

# ABSCENCE OF HYPERSCALING VIOLATIONS FOR PHASE TRASITIONS WITH POSITIVE SPECIFIC HEAT EXPONENT

R. HILFER

ABSTRACT. Finite size scaling theory and hyperscaling are analyzed in the ensemble limit which differs from the finite size scaling limit. Different scaling limits are discussed. Hyperscaling relations are related to the identification of thermodynamics as the infinite volume limit of statistical mechanics. This identification combined with finite ensemble scaling leads to the conclusion that hyperscaling relations cannot be violated for phase transitions with strictly positive specific heat exponent. The ensemble limit allows to derive analytical expressions for the universal part of the finite size scaling functions at the critical point. The analytical expressions are given in terms of general  $H$ -functions, scaling dimensions and a new universal shape parameter. The universal shape parameter is found to characterize the type of boundary conditions, symmetry and other universal influences on critical behaviour. The critical finite size scaling functions for the order parameter distribution are evaluated numerically for the cases  $\delta = 3, \delta = 5$  and  $\delta = 15$  where  $\delta$  is the equation of state exponent. Using a tentative assignment of periodic boundary conditions to the universal shape parameter yields good agreement between the analytical prediction and Monte-Carlo simulations for the twodimensional Ising model. Analytical expressions for critical amplitude ratios are derived in terms of critical exponents and the universal shape parameters. The paper offers an explanation for the numerical discrepancies and the pathological behaviour of the renormalized coupling constant in mean field theory. Low order moment ratios of difference variables are proposed and calculated which are independent of boundary conditions, and allow to extract estimates for a critical exponent.

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[page 63, §1]

## I. Introduction

[63.2.1.1] Analysis of finite size effects [1] has become an indispensable tool in the numerical simulation of critical phenomena [2, 3, 4, 5]. [63.2.1.2] According to the nonrigorous renormalization group derivations of finite size scaling [6] the singular part of the free energy  $f_{sing}(t, h, u, L)$  and the correlation length  $\xi$  have the scaling form

$$f_{sing}(t, h, u, L) = L^{-d} \tilde{f}(tL^{y_t}, hL^{y_h}, uL^{y_u}) \quad (1.1)$$

$$\xi(t, h, u, L) = L \tilde{\xi}(tL^{y_t}, hL^{y_h}, uL^{y_u}) \quad (1.2)$$

where  $t$  denotes the reduced temperature  $t = (T - T_c)/T_c$  relative to the critical temperature  $T_c$  of the infinite system,  $h$  is the field conjugate to the order parameter,  $u$  is an irrelevant variable,  $L$  the system size,  $d$  the spatial dimension, and  $y_t, y_h > 0$  and  $y_u < 0$  are the renormalization group eigenvalues for  $t, h$  and  $u$ .

[63.2.2.1] More heuristically there are several possibilities to introduce finite size scaling through a scaling hypothesis. [63.2.2.2] One such method [7, 8] assumes that the probability density  $p(\psi, L)$  for the order parameter  $\Psi$  of the transition can be written as

$$p(\psi, L, \xi) = L^{d(d_\Psi - d^*)/(d - d^*)} \tilde{p}_\Psi(\psi L^{d(d_\Psi - d^*)/(d - d^*)}, L/\xi_{d^*}) \quad (1.3)$$

where  $d_\Psi$  is the anomalous or scaling dimension of the order parameter,  $d^*$  is Fishers anomalous dimension of the vacuum [9], and  $\xi_{d^*}$  is Binders thermodynamic length [8]. [63.2.2.3] If hyperscaling holds then  $d^* = 0$ , the thermodynamic length becomes the correlation length,  $\xi_0 = \xi$ , and the exponent in (1.3) reduces to the familiar form  $d_\Psi = \beta/\nu$  where  $\beta$  is the order parameter exponent and  $\nu$  the correlation length exponent. [63.2.2.4] The finite size scaling Ansatz (1.3) can be extended to arbitrary composite operators, an important case being the energy density  $\mathcal{E}$  for which the exponent becomes  $d_\mathcal{E} = (1 - \alpha)/\nu$  if hyperscaling holds. [63.2.2.5] All finite size scaling relations (1.1)–(1.3) are assumed to hold in the finite size scaling limit [page 64, §0]

$$L \rightarrow \infty, \xi \rightarrow \infty \quad (1.4)$$

where  $L/\xi = c$  is kept constant.

[64.1.1.1] Despite their very plausible and seemingly general character finite size scaling relations are not generally valid [10]. [64.1.1.2] Violations of finite size scaling are closely related to violations of hyperscaling relations [10, 11]. [64.1.1.3] These violations have been rationalized via the so called mechanism of “dangerous irrelevant” variables [12] or by saying that the correlation length  $\xi$  is not the only relevant length [5]. [64.1.1.4] “Dangerous irrelevant” variables are relevant to critical behaviour

because by definition they induce a singularity in one or both of the scaling functions  $\tilde{f}(x, y, z)$  and  $\tilde{\xi}(x, y, z)$  as  $z \rightarrow 0$ . [64.1.1.5] The mechanism of dangerous irrelevant variables does not give general modelindependent criteria for the validity or violation of hyperscaling and finite size scaling. [64.1.1.6] The present paper attempts to establish positivity of the specific heat exponent as such a general criterion for the validity of hyperscaling relations.

[64.1.2.1] Given the scaling Ansatz (1.3) another well known problem with present finite size scaling theory concerns integrals of the scaling function appearing in (1.3). [64.1.2.2] To see this calculate the finite size scaling form for the absolute moments of order  $\sigma$  from (1.3) for the case  $d^* = 0$  as

$$\langle |\Psi|^\sigma \rangle(L, \xi) = L^{-\sigma\beta/\nu} \tilde{\Psi}_\sigma(L/\xi) \quad (1.5)$$

where the new scaling function  $\tilde{\Psi}_\sigma(z)$  is given in terms of  $\tilde{p}_\Psi(x, y)$  as

$$\tilde{\Psi}_\sigma(y) = \int |x|^\sigma \tilde{p}_\Psi(x, y) dx. \quad (1.6)$$

[64.1.2.3] From these moments one finds for the ratio related to the renormalized coupling constant the result

$$g(L, \xi) = \frac{\langle \Psi^4 \rangle}{\langle \Psi^2 \rangle^2} = \frac{\tilde{\Psi}_4(L/\xi)}{\tilde{\Psi}_2^2(L/\xi)}. \quad (1.7)$$

which implies that

$$g_\infty(c) = \lim_{\substack{L, \xi \rightarrow \infty \\ L/\xi = c}} g(L, \xi) = \frac{\tilde{\Psi}_4(c)}{\tilde{\Psi}_2^2(c)} \quad (1.8)$$

in the finite size scaling limit for which  $L/\xi = c$  is a constant. [64.1.2.4] While the value  $g_\infty(\infty) = 3$  for the trivial high temperature fixed point is universal, the value  $g_\infty(0)$  for the nontrivial fixed point is found to depend on seemingly nonuniversal factors. [64.1.2.5] Moreover, numerical difficulties arise in different methods of estimating  $g_\infty(0)$  [7, 13, 14, 15, 16]. [64.1.2.6] The problem is particularly apparent for the mean field universality class. [64.1.2.7] Twodimensional conformal field theory predicts that  $g_\infty(0) \propto \eta^{-1}$  in the limit  $\eta \rightarrow 0$  [17]. [64.1.2.8] Here  $\eta$  is the correlation function exponent, and  $\eta = 0$  in mean field theory. [64.1.2.9] Similarly for the  $n$ -vector models above four dimensions  $g_\infty(0)$  becomes  $n$ -dependent [15] in stark contrast to the “superuniversality” of mean field exponents and amplitude ratios. [64.1.2.10] The numerical agreement with Monte-Carlo simulations is poor and the authors of Ref. [13] have called for further studies to clarify the discrepancy. [64.1.2.11] The present paper attempts to contribute to this point.

[64.2.1.1] Let me summarize the objectives of this work resulting from the above exposition of two problems with current finite size scaling theory. [64.2.1.2] The first objective is to provide general criteria for the validity or violation of finite size scaling. [64.2.1.3] The second

objective is to investigate the finite size scaling functions and finite size amplitude ratios in the ensemble limit.

[64.2.2.1] Methodically, the results of this paper follow directly from a recently introduced classification theory of phase transition [18, 19, 20, 21, 22, 23]. [64.2.2.2] Let me briefly outline the basic idea. Within the classification theory it was shown that each phase transition in thermodynamics as well as in statistical mechanics is characterized by a set of generalized Ehrenfest orders plus a set of slowly varying functions. [64.2.2.3] This classification is macroscopic in the sense that it involves only thermodynamic averages while conformal field theory focusses on microscopic higher order correlation functions. [64.2.2.4] The classification in thermodynamics [18] is based upon the application of fractional calculus, the one in statistical mechanics [22] rests upon the theory of limit distributions for sums of independent random variables. [64.2.2.5] The latter theory, which cannot be employed in the traditional way of performing the scaling limit, became applicable by introducing a fundamentally new scaling limit, which was called *ensemble limit*. [64.2.2.6] In the ensemble limit critical systems decompose into an infinite ensemble of infinitely large, yet uncorrelated blocks. [64.2.2.7] The classification schemes in thermodynamics and statistical mechanics are mathematically very different but can be related to each other by studying the fluctuations in the ensemble of blocks. [64.2.2.8] The difference between the classification schemes is found to be related to violations of hyperscaling. [64.2.2.9] Moreover, a thermodynamic form of scaling, called *finite ensemble scaling*, emerges from the classification. [64.2.2.10] The basic idea of this paper is to regard finite ensemble scaling as a macroscopic or thermodynamic form of finite size scaling. [64.2.2.11] Thus the limit distributions in the classification theory ought to be related to the probability distributions, such as  $p(\psi, L, \xi)$ , appearing in finite size scaling theory. [64.2.2.12] To show that this expectation is indeed borne out it is first necessary to discuss in some detail the different scaling limits and finite ensemble scaling. [64.2.2.13] Subsequently the classification approach can be related to the theory of finite size scaling, hyperscaling and general scaling at critical points. [64.2.2.14] In the last two sections critical finite size scaling functions and amplitude ratios are discussed and compared with Monte Carlo simulations. [64.2.2.15] The comparison of the predicted universal part of the finite size scaling functions for the order parameter distribution at criticality with Monte Carlo simulations for Ising models shows good quantitative agreement.

## II. Scaling limits

[64.2.3.1] The finite size scaling limit  $L \rightarrow \infty, \xi \rightarrow \infty$  with  $L/\xi$  constant is a special kind of field theoretical

scaling limit. [64.2.3.2] A fieldtheoretic scaling limit involves three different limits: 1. The *thermodynamic limit*  $L \rightarrow \infty$  in which the system size becomes large, 2. the *continuum limit*  $a \rightarrow 0$  in which a microscopic length becomes small, and 3. the *critical* [page 65, §0] *limit*  $\xi \rightarrow \infty$  in which the correlation length of a particular observable (scaling field) diverges.

[65.1.1.1] This section discusses the recently introduced ensemble limit [20, 21, 22, 23] as a novel kind of field theoretic scaling limit, and relates it to traditional limiting procedures.

