not* determined by the degrees of homogeneity of s^m_{sing} of (3.14) (and therefore differ from the infinite-system exponents in general):

$$\Phi_{\tilde{m}}(x) \propto |x|^{\beta_{\varepsilon,L}} \Theta(-x) \Rightarrow \tilde{m}_{h=0}(\tilde{\varepsilon}, L^{-1}) = L^{d(a_\varepsilon \beta_{\varepsilon,L} - a_m)} |\tilde{\varepsilon}|^{\beta_{\varepsilon,L}} \Theta(-\tilde{\varepsilon}) \tag{3.23}$$

$$\Phi_{\tilde{\chi}}(x) \propto |x|^{-\gamma_{\varepsilon,L}} \Rightarrow \tilde{\chi}_{T;\,h=0}(\tilde{\varepsilon}, L^{-1}) = L^{d(1-2a_m - a_\varepsilon \gamma_{\varepsilon,L})} |\tilde{\varepsilon}|^{-\gamma_{\varepsilon,L}} \tag{3.24}$$

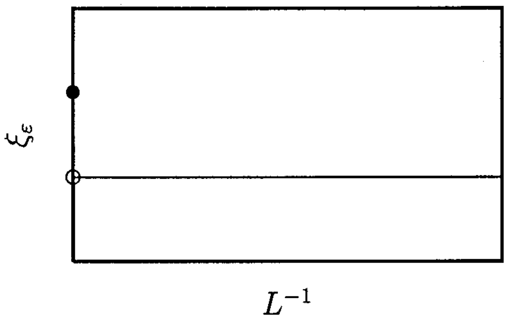

Fig. 8. "Sudden" change of an exponent $\xi_\varepsilon \in \{\beta_\varepsilon, \gamma_\varepsilon\}$ describing the properties of microcanonical zero-field quantities in the vicinity of the transition point.

As a consequence, the exponents characterizing the leading behavior of the microcanonical zero-field quantities in the vicinity of the corresponding transition points show a "sudden" change from their finite-system values to the respective infinite-system values (Fig. 8). This is discussed in detail in Remark (d).

(c) The power laws with finite-system exponents (3.23) and (3.24) suggest the introduction of a further homogeneity relation for the singular part of the microcanonical entropy:

$$\tilde{s}^m_{sing}(\tilde{\varepsilon}, m, L^{-1}) = \lambda^{-1} \tilde{s}^m_{sing}(\lambda^{a^+_\varepsilon} \tilde{\varepsilon}, \lambda^{a^+_m} m, L^{-1}) \qquad (3.25)$$

In analogy to the infinite-system case, this is a homogeneity with respect to *two* variables only (in contrast to the microcanonical finite size scaling assumption (3.14))! Then, the finite-system exponents can be expressed in terms of a^+_ε, a^+_m and these exponents are connected by scaling relations (which are equivalent to those of the infinite system since they merely reflect homogeneity properties). For Ising systems in $d = 2, 3$, the validity of these scaling relations is supported by experimental results.

(d) In Section 2, we found finite-system exponents $\beta_{\varepsilon, L}$ and $\gamma_{\varepsilon, L}$ which seem to be independent of system-size, but show values different from their infinite-system counterparts β_ε and γ_ε. Such a behavior is illustrated in Fig. 8 and appears to be alarming at first sight. For the purpose of an illustration how such a behavior can emerge from a "well-behaving" entropy function, we consider the following explicit form of $\tilde{s}^m_{sing}$ as an example:

$$\tilde{s}^*_m = |\tilde{\varepsilon}|^{\alpha_\varepsilon + 2} [A_\pm + \tilde{A}_\pm (|\tilde{\varepsilon}| L^{1/\nu_\varepsilon})^{\alpha_{\varepsilon, L} - \alpha_\varepsilon}] + |\tilde{\varepsilon}|^{\gamma_\varepsilon} m^2 [B_\pm + \tilde{B}_\pm (|\tilde{\varepsilon}| L^{1/\nu_\varepsilon})^{\gamma_{\varepsilon, L} - \gamma_\varepsilon}]$$
$$+ |m|^{1 + 1/\delta_m} [C_\pm + \tilde{C}_\pm (|m| L^{\beta_\varepsilon/\nu_\varepsilon})^{1/\delta_{m, L} - 1/\delta_m}] \qquad (3.26)$$