### II.A. Discretization in field theory

[65.1.2.1] Consider a macroscopic classical continuous system within a cubic subset of  $\mathbf{R}^d$  with volume  $V$  and linear extension  $L$ . [65.1.2.2] The finite macroscopic volume  $V = L^d$  is partitioned into  $N$  mesoscopic cubic blocks of linear size  $\xi$ . [65.1.2.3] The coordinate of the center of each block is denoted by  $\vec{y}_j$  ( $j = 1, \dots, N$ ). [65.1.2.4] Each block is further partitioned into  $M$  microscopic cells of linear size  $a$  whose coordinates with respect to the center of the block are denoted as  $\vec{x}_i$  ( $i = 1, \dots, M$ ). [65.1.2.5] The position vector for cell  $i$  in block  $j$  is  $\vec{y}_j + \vec{x}_i$ . [65.1.2.6] This partitioning of  $\mathbf{R}^d$  is depicted in Figure 1 for  $d = 2$  and  $M = N = 25$ . [65.1.2.7] The number of blocks is given by

$$N = \left(\frac{L}{\xi}\right)^d \quad (2.1)$$

while the number of cells within each block is

$$M = \left(\frac{\xi}{a}\right)^d. \quad (2.2)$$

[65.2.0.8] The total number of cells inside the volume  $V$  is then  $NM = (L/a)^d$ .

[65.2.0.9] Let the physical system enclosed in  $V$  be describable as a classical field theory with timeindependent fields  $\vec{\varphi}(\vec{z}, t = 0) = \vec{\varphi}(\vec{z})$  and a local microscopic configurational Hamiltonian density

$$\mathcal{H}(\vec{\varphi}) = \frac{J}{2}(\partial_\mu \vec{\varphi}(\vec{z}))^2 + U(\vec{\varphi}(\vec{z})) \quad (2.3)$$

where  $\partial_\mu = \partial/\partial x_\mu$  ( $\mu = 1, \dots, d$ ) denotes partial derivatives. [65.2.0.10] A particular example for the potential  $U(\vec{\varphi})$  would be the  $\phi^4$ -model for which

$$U(\vec{\varphi}) = m^2(\vec{\varphi}(\vec{z}))^2/2 + g(\vec{\varphi}(\vec{z}))^4/4!. \quad (2.4)$$

where the parameters  $m$  and  $g$  are the mass and the coupling constant. [65.2.0.11] For future convenience the parameters of the field theory are collected into the parameter vector  $\vec{\Pi} = (\Pi_1, \Pi_2, \dots) = (J, m, g, \dots)$ . [65.2.0.12] The partitioning introduced above allows two regularizations into a lattice field theory. [65.2.0.13] On the mesoscopic level the regularized block action representing

the total configurational energy of a single block (e.g. for block  $j$ ) reads

$$\begin{aligned} \mathcal{H}_{MN}(\vec{\varphi}(\vec{y}_j)) &= -J \sum_{\langle \vec{x}_i, \vec{x}_k \rangle_j} \vec{\varphi}(\vec{y}_j + \vec{x}_i) \cdot \vec{\varphi}(\vec{y}_j + \vec{x}_k) \\ &\quad + \sum_{i=1}^M U(\vec{\varphi}(\vec{y}_j + \vec{x}_i)) \end{aligned} \quad (2.5)$$

where  $\langle \vec{x}_i, \vec{x}_k \rangle_j$  denotes nearest neighbour pairs of cells inside block  $j$ , ( $j = 1, \dots, N$ ) such that each pair is counted once. [65.2.0.14] On the macroscopic level one has the discretized action between blocks (representing the total configurational energy)

$$\mathfrak{H}_{MN}(\vec{\phi}) = -\mathfrak{J} \sum_{\langle \vec{y}_j, \vec{y}_k \rangle} \vec{\phi}(\vec{y}_j) \cdot \vec{\phi}(\vec{y}_k) + \sum_{j=1}^N \mathfrak{U}(\vec{\phi}(\vec{y}_j)) \quad (2.6)$$

where now  $\langle \vec{y}_j, \vec{y}_k \rangle$  denotes nearest neighbour blocks. [65.2.0.15] Although the overall form of the discretizations is identical for  $\mathcal{H}_{MN}$  and  $\mathfrak{H}_{MN}$  the macroscopic discretized

fields  $\vec{\phi}$  and interactions  $\mathfrak{J}, \mathfrak{U}$  may in general require renormalization in the infinite volume and continuum limit, and are therefore denoted by different symbols. [65.2.0.16] Rearranging eq. (2.5) the macroscopic discretized action  $\mathfrak{H}_{MN}(\vec{\phi})$  is related to the mesoscopic discretized action  $\mathcal{H}_{MN}(\vec{\varphi}(\vec{y}_j))$  through

$$\begin{aligned} \mathfrak{H}_{MN}(\vec{\phi}) &= \mathfrak{H}_{MN}(\vec{\varphi}) = \sum_{j=1}^N \mathcal{H}_{MN}(\vec{\varphi}(\vec{y}_j)) \\ &\quad + \sum_{\langle \vec{y}_j + \vec{x}_i, \vec{y}_l + \vec{x}_k \rangle} \vec{\varphi}(\vec{y}_j + \vec{x}_i) \cdot \vec{\varphi}(\vec{y}_l + \vec{x}_k) \end{aligned} \quad (2.7)$$

expressing a decomposition into bulk plus surface energies. [65.2.0.17] Here  $\widetilde{\sum}$  expresses a summation over nearest neighbour [page 66, §0] cells in the surface layers of adjacent blocks such that each pair of adjacent block surface cells is counted once. [66.1.0.1] Conventional field theory or equilibrium statistical mechanics assumes that the surface term which is of order  $\mathcal{O}(NM^{(d-1)/d})$  becomes negligible compared to the bulk term which is of order  $\mathcal{O}(NM)$  in the field-theoretic continuum limit.

## II.B. Fieldtheoretic scaling limit

[66.1.1.1] Consider now a scalar local observable  $X_{MN}(\vec{\varphi}(\vec{x}_i + \vec{y}_j))$  (composite operator) fluctuating from cell to cell. [66.1.1.2] The fluctuations generally define a correlation length  $\xi_X(\vec{\Pi})$  whose magnitude depends on the observable in question and the parameters  $\vec{\Pi}$  in the Hamiltonian. [66.1.1.3] The reconstruction of the continuum theory from its discretization is usually carried out in two steps [24]. [66.1.1.4] First one takes the (thermodynamic) infinite volume limit  $L \rightarrow \infty$  at constant  $a$  as the limit of canonical (Boltzmann-Gibbs) probability measures in the finite volume. [66.1.1.5] The existence of this limit requires stability and temperedness of the interaction potentials [25]. The limit amounts to setting  $N = 1$  and thus  $\mathfrak{H}_{M1} = \mathcal{H}_{M1}$ .

[66.1.2.1] Given the existence of the infinite volume limit one studies the scaling limit  $a \rightarrow 0, \vec{\Pi} \rightarrow \vec{\Pi}_c$  of the regularized infinite-volume theory. [66.1.2.2] This field theoretic limit in general requires the renormalization of the action  $\mathcal{H}_{M1}(\vec{\varphi})$ . [66.1.2.3] The quantities of main interest are the correlation functions

$$\begin{aligned} &\langle X_{\infty 1}(\vec{x}_1) \dots X_{\infty 1}(\vec{x}_n) \rangle_{\vec{\Pi}} \\ &= \mathcal{Z}^{-1} \int X_{\infty 1}(\vec{\varphi}(\vec{x}_1)) \dots X_{\infty 1}(\vec{\varphi}(\vec{x}_n)) \\ &\quad \times \exp(-\mathcal{H}_{\infty 1}(\vec{\varphi}(\vec{0}))) \mathcal{D}[\vec{\varphi}] \quad (2.8) \\ &= \lim_{a \rightarrow 0} \lim_{L \rightarrow \infty} \int X_{M1}(\vec{\varphi}(\vec{x}_1)) \dots X_{M1}(\vec{\varphi}(\vec{x}_n)) \\ &\quad \times d\mu(\vec{\varphi}; a, L, \vec{\Pi}) \quad (2.9) \end{aligned}$$

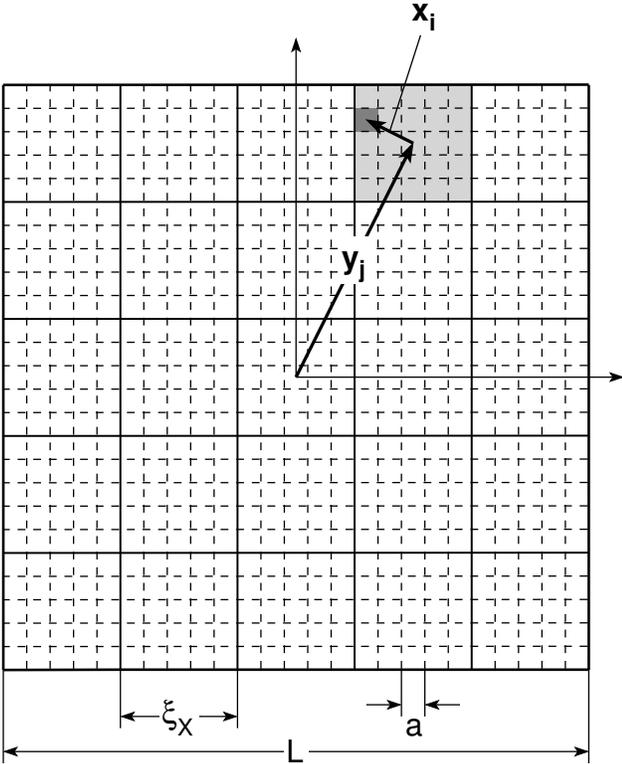


FIGURE 1. Discretization of a macroscopic classical continuum system of size  $L$  into mesoscopic blocks (solid lines) of size  $\xi_X$  and microscopic cells (dashed lines) of size  $a$ . The vector  $\vec{y}_j$  denotes the position of block  $j$ , the vector  $\vec{x}_i$  is the position vector for cell  $i$  relative to the block center.

within a single block here chosen to be the one at the origin, i.e.  $\vec{y}_1 = \vec{0}$ . [66.1.2.4] The normalization constant  $\mathcal{Z}$  is the partition function, the measure  $\mu(\vec{\varphi}; a, L, \vec{\Pi})$  is the finite volume lattice probability distribution on the space of field configurations, and the notation  $\langle \dots \rangle_{\vec{\Pi}}$  for the expectation value expresses its dependence on the parameters in the Hamiltonian. [66.1.2.5] The correlation functions (2.9) are plagued the well known short distance singularities in the continuum limit  $a \rightarrow 0$ . [66.1.2.6] The standard approach [24] to this problem is to keep  $a > 0$  fixed and to use instead a lattice rescaling procedure in which the auxiliary rescaling factor  $b \propto a^{-1} \rightarrow \infty$  diverges. [66.1.2.7] This keeps the theory explicitly finite at all steps. [66.1.2.8] Thus the field theoretic continuum theory is defined through the limiting renormalized correlation functions

$$\langle X_{\infty 1}(\vec{x}_1) \dots X_{\infty 1}(\vec{x}_n) \rangle_{\vec{\Pi}_c} = \lim_{b \rightarrow \infty} A(b)^n \langle X_{\infty 1}(b\vec{x}_1) \dots X_{\infty 1}(b\vec{x}_n) \rangle_{\vec{\Pi}(b)} \quad (2.10)$$

where  $A(b)$  is the field renormalization. [66.1.2.9] The parameters  $\vec{\Pi}$  approach a critical point  $\vec{\Pi}_c = \vec{\Pi}(\infty)$  such that the rescaled correlation length

$$\lim_{b \rightarrow \infty} \xi_X(\vec{\Pi}(b))/b > 0 \quad (2.11)$$

remains nonzero. [66.2.0.10] The field theoretical continuum or scaling limit is called ‘‘massive’’ or ‘‘massless’’ depending on whether the rescaled correlation length approaches a finite constant or diverges to infinity. [66.2.0.11] Because  $a > 0$  is fixed equations (2.2) and (2.11) imply  $b \propto \xi \propto M^{1/d}$  in the massive scaling limit, and this allows to rewrite equation (2.10) as

$$\langle X_{\infty 1}(\vec{x}_1) \dots X_{\infty 1}(\vec{x}_n) \rangle_{\vec{\Pi}_c} = \lim_{M \rightarrow \infty} D(M)^n \langle X_{\infty 1}(M^{1/d}\vec{x}_1) \dots X_{\infty 1}(M^{1/d}\vec{x}_n) \rangle_{\vec{\Pi}(M^{1/d})} \quad (2.12)$$

if the limit exists. [66.2.0.12] In that case the renormalization factor  $D(M)$  has the form

$$D(M) \sim M^{d_X/d} \quad (2.13)$$

by virtue of the relation

$$A(b) \sim b^{d_X}, \quad (2.14)$$

which follows generally from renormalization group theory [26]. [66.2.0.13] Here  $d_X$  is the anomalous dimension of the operator  $X$ .

## II.C. Ensemble limit

[66.2.1.1] The ensemble limit introduced in [20] is a way of defining infinite volume continuum averages from the discretized theory in a finite volume without actually calculating the measure  $\mu(\vec{\varphi}, 0, \infty, \vec{\Pi}_c)$  explicitly. [66.2.1.2] The idea is to focus on the one point functions given

by (2.12) with  $n = 1$  as

$$\langle X_{\infty 1} \rangle_{\vec{\Pi}_c} = \langle X_{\infty 1}(\vec{x}_i) \rangle_{\vec{\Pi}_c} \quad (2.15)$$

$$= \lim_{M \rightarrow \infty} D(M) \langle X_{\infty 1}(M^{1/d}\vec{x}_i) \rangle_{\vec{\Pi}(M)} \quad (2.16)$$

$$= \lim_{M \rightarrow \infty} \frac{D(M)}{M} \left\langle \sum_{i=1}^M X_{\infty 1}(M^{1/d}\vec{x}_i) \right\rangle_{\vec{\Pi}(M)} \quad (2.17)$$

where independence of  $\vec{x}_i$  by virtue of translation invariance has been used in the first and the last equality. [66.2.1.3] At criticality these functions contain information about fluctuations through the renormalization factor  $D(M)$  for field averages.

[66.2.2.1] For a given field configuration the fluctuating local observable inside cell  $i$  ( $i = 1, \dots, M$ ) of block  $j$  ( $j = 1, \dots, N$ ) will again be denoted by  $X_{MN}(\vec{\varphi}(\vec{y}_j + \vec{x}_i))$  as defined above and illustrated in Figure 1. [66.2.2.2] The block variables

$$X_{MN}(\vec{\varphi}(\vec{y}_j)) = \sum_{i=1}^M X_{MN}(\vec{\varphi}(\vec{y}_j + \vec{x}_i)) \quad (2.18)$$

( $j = 1, \dots, N$ ) are defined by summing the cell variables and the ensemble variable [page 67, §0]

$$X_{MN}(\vec{\varphi}) = \sum_{j=1}^N X_{MN}(\vec{\varphi}(\vec{y}_j)) \quad (2.19)$$

is obtained by summing the block variables. For  $a > 0$  the *ensemble limit* is defined as the limit

$$M \rightarrow \infty, N \rightarrow \infty, \frac{N}{M} = \frac{aL}{\xi_X(\vec{\Pi})^2} = C_0 \quad (2.20)$$

where  $C_0$  is a constant. [67.1.0.1] In the ensemble limit  $L \sim (\xi_X(\vec{\Pi}))^2$  as compared to  $L \sim \xi_X(\vec{\Pi})$  in the field theoretic scaling limit. [67.1.0.2] The difference to the field theoretic scaling limit is that thermodynamic ( $L \rightarrow \infty$ ), continuum ( $a \rightarrow 0$ ) and critical ( $\vec{\Pi} \rightarrow \vec{\Pi}_c$ ) limit are taken simultaneously. [67.1.0.3] In this way an infinite ensemble of regularized infinite classical continuum systems is generated. [67.1.0.4] The elements of the ensemble are replicas of one and the same system governed by the Hamiltonian density  $\mathcal{H}(\vec{\varphi})$ . [67.1.0.5] Thus the ensemble limit generates an ensemble in the sense of statistical mechanics.

[67.1.1.1] The critical or noncritical averages  $\langle X_{\infty 1} \rangle_{\vec{\Pi}}$  can be calculated in the ensemble limit as

$$\langle X_{\infty 1} \rangle_{\vec{\Pi}} = \lim_{M, N \rightarrow \infty} \frac{1}{MN} X_{MN}(\vec{\varphi}). \quad (2.21)$$

[67.1.1.2] This equation states that macroscopic ensemble averages can either be calculated using equations (2.9) in the traditional scaling limit or directly using equations (2.18) and (2.19) in the ensemble limit. [67.1.1.3] Equation (2.21) gives the connection between the scaling limit

and the ensemble limit. [67.1.1.4] Note that the validity of eq. (2.21) requires the existence of the renormalized field theory. [67.1.1.5] Thus the left hand side of (2.21) cannot be calculated at anequilibrium phase transitions [21, 22] while the right hand side can still be calculated in such cases.

## II.D. Summary of different scaling limits

[67.1.2.1] The main difference of the ensemble limit as compared to other scaling limits is that the three limits  $a \rightarrow 0, L \rightarrow \infty, \vec{\Pi} \rightarrow \vec{\Pi}_c$  are simultaneously performed while in other limits only two of these limits are taken simultaneously. [67.1.2.2] There are  $2^3 = 8$  ways of performing the scaling limit with the three variables  $a, L, \vec{\Pi}$  depending on whether a particular variable is set equal to its limiting value or not. [67.2.0.3] The different possibilities are summarized in Table I. [67.2.0.4] Note that only the ensemble limit (1.) and the related critical limit (7.) in an infinite continuum theory yield an infinite number of uncorrelated blocks. [67.2.0.5] The close relation between the ensemble limit and the massive finite size scaling limit (5.) is apparent if  $N_0 \gg 1$ .

## III. Finite ensemble scaling

[67.2.1.1] The quantity of main interest for finite ensemble scaling [21, 22, 23] is the macroscopic ensemble sum  $X_{MN}(\vec{\varphi})$  given by (2.19). [67.2.1.2] The idea is to neglect completely its microscopic definition (2.18) in terms of cell variables, and to consider the mesoscopic block variables  $X_{MN}(\vec{\varphi}(\vec{y}))$  as a starting point. [67.2.1.3] The univariate probability distribution of the ensemble variable is defined as

$$P_{X_{MN}}(x) = \text{Prob}\{X_{MN}(\vec{\varphi}) \leq x\}. \quad (3.1)$$

[67.2.1.4] Because the ensemble limit automatically generates independent and identically distributed block variables  $X_{MN}(\vec{\varphi}(\vec{y}_j))$  the standard theory of stable laws [27, 28] can be applied. [67.2.1.5] It yields the existence and uniqueness of limiting distributions for the linearly renormalized ensemble sums

$$\begin{aligned} Z_{MN}(\vec{\varphi}) &= \frac{X_{MN}(\vec{\varphi}) - C_N}{D_N} \\ &= \frac{\sum_{j=1}^N X_{MN}(\vec{\varphi}(\vec{y}_j)) - C_N}{D_N} \end{aligned} \quad (3.2)$$

where  $D_N > 0$  and  $C_N$  are real numbers. [67.2.1.6] Remember that this holds for sums of arbitrary block variables independent of their microscopic definition. [67.2.1.7] The index  $M$  serves only as a reminder for the fact that the ensemble limit is used.

[page 68, §1] [68.1.1.1] The distribution function  $P_{Z_{MN}}(x)$  for  $Z_{MN}(\vec{\varphi})$  is given in terms of  $P_{X_{MN}}(x)$  as  $P_{X_{MN}}(D_N x + C_N)$  and it is thus sufficient to consider  $P_{X_{MN}}(x)$ . [68.

1.1.2] The (weak) ensemble limit of these probability distribution functions

$$\lim_{\substack{M, N \rightarrow \infty \\ N/M=c}} P_{X_{MN}}(D_N x + C_N) = H(x; \varpi_X(c), \zeta_X(c), C(c), D(c)) \quad (3.3)$$

exists if and only if  $H(x; \varpi_X(c), \zeta_X(c), C(c), D(c))$  is a stable distribution function whose characteristic function

$$h(k) = \langle e^{ikX} \rangle = \int_{-\infty}^{\infty} e^{ikx} dH(x) \quad (3.4)$$

has the form

$$\begin{aligned} h(k; \varpi_X, \zeta_X, C, D) &= \\ \exp\left(iCk - D|k|^{\varpi_X} e^{\frac{i\pi}{2}(1-|\varpi_X|)\zeta_X \text{sgn}k}\right) \end{aligned} \quad (3.5)$$

for  $\varpi_X \neq 1$  and

$$\begin{aligned} h(k; 1, \zeta_X, C, D) &= \\ \exp\left(iCk - D|k|(1 - i\zeta_X \frac{2}{\pi} \text{sgn}k \log|k|)\right) \end{aligned} \quad (3.6)$$

for  $\varpi_X = 1$ . [68.1.1.3] The  $c$ -dependence of the parameters  $\varpi_X(c), \zeta_X(c), C(c), D(c)$  has been suppressed to shorten the notation. [68.1.1.4] The parameters  $\varpi_X, \zeta_X, C, D$  obey

$$\begin{aligned} 0 &< \varpi_X \leq 2 \\ -1 &\leq \zeta_X \leq 1 \\ -\infty &< C < \infty \\ 0 &\leq D. \end{aligned} \quad (3.7)$$

[68.1.1.5] If the limit exists, and  $D \neq 0$ , the constants  $D_N$  must have the form

$$D_N = (N\Lambda(N))^{1/\varpi_X} \quad (3.8)$$

where  $\Lambda(N)$  is a slowly varying function [28], i.e.

$$\lim_{x \rightarrow \infty} \frac{\Lambda(bx)}{\Lambda(x)} = 1 \quad (3.9)$$

for all  $b > 0$ .

[68.1.1.6] The forms (3.5) and (3.6) of the limiting characteristic functions imply the following scaling relations for the stable probability densities  $h(x; \varpi_X, \zeta_X, C, D)$ . [68.1.1.7] If  $\varpi_X \neq 1$  then

$$\begin{aligned} h(x; \varpi_X, \zeta_X, C, D) &= \\ D^{-1/\varpi_X} h((x - C)D^{-1/\varpi_X}; \varpi_X, \zeta_X, 0, 1) \end{aligned} \quad (3.10)$$

holds, while for  $\varpi_X = 1$  one has

$$\begin{aligned} h(x; \varpi_X, \zeta_X, C, D) &= \\ D^{-1} h((x - C)D^{-1} - 2\frac{\zeta_X}{\pi} \log D; \varpi_X, \zeta_X, 0, 1). \end{aligned} \quad (3.11)$$

[68.2.0.8] The parameters  $C$  and  $D$  correspond to the centering and the width of the distribution.

TABLE 1. Different possible scaling limits. FSS stands for finite size scaling, and ES for ensemble scaling.