with

$$\tilde{\varepsilon} = \varepsilon^* + DL^{-1/\nu_\varepsilon} \tag{3.27}$$

where $A_\pm$, $\tilde{A}_\pm$, $B_\pm$, $\tilde{B}_\pm$, $C_\pm$, $\tilde{C}_\pm$ are arbitrary amplitudes which may take on different values below $(-)$ and above $(+)$ the transition interaction energy ε_{TR}. It can be shown easily that $\tilde{s}^m_{sing}$ is a homogeneous function according to (3.14) and (3.19) for arbitrary values of $\alpha_{\varepsilon,L}$, $\gamma_{\varepsilon,L}$ and $\delta_{m,L}$. For finite-system exponents $\alpha_{\varepsilon,L} < \alpha_\varepsilon$, $\gamma_{\varepsilon,L} < \gamma_\varepsilon$ and $1/\delta_{m,L} < 1/\delta_m$, the leading asymptotic behavior of microcanonical observables calculated from (3.26) is governed by the $\tilde{A}_\pm$-, $\tilde{B}_\pm$- and $\tilde{C}_\pm$-terms for all finite L, and therefore the non-analyticities are subject to the *finite-system exponents* $\alpha_{\varepsilon,L}$, $\gamma_{\varepsilon,L}$ and $\delta_{m,L}$. The $A_\pm$-, $B_\pm$- and $C_\pm$-terms are subdominant and therefore irrelevant for the leading asymptotic behavior. However, considering $\tilde{s}^m_{sing}$ in the limit $L \to \infty$, the L-dependent terms vanish:

$$\lim_{L^{-1}\to 0} \tilde{s}^m_{sing} = A_\pm \, |\tilde{\varepsilon}|^{\alpha_\varepsilon+2} + B_\pm m^2 \, |\tilde{\varepsilon}|^{\gamma_\varepsilon} + C_\pm \, |m|^{1/\delta_m+1} \tag{3.28}$$

Calculating the asymptotic behavior of the microcanonical observables from the remaining $A_\pm$-, $B_\pm$- and $C_\pm$-terms leads to non-analyticities governed by the *critical exponents of the infinite system* α_ε, γ_ε and δ_m. This results in a sudden change of the leading asymptotic behavior, and therefore in a switching of the exponents from their finite-system to their infinite-system value. Put briefly, the switching turns out to be a consequence of the fact that limiting procedures do not commute in general.

For simplicity, we disregarded the fact that the entropy is a concave function in the thermodynamic limit. However, this property could easily be included in (3.26). Note that this function is not the most general form of $\tilde{s}^m_{sing}$—but sufficient as an illustrative example—and leads to relations between the finite-system exponents. These relations can be avoided when additional terms in $\tilde{s}^m_{sing}$ are considered.

(e) Note that (3.14) even accounts for the possibility of s^m_{sing} showing no system-size dependence at all. Nevertheless, this case results in a system size dependence of the free energy density g^c_{sing} and in canonical finite-size scaling (see refs. 10 and 6 for details).

(f) The canonical free energy density g^c is analytic for all finite L and shows nonanalyticities only in the thermodynamic limit. To the best of our knowledge, no proof exists that the microcanonical specific entropy s^m is analytic for finite systems. Depending on the values of $\beta_{\varepsilon,L}$ and $\gamma_{\varepsilon,L}$, Eq. (3.26) implies the possibility for $\tilde{s}^m_{sing}$ to be either an analytic or a non-analytic function. Due to the particular form of the microcanonical observables (2.2) and (2.3), even a completely analytic entropy function can result in non-analyticities of microcanonical observables,[6] whether for the infinite system or for finite system-sizes. Mean-field values are a prominent example of exponents which are in accord with an analytic entropy function.

4. CONCLUSION

A microcanonical finite-size scaling theory has been developed in accordance with the demanded properties (i)–(iii) stated in Section 2. Amazingly, although the scaling laws (3.4) and (3.14) comprise identical degrees of homogeneity a_ε and a_m for the singular parts of the entropy of the finite *and* the infinite system respectively, they nevertheless can account for power law behaviour with different values for the critical exponents of the infinite system β_ε, γ_ε and for the finite-system exponents $\beta_{\varepsilon, L}$, $\gamma_{\varepsilon, L}$, where the latter ones are independent of system-size for all finite L. Therefore, an extrapolation of the finite-system exponents toward the thermodynamic limit is *not* an appropriate procedure to determine the critical exponents of the infinite system. However, the microcanonical finite-size scaling theory can provide another approach to the critical exponents: Finite-size scaling laws, similar to the canonical ones in structure, have been found, which relate the system-size dependence of the *amplitudes* of microcanonical observables of finite systems to the critical exponents of the infinite system.

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