Type of scaling limit	$a$	$L$	$\vec{\Pi}$	$\frac{aL}{\xi^2}$	$M$	$N$	$\frac{N}{M}$
1. discrete ES limit	$\rightarrow 0$	$\rightarrow \infty$	$\rightarrow \vec{\Pi}_c$	$\rightarrow c^{1/d}$	$\rightarrow \infty$	$\rightarrow \infty$	$\rightarrow c$
2.	$\rightarrow 0$	$\rightarrow \infty$	$= \vec{\Pi}_c$	$= 0$	$= \infty$	$= 1$	$= 0$
3. massive scaling limit	$\rightarrow 0$	$= \infty$	$\rightarrow \vec{\Pi}_c$	$= \infty$	$= \infty$	$\rightarrow 1$	$= 0$
4. massless scaling limit	$\rightarrow 0$	$= \infty$	$= \vec{\Pi}_c$	$= \frac{\infty}{\infty^2}$	$= \infty$	$= 1$	$= 0$
5. massive FSS limit	$= 0$	$\rightarrow \infty$	$\rightarrow \vec{\Pi}_c$	$= 0$	$= \infty$	$\rightarrow N_0$	$= 0$
6. massless FSS limit	$= 0$	$\rightarrow \infty$	$= \vec{\Pi}_c$	$= \frac{0}{\infty^2}$	$= \infty$	$= 1$	$= 0$
7. continuum ES limit	$= 0$	$= \infty$	$\rightarrow \vec{\Pi}_c$	$= 0 \cdot \infty$	$= \infty$	$= \infty$	$= \frac{\infty}{\infty}$
8.	$= 0$	$= \infty$	$= \vec{\Pi}_c$	$= \frac{0 \cdot \infty}{\infty^2}$	$= \infty$	$= 1$	$= 0$

[68.2.1.1] Strictly stable probability densities (i.e. those with  $\varpi_X \neq 1$ ) are conveniently written in terms of Mellin transforms [29, 30]. [68.2.1.2] This representation is useful for computations and involves the general class of  $H$ -functions [31, 32]. [68.2.1.3] For  $1 < \varpi_X < 2$  corresponding to equilibrium phase transitions two cases are distinguished. [68.2.1.4] If  $|\zeta_X| \neq 1$  then [30, 22]

$$h(x; \varpi_X, \zeta_X, 0, 1) = \quad (3.12)$$

$$\frac{1}{\varpi_X} H_{22}^{11} \left( x \left| \begin{array}{cc} (1 - 1/\varpi_X, 1/\varpi_X) & (1 - \varrho, \varrho) \\ (0, 1) & (1 - \varrho, \varrho) \end{array} \right. \right)$$

where  $\varrho = \frac{1}{2} - \frac{\zeta_X}{\varpi_X} + \frac{\zeta_X}{2}$  and the definition of the general  $H$ -function  $H_{PQ}^{mn}$  is given in the appendix. [68.2.1.5] If  $|\zeta_X| = 1$  then for  $1 < \varpi_X < 2$

$$h(x; \varpi_X, \pm 1, 0, 1) =$$

$$\frac{1}{\varpi_X} H_{11}^{10} \left( x \left| \begin{array}{cc} (1 - 1/\varpi_X, 1/\varpi_X) \\ (0, 1) \end{array} \right. \right) \quad (3.13)$$

[68.2.1.6] Similar expressions hold for  $0 < \varpi_X < 1$  [30, 22]. [68.2.1.7] The special case  $\varpi_X = 2$  of the general limit theorem (3.3) is the central limit theorem [28] and in this case the stable probability density

$$h(x; 2, \zeta_X, C, D) = \frac{1}{\sqrt{4D\pi}} e^{-(x-C)^2/(4D)} \quad (3.14)$$

is the Gaussian distribution with mean  $C$  and variance  $\sigma^2 = 4D$ . [68.2.1.8] Note that the right hand side is independent of  $\zeta_X$  in this case. [68.2.1.9] Another special case expressible in terms of elementary functions is  $\varpi_X = 1, \zeta_X = 0$  where

$$h(x; 1, 0, C, D) = \frac{1}{\pi D} \frac{D^2}{D^2 + (x - C)^2} \quad (3.15)$$

is the Cauchy distribution centered at  $C$  and having width  $D$ .

[68.2.2.1] For sufficiently large but finite  $N = (L/\xi)^d$  equation (3.3) implies that the distribution function of

ensemble variables may be approximately written as

$$P_{X_{MN}}(x) = \quad (3.16)$$

$$\begin{cases} R(x, M, N, c) H\left(\frac{x - C_N}{D_N}; \varpi_X, \zeta_X, C, D\right) : x \leq 0 \\ 1 - R(x, M, N, c) \left(1 - H\left(\frac{x - C_N}{D_N}; \varpi_X, \zeta_X, C, D\right)\right) : x > 0 \end{cases}$$

[page 69, §0] involving a nonuniversal cutoff function  $R(x, M, N, c)$  such that  $R(0, M, N, c) = 1$  and  $\lim_{x \rightarrow \pm\infty} R(x, M, N, c) = 0$  for all  $M, N < \infty$ . In the ensemble limit the cutoff function must obey

$$\lim_{\substack{M, N \rightarrow \infty \\ N/M = c}} R(x; M, N, c) = 1, \quad (3.17)$$

for all  $x$  and  $c$  as a result of equation (3.3). [69.1.0.1] Note that equation (3.17) does not hold for the finite size scaling limit. [69.1.0.2] Instead Table I implies that for the finite size scaling limit

$$\lim_{\substack{L, \xi \rightarrow \infty \\ L/\xi = c}} R(x; M, N, N/M) = R(x; \infty, c^d, 0) \quad (3.18)$$

if the limit exists, and where now  $c = L/\xi$ . [69.1.0.3] The function  $R(x; \infty, (L/\xi)^d, 0)$  may in general differ from unity, and thus the *finite size scaling limit may involve a nonuniversal cutoff function which is absent in the finite ensemble limit*.

[69.1.1.1] Wherever possible equation (3.16) will be abbreviated as

$$P_{X_{MN}}(x) \approx H\left(\frac{x - C_N}{D_N}; \varpi_X, \zeta_X, C, D\right). \quad (3.19)$$

to shorten the equations. [69.1.1.2] If the centering con-

stants are now chosen as

$$C_N = \begin{cases} -D_N C & : \varpi_X \neq 1 \\ -D_N(C + \frac{2}{\pi} \zeta_X D \log D) & : \varpi_X = 1 \end{cases} \quad (3.20)$$

then using equations (3.10), (3.11) and (3.8) the basic finite ensemble scaling result [21, 22]

$$p_{X_{MN}}(x) \approx h(x; \varpi_X, \zeta_X, 0, DN\Lambda(N)) \quad (3.21)$$

is obtained for the probability density function  $p_{X_{MN}}(x)$  of suitably centered and renormalized ensemble sums. [69.1.1.3] The approximate result (3.21) has formed the basis for the statistical mechanical classification of phase transitions [21, 22].

[69.1.2.1] From the basic result (3.21) the scaling form for the probability density of ensemble averaged block variables  $\bar{X}_{MN}(\vec{\varphi}) = X_{MN}(\vec{\varphi})/(MN)$  is readily obtained using eq. (3.10) as

$$\bar{p}_{\bar{X}_{MN}}(x) \approx \frac{(L/\xi)^{d(1-(1/\varpi_X))}}{(D\Lambda((L/\xi)^d))^{1/\varpi_X}} \times h\left(\frac{x(L/\xi)^{d(1-(1/\varpi_X))}}{(D\Lambda((L/\xi)^d))^{1/\varpi_X}}; \varpi_X, \zeta_X, 0, 1\right). \quad (3.22)$$

[69.1.2.2] Setting  $X = \Psi$  this result is found to be distinctly different from equation (1.3). This shows that finite ensemble scaling (3.22) and finite size scaling (1.3) are not equivalent.

## IV. Finite size scaling

[69.1.3.1] This section discusses the implications of finite ensemble scaling for finite size scaling at a critical point. [69.1.3.2] Contrary to finite ensemble scaling the theory of finite size scaling includes the strongly correlated microscopic cell variables into the theoretical consideration. [69.2.0.3] This can be done in two ways. [69.2.0.4] Thermodynamic finite size scaling concentrates on the thermodynamic fluctuations within the ensemble, while statistical mechanical (or fieldtheoretical) finite size scaling focusses on the correlation functions on the block level. [69.2.0.5] The distinction appears already in equations (1.1) and (1.2). [69.2.0.6] The general identification of thermodynamics as the infinite volume limit of statistical mechanics implies a relation between the two parts which is at the origin of hyperscaling relations.

### IV.A. Thermodynamic finite size scaling

[69.2.1.1] The thermodynamic method of reintroducing the strongly correlated cell variables is to use the

definition of block variables (2.18) and to define

$$Z_{MN}(\vec{\varphi}) = \frac{X_{MN}(\vec{\varphi}) - C_{MN}}{D_{MN}} = \frac{\sum_{j=1}^N \sum_{i=1}^M X_{MN}(\vec{\varphi}(\vec{y}_j + \vec{x}_i)) - C_{MN}}{D_{MN}} \quad (4.1)$$

as a double sum over correlated microscopic cell variables. [69.2.1.2] Although the microscopic variables are strongly correlated inside the blocks they remain uncorrelated at separations larger than  $\xi$ . [69.2.1.3] Therefore the property of strong mixing [33, 34] continues to hold in the ensemble limit. [69.2.1.4] Therefore the same considerations as in the previous section can also be applied to the double sums (4.1) to give the finite size scaling result

$$P_{X_{MN}}(x) \approx H(x; \varpi_X, \zeta_X, 0, DD_{MN}^{\varpi_X}) \quad (4.2)$$

where now

$$D_{NM} = (MN \Lambda(MN))^{1/\varpi_X} \quad (4.3)$$

similar to equation (3.8).

[69.2.1.5] To exhibit the relation of the result (4.2) with the usual thermodynamic finite size scaling Ansatz (1.3) [8] for the order parameter distribution it is first necessary to rewrite the results in terms of the probability density for the ensemble averages  $\bar{X}_{MN}(\vec{\varphi}) = X_{MN}(\vec{\varphi})/(MN)$ . [69.2.1.6] This gives the thermodynamic finite size scaling result

$$\bar{p}_{\bar{X}_{MN}}(x) \approx \frac{(L/a)^{d-(d/\varpi_X)}}{(\Lambda((L/a)^d))^{1/\varpi_X}} \times h\left(\frac{x(L/a)^{d-(d/\varpi_X)}}{(\Lambda((L/a)^d))^{1/\varpi_X}}; \varpi_X, \zeta_X, 0, D\right). \quad (4.4)$$

[69.2.1.7] Setting  $X = \Psi$  and comparing with [5] yields the identification [21, 22]

$$\varpi_\Psi = \min\left(2, \frac{\gamma_\Psi \Psi + 2\beta_\Psi}{\gamma_\Psi \Psi + \beta_\Psi}\right) = \min(2, \lambda_\Psi) \quad (4.5)$$

where  $\gamma_\Psi$  is the order parameter susceptibility exponent,  $\beta_\Psi$  is the order parameter exponent, and  $\lambda_\Psi$  is the [page 70, §0] generalized Ehrenfest order [19] in the conjugate field direction. [70.1.0.1] The appearance of the minimum function results from the general inequality (3.7). [70.1.0.2] Similarly for the energy density  $X = \mathcal{E}$  the result

$$\varpi_\mathcal{E} = \min(2, 2 - \alpha_\mathcal{E}) = \min(2, \lambda_\mathcal{E}) \quad (4.6)$$

is obtained with  $\alpha_\mathcal{E} = \alpha$  the specific heat exponent. [70.1.0.3] In general the identification is given as  $\varpi_X = \min(2, 2 - \alpha_X) = \min(2, \lambda_X)$  where  $\alpha_X$  is the thermodynamic fluctuation exponent [9] defined in terms of derivatives of the free energy. [70.1.0.4] Equation (4.4) in combination with equations (4.5) and (3.16) determines the thermodynamic finite size scaling function for the order

parameter distribution in (1.3) explicitly as

$$\tilde{p}_\Psi(x, y) = \begin{cases} R(x, y) h_\Psi(x) + H_\Psi(x) \frac{\partial R(x, y)}{\partial x} & : x \leq 0 \\ R(x, y) h_\Psi(x) - (1 - H_\Psi(x)) \frac{\partial R(x, y)}{\partial x} & : x > 0 \end{cases} \quad (4.7)$$

where

$$h_\Psi(x, y) = h\left(x; \frac{\gamma_{\Psi\Psi} + 2\beta_\Psi}{\gamma_{\Psi\Psi} + \beta_\Psi}, \zeta_\Psi, 0, D\right) = \frac{dH_\Psi(x)}{dx} \quad (4.8)$$

and  $h$  is defined through the  $H$ -functions in equations (3.12), (3.13) and the appendix. [70.1.0.5] Note that the thermodynamic finite size scaling function depends on  $y$  only through the nonuniversal cutoff function  $R(x; M, y, c)$ . [70.1.0.6] It will be seen below that the dependence on  $y$  in the universal function  $h$  reappears in fieldtheoretical finite size scaling. [70.1.0.7] Note also that the general inequalities  $\beta_\Psi > 0$  and  $\gamma_{\Psi\Psi} > 0$  imply  $\varpi_\Psi < 2$ .

#### IV.B. Fieldtheoretical finite size scaling

[70.1.1.1] The fieldtheoretical or statistical mechanical method of reintroducing the microscopic cell variables uses the same uncorrelated block sums as in finite ensemble scaling (3.2), but multiplies them with the  $M$ -dependent field theoretic renormalization factor for block sums  $D(M)/M$  from (2.17) which has to be calculated independently. [70.1.1.2] In this case the renormalized ensemble sums are defined as

$$Z_{MN}(\vec{\varphi}) = \frac{(D(M)/M)Y_{MN}(\vec{\varphi}) - C_N}{D_N} = \frac{(D(M)/M) \sum_{j=1}^N Y_{MN}(\vec{\varphi}(\vec{y}_j)) - C_N}{D_N} \quad (4.9)$$

where  $C_N$  and  $D_N$  are constants as in (3.2). [70.1.1.3] The composite operators  $Y_{MN}(\vec{\varphi}(\vec{y}_j))$  have been denoted differently from the thermodynamic case to indicate that the variables of interest in mesoscopic fieldtheoretic or statistical mechanical calculations (block level) may in general differ from those accessible to macroscopic thermodynamic experiments (ensemble level). [70.2.0.4] Particular examples are the staggered magnetization for antiferromagnets or the quantum mechanical wave function. [70.2.0.5] Applying the same limit theorem as in the previous section now gives the fieldtheoretic finite size scaling result

$$P_{Y_{MN}}(x) \approx H\left(x; \varpi_Y, \zeta_Y, 0, D' \left(\frac{MD_N}{D(M)}\right)^{\varpi_Y}\right) \quad (4.10)$$

for the limiting probability distribution function of ensemble sums in the ensemble limit. [70.2.0.6] Using (2.13) and going over to averages the finite size scaling

form for the probability density of ensemble averages is found as

$$\bar{p}_{Y_{MN}}(x) \approx \left(\frac{L}{a}\right)^{d_Y} h\left(x \left(\frac{L}{a}\right)^{d_Y}; \varpi_Y, \zeta_Y, 0, D' \left(\frac{L}{\xi}\right)^{d - \varpi_Y(d - d_Y)} \Lambda\left(\frac{L}{\xi}\right)\right) \quad (4.11)$$

which is exactly of the form (1.3) with  $d^* = 0$ . [70.2.0.7] Thus the validity of (2.13), which has to be established by independent calculation, implies the validity of hyperscaling. [70.2.0.8] Note that the fieldtheoretic finite size scaling result (4.11) appears to be different from the thermodynamic one (4.4) in that it depends on  $L/\xi$ . [70.2.0.9] It will be seen below however that the two forms are generally identical except for  $\varpi_X = 2$ .

#### IV.C. Hyperscaling and the Structure of the Gaussian Fixed Point

[70.2.1.1] To establish the connection between thermodynamic fluctuation exponents  $\varpi_X$  and fieldtheoretic correlation exponents  $\varpi_Y$  it is necessary to compare the scaling results (4.4) and (4.11). [70.2.1.2] Note that (4.4) holds generally by virtue of the ensemble limit while the validity of (4.11) depends upon the validity of (2.13). [70.2.1.3] The connection between thermodynamics and statistical mechanics is generally given by identifying  $-\log \mathcal{Z}$  with the free energy or, in the microcanonical ensemble, by inverting the logarithm of the density of states to give the internal energy as function of entropy. [70.2.1.4] Thus the identification rests upon the identification of microscopic and macroscopic energies. [70.2.1.5] In fact the energy is the only observable which will always exist microscopically and macroscopically for thermal systems because it is a defining property of the system, and generates the thermal fluctuations of interest. [70.2.1.6] Thus the connection between thermodynamics and statistical mechanics in the present probabilistic approach is provided by identifying equation (4.4) for  $X = \mathfrak{H}$  with equation (4.11) for  $Y = \mathcal{H}$ . [70.2.1.7] This yields the algebraic form

$$D(M) = M^{1 - (1/\varpi_\mathcal{E})} \left(\frac{D' \Lambda(N)}{D \Lambda(MN)}\right)^{1/\varpi_\mathcal{E}} \quad (4.12)$$

for the energy renormalization. [70.2.1.8] Comparison with (2.13) and (4.6) gives the identification (first obtained in [21, 22]) [page 71, §0]

$$\begin{aligned} \varpi_\mathcal{E} &= \min\left(2, \frac{d}{d - d_\mathcal{E}}\right) \\ &= \min(2, d\nu) = \min(2, 2 - \alpha) \end{aligned} \quad (4.13)$$

where  $\nu = \nu_\mathcal{E}$  is the correlation length exponent, and  $\alpha = \alpha_\mathcal{E}$  is the specific heat exponent. [71.1.0.1] Thus equation

(4.12) and (4.13) combined with the general relation [9]

$$\frac{2 - \alpha_X}{\nu_X} = \frac{2 - \alpha_Y}{\nu_Y} \quad (4.14)$$

establish the general validity of hyperscaling for all microscopically and macroscopically accessible observables whenever the specific heat exponent is positive. [71.1.0.2] Therefore the hyperscaling relation

$$\begin{aligned} \varpi_X &= \min\left(2, \frac{d}{d - d_X}\right) \\ &= \min(2, d\nu_X) = \min(2, 2 - \alpha_X) \end{aligned} \quad (4.15)$$

holds for all phase transitions with  $\alpha > 0$ . [71.1.0.3] This result is a direct consequence of identifying thermal fluctuations in thermodynamics with those in statistical mechanics or field theory.

[71.1.1.1] The violation of hyperscaling above four dimensions in field theory is now a simple consequence of the renormalization group eigenvalues  $y_E = 1/\nu_E = 2$  and  $y_\Psi = 1/\nu_\Psi = (d+2)/2$  for the Gaussian fixed point. [71.1.1.2] Equation (4.13) implies  $\varpi_E = 2$  at  $d = 4$ .

[71.1.2.1] Of course the present theory does not allow to conclude that hyperscaling is generally violated for  $\alpha \leq 0$ . [71.1.2.2] In fact very often hyperscaling continues to be valid in such cases. [71.1.2.3] To see how this is possible it is instructive to consider the domains of attraction for the stable laws appearing in the finite size and finite ensemble scaling formulas. [71.1.2.4] Within the present approach the fact that only stable distributions have nonempty domains of attraction [28] is the reason for the existence of fixed points in the renormalization group picture and for *universality* of critical behaviour [35]. [71.1.2.5] It is well known [27, 28] that the domain of attraction is very different for gaussian and nongaussian fixed points.

[71.1.3.1] The existence of the limit distribution in (4.2) for the correlated ensemble sums implies by virtue of (2.18) and (2.19) that the limiting distribution of the correlated block sums

$$P_{X_{MNj}}(x) = \text{Prob}\{X_{MN}(\vec{\varphi}(\vec{y}_j)) \leq x\} \quad (4.16)$$

must approach a distribution within the domain of attraction of the stable distribution (4.2) for all blocks  $j = 1, \dots, N$ . [71.1.3.2] In order that a distribution  $P_{X_{MNj}}(x)$  belongs to the domain of attraction of the stable law with index  $0 < \varpi_X < 2$  and parameters  $\zeta_X, D$  it is necessary and sufficient [28] that, as  $|x| \rightarrow \infty$ ,

$$P_{X_{MNj}}(x) = \begin{cases} c_- \Lambda(-x) (-x)^{-\varpi_X} & : x < 0 \\ 1 - c_+ \Lambda(x) x^{-\varpi_X} & : x > 0 \end{cases} \quad (4.17)$$

where  $\Lambda(x)$  is slowly varying and the constants  $c_-, c_+ \geq 0, c_- + c_+ > 0$  are related to the parameters  $\varpi_X, \zeta_X, D$

by

$$c_\pm = \begin{cases} \frac{D \cos(\omega_1 \zeta_X)}{2\Gamma(1 - \varpi_X) \cos(\omega_1)} (1 \mp \cot(\omega_1) \tan(\omega_1 \zeta_X)) & : 0 < \varpi_X < 1 \\ \frac{D}{\pi} \cos(\pi \zeta_X / 2) (1 \mp \cot(\omega_1) \tan(\pi \zeta_X / 2)) & : \varpi_X = 1 \\ \frac{D(1 - \varpi_X) \cos(\omega_2 \zeta_X)}{2\Gamma(2 - \varpi_X) \cos(\omega_1)} (1 \mp \cot(\omega_1) \tan(\omega_2 \zeta_X)) & : 1 < \varpi_X < 2 \end{cases} \quad (4.18)$$

with  $\omega_1 = \pi \varpi_X / 2$  and  $\omega_2 = \pi(2 - \varpi_X) / 2$ . [71.2.0.3] For  $\varpi_X = 2$  on the other hand the domain of attraction is much larger. A distribution  $P_{X_{MNj}}(x)$  belongs to the domain of attraction of the Gaussian if it has a finite variance or if, for  $x > 0$ ,

$$1 - P_{X_{MNj}}(x) + P_{X_{MNj}}(-x) = x^{-2} \Lambda(x) \quad (4.19)$$

where  $\Lambda(x)$  is slowly varying.

[71.2.1.1] Equation (4.17) implies that for  $\varpi_X < 2$  the generalized susceptibility which is proportional to the second moment of the renormalized block variables

$$\infty = \lim_{M, N \rightarrow \infty} \int_{-\infty}^{\infty} x^2 dP_{X_{MNj}}(x) \sim \chi_{XX} \quad (4.20)$$

diverges in each block  $j = 1, \dots, N$ . [71.2.1.2] For  $\varpi_X = 2$  on the other hand the second moment may either diverge or else it is finite and nonzero. [71.2.1.3] (A zero value occurs only away from the critical point). [71.2.1.4] This result underlines the general validity of the algebraic form (2.13) derived in (4.12) for nongaussian fixed points, i.e.  $\varpi_E < 2$ , which then implies the validity of hyperscaling. [71.2.1.5] The Gaussian fixed point  $\varpi_E = 2$  on the other hand has a much larger domain of attraction. [71.2.1.6] In particular it contains both distribution functions with algebraic tails and distributions without algebraic tails. [71.2.1.7] No general conclusion about the validity or violation of hyperscaling can be drawn in the present approach for the Gaussian fixed point.

## V. Relation with general scaling theory

[71.2.2.1] The results of the previous section are closely related with the general classification theory of phase transitions [18, 19, 20, 21, 22, 23], the probabilistic approach in the theory of critical phenomena [34, 35, 36], and finite size scaling theory for the order parameter distribution [7]. [71.2.2.2] The relation with the general classification theory of phase transitions [21, 22] has already been given above. [71.2.2.3] The relation with the probabilistic approach to critical phenomena [35] is that scaling and universality are obtained probabilistically from stability and nonempty domains of attraction

for stable distributions. [71.2.2.4] The difference to [34, 35, 36] is that in those works the usual scaling limit of the measure [page 72, §0]  $\mu(\vec{\varphi}, a, L, \vec{\Pi})$  is studied instead of the much simpler distributions appearing in the ensemble limit. [72.1.0.1] Similarly the differences with finite size scaling theory of the order parameter distribution [7] arise from the difference between the finite size scaling limit and the ensemble limit.

[72.1.1.1] The relation with the renormalization group scaling theory of critical points [37] is provided by the identification (4.15) relating the thermodynamic fluctuation exponents to the field theoretic correlation exponents, i.e. by hyperscaling. [72.1.1.2] The present theory considers only relevant operators by virtue of the general inequality  $\varpi_X > 0$ . [72.1.1.3] Note that marginal operators correspond formally to  $\varpi_X \rightarrow \pm\infty$ , not to  $\varpi_X \rightarrow 0$ . [72.1.1.4] The influence of irrelevant operators is reflected in the general presence of a slowly varying function  $\Lambda(x)$  in all scaling relations.

[72.1.2.1] The traditional classification into irrelevant (IO), marginal (MO) and relevant operators (RO) can be extended by three additional distinctions. [72.1.2.2] The first refinement is into equilibrium (ERO) and anequilibrium relevant operators (ARO) according to  $y_{ERO} \leq d$  for equilibrium relevant operators and  $y_{ARO} > d$  for anequilibrium relevant operators. [72.1.2.3] ARO's are readily constructed from ERO's and are well known to occur in many models. [72.1.2.4] Examples are non-primary operators in conformal field theory [17], the energy and order parameter in anequilibrium phase transitions [21, 22], high gradient operators in the  $O(n)$  nonlinear  $\sigma$  models [38, 39] or the hierarchical shell number modes in shell models for turbulence [40]. [72.1.2.5] An intriguing formal analogy exists between the random local events building up a multifractal measure and anequilibrium relevant operators [41].

[72.1.3.1] A second refinement of the traditional classification is to distinguish between gaussian and nongaussian relevant operators. [72.1.3.2] A relevant operator  $X$  is called gaussian if  $y_X \leq d/2$  and nongaussian if  $y_X > d/2$ . [72.1.3.3] By virtue of the duality law [28]

$$h(x; \varpi_X, \zeta_X, 0, 1) = x^{-1-\varpi_X} h(x^{-\varpi_X}; 1/\varpi_X, \zeta'_X, 0, 1), \quad (5.1)$$

where  $\zeta'_X = \zeta'_X(\varpi_X, \zeta_X)$  an additional third distinction is expected for operators with  $y_X < 2d$  as compared to those with  $y_X \geq 2d$ . [72.1.3.4] The precise nature of this distinction remains to be explored.

[72.1.3.5] The new extended classification of the spectrum of critical operators may (in obvious notation) be

summarized by the inequalities

$$y_{IO} < 0 = y_{MO} < y_{GERO} \leq d/2 < y_{NERO} \leq d < y_{ARO_1} \leq 2d < y_{ARO_2} \quad (5.2)$$

in which the relevance increases from left to right.

## VI. Scaling functions

[72.1.4.1] This section discusses how the general theory above may be used to obtain finite size scaling functions at the critical point.

[72.2.1.1] The finite size scaling function  $\tilde{p}_X(x, y)$  for the probability density  $p(x, \xi, L)$  of the observable  $X$  is defined through an equation analogous to (1.3) by

$$p(x, L, \xi) = L^{d(d_X - d^*)/(d - d^*)} \tilde{p}_X(x L^{d(d_X - d^*)/(d - d^*)}, L/\xi_{d^*}) \quad (6.1)$$

where  $d_X$  is the anomalous dimension of  $X$ . [72.2.1.2] The ensemble limit yields explicit analytical expressions for the scaling functions  $\tilde{p}_X(x, y)$  at the critical point. [72.2.1.3] This is seen from (4.11) as well as from (4.4) which become identical in the ensemble limit if  $\varpi_X < 2$ . [72.2.1.4] If  $X$  is identified as the macroscopic (thermodynamic) equivalent of the microscopic observable  $Y$  then it follows from (4.4) and (4.11) that the finite ensemble scaling functions are given as

$$\tilde{p}_X^{ES}(x, y) = \tilde{p}_Y^{ES}(x, y) = h(x; \varpi_X, \zeta_X, 0, D) \quad (6.2)$$

if  $1 < \varpi_X < 2$ . [72.2.1.5] The superscript is a reminder for the ensemble limit. [72.2.1.6] The point  $\varpi_X = 1$  corresponding to first order transitions is singular and will not be discussed here. [72.2.1.7] For  $\varpi_X = 2$  on the other hand the thermodynamic form (4.4) yields a simple Gaussian while the fieldtheoretic form (4.11) gives

$$\tilde{p}_X^{ES}(x, y) = \frac{1}{\sqrt{4\pi D y^{2d_X - d}}} \exp\left(-\frac{x^2}{4D y^{2d_X - d}}\right). \quad (6.3)$$

[72.2.1.8] This is the scaling function conjectured in [7] for the order parameter density on the basis of a Gaussian approximation. [72.2.1.9] Note that this scaling function, contrary to those for  $\varpi_X < 2$ , does depend on the variable  $y$  separately. [72.2.1.10] Note also that the order parameter generally has anomalous dimension  $d_\Psi < d/2$  and thus this scaling form for the order parameter distribution is expected to arise in the vicinity but not directly at the critical point.

[72.2.2.1] Another source for the dependence of the scaling function  $\tilde{p}_\Psi(x, y)$  for the order parameter distribution on  $y$  is the appearance of the nonuniversal cut-off function  $R$  in the finite size scaling limit of equation (3.18). [72.2.2.2] With equation (3.18) and introducing the abbreviations  $R(x, L/\xi) = R(x, \infty, (L/\xi)^d, \infty)$ ,

$h(x) = h(x; \varpi_X, \zeta_X, 0, D)$  and  $H(x) = H(x; \varpi_X, \zeta_X, 0, D)$  the analogue of equation (6.2) reads

$$\tilde{p}_X^{FSS}(x, y) = \begin{cases} R(x, y) h(x) + H(x) \frac{\partial R(x, y)}{\partial x} & : x \leq 0 \\ R(x, y) h(x) - (1 - H(x)) \frac{\partial R(x, y)}{\partial x} & : x > 0 \end{cases} \quad (6.4)$$

for the finite size scaling limit. [72.2.2.3] Thus it is seen that the finite ensemble scaling function  $h$  corresponds to the universal part of the finite size scaling function which is independent of  $y$  while the cutoff function  $R$  is responsible [page 73, §0] for the dependence on  $y$  and adds a nonuniversal part.

[73.1.1.1] The analytical expressions (3.5) and (3.12) for the universal part of critical finite size scaling functions can be employed to evaluate the scaling functions numerically. [73.1.1.2] In this effort the symmetry relation [28]

$$h(-x, \varpi_X, \zeta_X, 0, 1) = h(x; \varpi_X, -\zeta_X, 0, 1) \quad (6.5)$$

reduces the computational effort. [73.1.1.3] Moreover equation (6.5) suggests a relation with the phenomenon of *spontaneous symmetry breaking* within the present approach. [73.1.1.4] In this view the two scaling functions  $h(x; \varpi_X, \pm\zeta_X, 0, 1)$  represent the two pure phases, and thus on general thermodynamic grounds the full scaling function is expected to become a convex combination

$$\tilde{p}_X(x) = \tilde{p}_X^{ES}(x, y) = s h(x; \varpi_X, \zeta_X, 0, D) + (1 - s) h(x; \varpi_X, -\zeta_X, 0, D) \quad (6.6)$$

of two extremal phases. [73.1.1.5] The relation may be generalized to several phases or asymmetric situations.

[73.1.2.1] Consider now an ordinary critical point with a global symmetry such as in the Ising models. [73.1.2.2] Let  $X = \Psi$  be the order parameter which is assumed to be normalized such that  $D = 1$ . [73.1.2.3] Then  $\varpi_X$  becomes  $\varpi_\Psi = 1 + (1/\delta)$  where  $\delta$  is the equation of state exponent. [73.1.2.4] Abbreviating  $\zeta_\Psi$  as  $\zeta$  the scaling function in equation (6.6) becomes

$$\tilde{p}_\Psi(x; \delta, \zeta, s) = s h(x; 1 + 1/\delta, \zeta, 0, 1) + (1 - s) h(x; 1 + 1/\delta, -\zeta, 0, 1). \quad (6.7)$$

[73.1.2.5] For the symmetric case  $s = 1/2$  the function  $\tilde{p}_\Psi(x; \delta, \zeta, s)$  is displayed in Figures 2, 3 and 4 for  $\delta = 3, 5, 15$  and several choices of  $\zeta$ . [73.1.2.6] The symmetrization  $s = 1/2$  in (6.7) corresponds to an ‘‘equal weight rule’’ which is known to apply for first order transitions [42]. [73.1.2.7] Figure 2 shows the case  $\delta = 3$  which is the value for the universality class of mean field models. [73.1.2.8] The six values for  $\zeta$  in Figure 2 through 4 are  $\zeta = 0.0, 0.6, 0.7, 0.8, 0.9, 1.0$ . [73.1.2.9] The case  $\zeta = 1.0$  corresponds to the double peak structure with

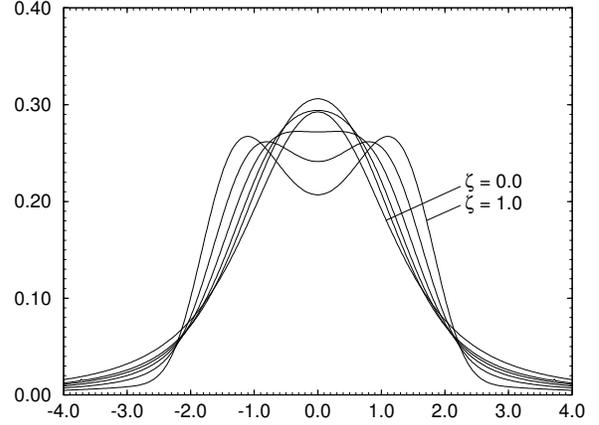


FIGURE 2. Universal part of the finite size scaling functions  $\tilde{p}_\Psi(x; 3, \zeta, 1/2)$  for the order parameter probability density function for the mean field universality class corresponding to  $\delta = 3$  for the equation of state exponent (or  $\varpi_\Psi = 1 + (1/\delta) = 4/3$ ). All curves have width  $D = 1$ , and symmetrization  $s = 1/2$ . Different curves correspond to different choices of the universal symmetry or shape parameter  $\zeta = 0.0, 0.6, 0.7, 0.8, 0.9, 1.0$ . The curves for  $\zeta = 0.0$  and  $\zeta = 1.0$  are labelled explicitly, the curves for other values of  $\zeta$  interpolate between them.

the widest peak separation while the value  $\zeta = 0.0$  corresponds to the singly peaked function whose maximum has the smallest height. [73.1.2.10] Figure 3 shows the case  $\delta = 5$  which is close to the value of  $\delta \approx 4.8$  [16] for the three-dimensional Ising model. [73.1.2.11] The value  $\delta = 15$  in Figure 4 is the value for the two dimensional Ising universality class.

[73.1.2.12] The scaling functions displayed in Figures 2 through 4 are consistent with published data on critical scaling functions [7, 43, 44]. [73.1.2.13] Moreover it is seen that the universal shape parameter  $\zeta$  is related to the type of boundary conditions. [73.1.2.14] Free boundary conditions apparently correspond to smaller values of the universal shape parameter  $\zeta$  than periodic boundary conditions. [73.1.2.15] This correspondence between the value of  $\zeta$  and the applied boundary conditions is not expected to be one to one. [73.1.2.16] The value of  $\zeta$  may be influenced by other universal factors such as the type or symmetry of the pure phases. [page 74, §0] [74.1.0.1] On the other hand the boundary conditions may also influence other parameters such as the value of the symmetrization  $s$ . [74.1.0.2] This is expected for boundary conditions which do not preserve the symmetry.

[74.1.1.1] Figure 5 shows that the scaling functions are not merely consistent but also in good quantitative

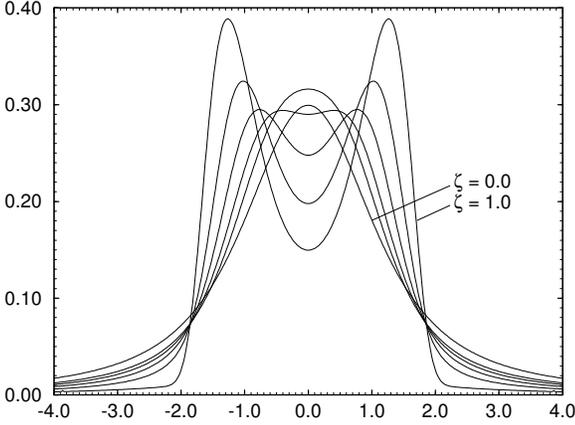


FIGURE 3. Same as Figure 2 with  $\delta = 5$  close to the  $d = 3$  Ising ( $\delta \approx 4.8$ ) universality class.

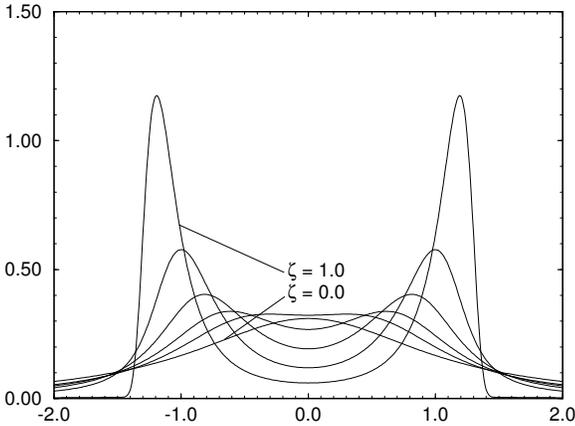


FIGURE 4. Same as Figure 2 with  $\delta = 15$  corresponding to the  $d = 2$  Ising universality class.

agreement with Monte-Carlo simulations of the two-dimensional Ising model [43, 44, 45] where the exact value of  $\delta$  and the location of the critical point for the infinite system are known. [74.1.1.2] The open circles in Figure 5 represent the smooth interpolation through the data published in [43, 44, 45]. [74.1.1.3] The solid line is the analytical prediction shown in Figure 4 for  $\zeta = 1$ . [74.1.1.4] For the comparison the nonuniversal scaling factors which were chosen to yield unit norm and variance in [43, 44, 45] were matched to those of the theoretical curve. [74.1.1.5] The excellent agreement between theory and simulation suggests to identify the value  $\zeta = 1$  with periodic boundary conditions. [74.1.1.6] It is however not clear whether this identification will hold more generally.

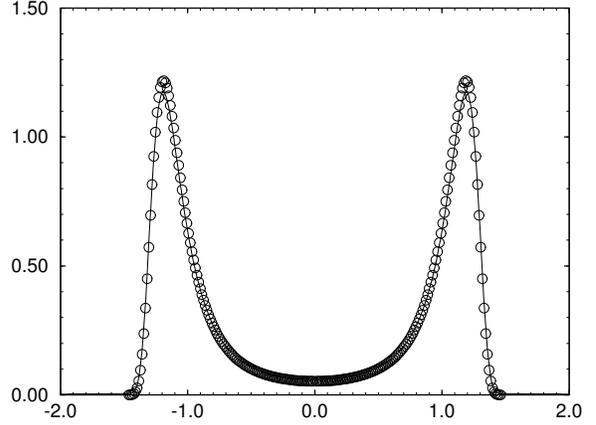


FIGURE 5. Comparison between the scaling function  $\tilde{p}_\Psi(x; 15, 1, 1/2)$  (solid line) for the order parameter density of the two dimensional Ising universality class ( $\delta = 15$ ) with a smoothed interpolation through the simulation results of Refs.[43, 44, 45], (open circles) under the assumption that  $\zeta = 1$  corresponds to periodic boundary conditions.

## VII. Amplitude ratios

[74.1.2.1] This section discusses universal amplitudes such as those defined in (1.6) and their ratios. [74.1.2.2] In numerical simulations of critical phenomena amplitude ratios such as (1.7) are used routinely to extract critical parameters  $\tilde{\mathbf{I}}_c$  and exponents from simulations of finite systems. [74.1.2.3] It is then of interest to analyze finite size amplitude ratios within the present framework.

[74.1.3.1] The absolute moment of order  $\sigma$  for the ensemble averages of  $X$  in a *finite and noncritical* system is found from equations (4.4) and (3.16) as

$$\langle |X|^\sigma \rangle = \int_{-\infty}^{\infty} |x|^\sigma \tilde{p}_{\bar{X}_{MN}}(x) dx \quad (7.1)$$

$$= \frac{(\Lambda((L/a)^d))^{\sigma/\varpi_X}}{(L/a)^{d\sigma(1-(1/\varpi_X))}} \tilde{X}(\sigma; a, \xi, L) \quad (7.2)$$

where the amplitude  $\tilde{X}(\sigma; a, \xi, L)$  of the finite, discrete and noncritical system is given as

$$\tilde{X}(\sigma; a, \xi, L) = \int_{-\infty}^{\infty} |x|^\sigma h(x; \varpi_X, \zeta_X, 0, D) \times r \left( \frac{x (\Lambda((L/a)^d))^{1/\varpi_X}}{(L/a)^{d-(d/\varpi_X)}}; \frac{\xi}{a}, \frac{L}{\xi}, \frac{aL}{\xi^2} \right) dx \quad (7.3)$$

and the function  $r(x; \xi/a, L/\xi, aL/\xi^2)$  is defined from equation (4.7) by replacing  $\Psi$  with  $X$  and extracting a factor  $h(x; \varpi_X, \zeta_X, 0, D)$ . [74.2.0.2] In the ensemble limit one

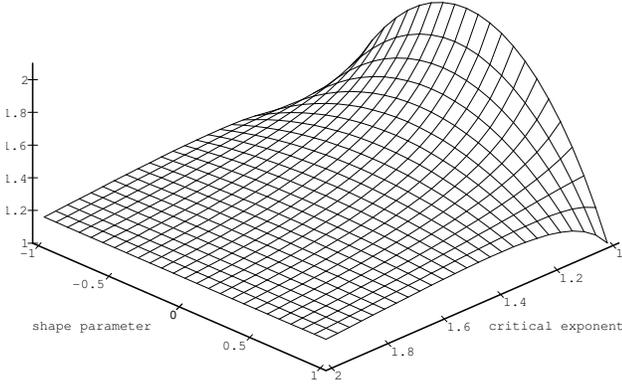


FIGURE 6. The moment ratio  $g(3/4, 1/4; \varpi_X, \zeta_X) = \langle |X|^{3/4} \rangle / \langle |X|^{1/4} \rangle^3$  as a function of the critical exponent  $\varpi_X$  and the universal shape parameter  $\zeta_X$ .

obtains from this and (3.17) the result

$$\begin{aligned} \tilde{X}_{ES}(\sigma) &= \lim_{\substack{M, N \rightarrow \infty \\ N/M=c}} \tilde{X}(\sigma; a, \xi, L) \\ &= \int_{-\infty}^{\infty} |x|^\sigma h(x; \varpi_X, \zeta_X, 0, D) dx \end{aligned} \quad (7.4)$$

for the critical ensemble scaling amplitude of order  $\sigma$  in an infinite system. [74.2.0.3] The subscript is again a reminder for the ensemble scaling limit. [74.2.0.4] The integral in (7.4) can be evaluated for  $D = 1$  as

$$\begin{aligned} \tilde{X}_{ES}(\sigma) &= \frac{2}{\pi} \Gamma(\sigma) \Gamma\left(1 - \frac{\sigma}{\varpi_X}\right) \\ &\quad \times \sin(\pi\sigma/2) \cos\left(\frac{\pi\sigma\zeta_X(\varpi_X - 2)}{2\varpi_X}\right), \end{aligned} \quad (7.5)$$

which is valid for  $-1 < \text{Re}\sigma < \varpi_X, 1 < \varpi_X < 2$  and  $-1 < \zeta_X < 1$ . [74.2.0.5] A derivaton of this result is given in Appendix B. [74.2.0.6] This allows to calculate the general moment ratios

$$\begin{aligned} g(\sigma_1, \sigma_2; \varpi_X, \zeta_X) &= \lim_{\substack{M, N \rightarrow \infty \\ N/M=c}} \frac{\langle |X|_1^{\sigma_1} \rangle}{\langle |X|_2^{\sigma_2} \rangle^{\sigma_1/\sigma_2}} \\ &= \frac{\tilde{X}_{ES}(\sigma_1)}{\left(\tilde{X}_{ES}(\sigma_2)\right)^{\sigma_1/\sigma_2}} \end{aligned} \quad (7.6)$$

with  $-1 < \sigma_1, \sigma_2 < \varpi_X$  in the ensemble limit. [74.2.0.7] Figure 6 shows a twodimensional plot of the ratio  $g(3/4, 1/4; \varpi_X, \zeta_X)$ .

[74.2.1.1] If equation (7.5) is used to analytically continue  $g(\sigma_1, \sigma_2; \varpi_X, \zeta_X)$  beyond the regime  $-1 < \sigma_1, \sigma_2 < \varpi_X$  the traditional fourth order cumulant  $g(4, 2; \varpi_\Psi, \zeta_\Psi)$  for the order parameter is found to exhibit special problems if  $\varpi_\Psi < 2$ . [74.2.1.2] This is mainly due to the

presence of the factor  $\sin(\pi\sigma/2)$  in (7.5). [74.2.1.3] The divergence must somehow become absorbed by the cutoff factor  $r(0; \infty, c, 0)$  in the finite size scaling limit. [74.2.1.4] Assuming that this is indeed the case it is then of interest to consider the quantity

$$g_{FSS}(\sigma_1, \sigma_2; \varpi_X, \zeta_X) = \lim_{\substack{L, \xi \rightarrow \infty \\ L/\xi=c}} \frac{(\sin(\pi\sigma_2/2))^{\sigma_1/\sigma_2} \langle |X|^{\sigma_1} \rangle}{\sin(\pi\sigma_1/2) \langle |X|^{\sigma_2} \rangle^{\sigma_1/\sigma_2}} \quad (7.7)$$

[page 75, §0] in the finite size scaling limit assuming that it exists. [75.1.0.1] Then the traditional finite size cumulant becomes

$$g_{FSS}(4, 2; \varpi_X, \zeta_X) = \frac{\Gamma\left(1 - \frac{4}{\varpi_X}\right) \cos(2\pi\zeta_X(\varpi_X - 2)/\varpi_X)}{3\pi \Gamma^2\left(1 - \frac{2}{\varpi_X}\right) \cos^2(\pi\zeta_X(\varpi_X - 2)/\varpi_X)}. \quad (7.8)$$

[75.1.0.2] The interest in this formal expression is that it is still singular. [75.1.0.3] Within the domain  $1 < \varpi_X < 2, -1 < \zeta_X < 1$  it has simple poles along the lines

$$\begin{aligned} \varpi_X &= \frac{4}{3} \\ \varpi_X &= \frac{4\zeta_X}{2\zeta_X \pm 1} \end{aligned} \quad (7.9)$$

and zeros along the lines

$$\begin{aligned} \varpi_X &= \frac{8\zeta_X}{4\zeta_X \pm 1} \\ \varpi_X &= \frac{8\zeta_X}{4\zeta_X \pm 3}. \end{aligned} \quad (7.10)$$

[75.1.0.4] For the traditionally studied order parameter cumulant, i.e. setting  $X = \Psi$ , the pole at  $4/3$  implies a divergence whenever  $\delta = 3$ , i.e. in mean field theory. [75.1.0.5] This result is consistent with the divergence  $g_\infty(0) \propto \eta^{-1}$  found in conformal field theory [17]. [75.1.0.6] Note that the points  $\zeta = \pm 1/2$  along the singular mean field line  $\varpi_\Psi = 4/3$  are intersection points with a line of zeros.

[75.1.1.1] Irrespective of these problems it is of interest to estimate values for the traditional order parameter cumulant ratio  $g_\infty(0)$  because much previous work has focussed on it. [75.1.1.2] Within the present approach this is possible from the knowledge of the scaling functions if it is assumed that the identification of  $\zeta = 1$  with periodic boundary conditions holds generally. [75.1.1.3] If the scaling functions with  $\zeta = 1$  in Figures 2 through 4 are simply truncated sharply at  $\pm x_{max}$ , and subsequently rescaled to unit norm and variance, the order parameter cumulant  $g_\infty(0)$  may be calculated as usual, and it will depend upon the nonuniversal cutoff at  $x_{max}$ . [75.2.0.4] The results of such a cutoff procedure are displayed in Figure 7 for the cases  $\delta = 3, 5, 15$ . [75.2.0.5] It is seen

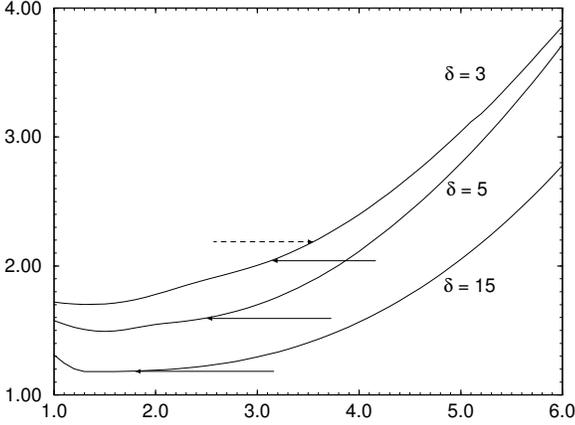


FIGURE 7. Plot of  $g_\infty(0)$  calculated by truncating  $\tilde{p}_\Psi(x; \delta, 1, 1/2)$  at  $\pm x_{max}$  and choosing the scale factors to give unit norm and variance. Solid arrows indicate numerical estimates from Monte-Carlo simulations on Ising models as  $g_\infty(0) = 1.168 \pm 0.002$  for  $d = 2$  Ref. [43],  $g_\infty(0) = 1.59 \pm 0.03$  for  $d = 3$  Ref. [16] and  $g_\infty(0) = 2.04 \pm 0.05$  for  $d = 5$  Ref. [46]. The dashed arrow represents the analytical result  $g_\infty(0) = 2.188\dots$  from Ref. [15].

that the cumulant is distinctly cutoff dependent. [75.2.0.6] Note that all curves appear to diverge as the cutoff increases. [75.2.0.7] For the cases  $\delta = 3$  and  $\delta = 5$  some structure appears between  $x_{max} = 2$  and 3 corresponding to the strong curvature in this region seen in Figures 2 and 3. [75.2.0.8] For the  $2d$ -Ising case the curve is flat up to about twice the maximal value 1.39 for the simulations of Bruce and coworkers [43, 45]. [75.2.0.9] Figure 5 provides a possible explanation for the poor agreement between the value  $g_\infty(0) = 2.042 \pm 0.05$  observed in simulations of the five-dimensional Ising model [11, 46] and the mean field calculation  $g_\infty(0) = 2.188\dots$  from [15]. [75.2.0.10] The simulation result is indicated as the solid arrow, the analytical result as the dashed arrow pointing to the curve  $\delta = 3$ . [75.2.0.11] The small difference in the cutoff  $x_{max}$  corresponding to these values suggests that the discrepancy may result from different nonuniversal (but most likely smooth) cutoffs in the two estimates.

[75.2.1.1] Finally, the fact that the value of the universal shape parameter  $\zeta_X$  appears to be related to the choice of boundary conditions suggests a method of constructing critical amplitude ratios which do not depend on boundary conditions, or other factors influencing  $\zeta_X$ . [75.2.1.2] The basic idea is to use the difference of two independent observations of ensemble averages or sums. [75.2.1.3] Let  $X_{MN}$  and  $X'_{MN}$  be two independent measurements and  $Y_{MN} = X_{MN} - X'_{MN}$  their difference. [75.2.1.4] The limiting distribution function  $P_{X_{MN}}(x)$  for

$X_{MN}$  and  $X'_{MN}$  at criticality is given in equation (4.2). [75.2.1.5] Then the difference  $Y_{MN}$  has the distribution function

$$P_{Y_{MN}}(x) \approx H(x; \varpi_X, 0, 0, 2DD_{MN}^{\varpi_X}) \quad (7.11)$$

[page 76, §0] in which the width is doubled, but  $\zeta_X$  has disappeared. [76.1.0.1] The fractional difference moment ratio  $\Delta(\sigma_1, \sigma_2, \varpi_X)$  is formed analogously to the moment ratio  $g$  as

$$\begin{aligned} \Delta(\sigma_1, \sigma_2, \varpi_X) &= \frac{\langle |Y_{MN}|^{\sigma_1} \rangle}{\langle |Y_{MN}|^{\sigma_2} \rangle^{\sigma_1/\sigma_2}} \\ &= \frac{(2/\pi)\Gamma(1 - (\sigma_1/\varpi_X))\Gamma(\sigma_1)\sin(\pi\sigma_1/2)}{[(2/\pi)\Gamma(1 - (\sigma_2/\varpi_X))\Gamma(\sigma_2)\sin(\pi\sigma_2/2)]^{\sigma_1/\sigma_2}} \quad (7.12) \end{aligned}$$

and it has a universal value depending only on the scaling dimension of  $X$  as long as  $\sigma_1, \sigma_2 < \varpi_X$ . [76.1.0.2] If the scaling dimension is universal then the fractional difference moment ratio is independent of boundary conditions. [76.1.0.3] Plotting  $\Delta(\sigma_1, \sigma_2, \varpi_X)$  as a function of length scale and temperature should then allow to extract the critical exponent.

## Acknowledgements

[76.1.1.1] The author is grateful to Dr. N. B. Wilding for providing him with the data of Ref. [44, 45], and to Prof. Dr. K. Binder, Dr. B. Dünweg and Dr. G. Schreider for useful discussions and critically reading the manuscript.

## Appendix A. Definition of $H$ -functions

[76.1.1.2] The general  $H$ -function is defined as the inverse Mellin transform [32]

$$H_{PQ}^{mn} \left( z \left| \begin{array}{ccc} (a_1, A_1) & \dots & (a_P, A_P) \\ (b_1, B_1) & \dots & (b_Q, B_Q) \end{array} \right. \right) = \quad (A.1)$$

$$\frac{1}{2\pi i} \int_{\mathcal{C}} \frac{\prod_{j=1}^m \Gamma(b_j - B_j s) \prod_{j=1}^n \Gamma(1 - a_j + A_j s)}{\prod_{j=m+1}^Q \Gamma(1 - b_j + B_j s) \prod_{j=n+1}^P \Gamma(a_j - A_j s)} z^s ds$$

where the contour  $\mathcal{C}$  runs from  $c - i\infty$  to  $c + i\infty$  separating the poles of  $\Gamma(b_j - B_j s)$ , ( $j = 1, \dots, m$ ) from those of  $\Gamma(1 - a_j + A_j s)$ , ( $j = 1, \dots, n$ ). [76.1.1.3] Empty products are interpreted as unity. [76.1.1.4] The integers  $m, n, P, Q$  satisfy  $0 \leq m \leq Q$  and  $0 \leq n \leq P$ . [76.1.1.5] The coefficients  $A_j$  and  $B_j$  are positive real numbers and the

complex parameters  $a_j, b_j$  are such that no poles in the integrand coincide. [76.1.1.6] If

$$\Omega = \sum_{j=1}^n A_j - \sum_{j=n+1}^P A_j + \sum_{j=1}^m B_j - \sum_{j=m+1}^Q B_j > 0 \quad (\text{A.2})$$

then the integral converges absolutely and defines the  $H$ -function in the sector  $|\arg z| < \Omega\pi/2$ . [76.2.0.7] The  $H$ -function is also well defined when either

$$\delta = \sum_{j=1}^Q B_j - \sum_{j=1}^P A_j > 0 \quad \text{with} \quad 0 < |z| < \infty \quad (\text{A.3})$$

or

$$\delta = 0 \quad \text{and} \quad 0 < |z| < R = \prod_{j=1}^P A_j^{-A_j} \prod_{j=1}^Q B_j^{B_j}. \quad (\text{A.4})$$

[76.3.0.8] The  $H$ -function is a generalization of Meijers  $G$ -function and many of the known special functions are special cases of it.

## Appendix B. Derivation of equation (7.5)

[76.3.1.1] By virtue of the symmetry relation (6.5) the integral in (7.4) may be written as

$$\int_{-\infty}^{\infty} |x|^\sigma h(x; \varpi, \zeta, 0, 1) dx = \int_0^{\infty} x^\sigma h(x; \varpi, \zeta, 0, 1) dx + \int_0^{\infty} x^\sigma h(x; \varpi, -\zeta, 0, 1) dx \quad (\text{B.1})$$

The definition (A.1) implies the general formula [32]

$$\int_0^{\infty} x^{s-1} H_{PQ}^{mn} \left( ax \left| \begin{matrix} (a_1, A_1) & \dots & (a_P, A_P) \\ (b_1, B_1) & \dots & (b_Q, B_Q) \end{matrix} \right. \right) dx = a^{-s} \frac{\prod_{j=1}^m \Gamma(b_j + B_j s) \prod_{j=1}^n \Gamma(1 - a_j - A_j s)}{\prod_{j=m+1}^Q \Gamma(1 - b_j - B_j s) \prod_{j=n+1}^P \Gamma(a_j + A_j s)} \quad (\text{B.2})$$

by virtue of the Mellin inversion theorem. [76.3.1.2] Specializing to the case at hand

$$\int_0^{\infty} x^\sigma h(x; \varpi, \zeta, 0, 1) dx = \frac{1}{\varpi} \int_0^{\infty} x^\sigma H_{22}^{11} \left( x \left| \begin{matrix} (1 - 1/\varpi, 1/\varpi) & (1 - \varrho, \varrho) \\ (0, 1) & (1 - \varrho, \varrho) \end{matrix} \right. \right) dx \quad (\text{B.3})$$

$$= \frac{\Gamma(\sigma + 1)\Gamma(-\sigma/\varpi)}{\varpi\Gamma(1 + \varrho\sigma)\Gamma(-\varrho\sigma)} \quad (\text{B.4})$$

where  $\varrho = \frac{1}{2} - \frac{\zeta}{\varpi} + \frac{\zeta}{2}$ . [76.3.1.3] Using  $\Gamma(x)\Gamma(-x) = -\pi/(x \sin(\pi x))$  and the functional equation for the  $\Gamma$ -function gives

$$\int_0^{\infty} x^\sigma h(x; \varpi, \zeta, 0, 1) dx = \frac{1}{\pi} \sin(\pi\varrho\sigma)\Gamma(\sigma)\Gamma\left(1 - \frac{\sigma}{\varpi}\right) \quad (\text{B.5})$$

which inserted into (B.1) readily yields the desired result (7.5).

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INSTITUT FÜR PHYSIK, UNIVERSITÄT MAINZ, 55099 MAINZ, GERMANY