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Short Communication

On Finite-Size Scaling in the Presence of Dangerous Irrelevant Variables

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A scaling hypothesis on finite-size scaling in the presence of a dangerous irrelevant variable is formulated for systems with long-range interaction and general geometry $L^{d-d'} \times \infty^{d'}$. A characteristic length which obeys a universal finite-size scaling relation is defined. The general conjectures are based on exact results for the mean spherical model with inverse power law interaction.

KEY WORDS: Finite-size scaling; dangerous irrelevant variables; spherical model; long-range interactions.

1. INTRODUCTION

According to the finite-size scaling hypothesis due to Fisher,[1,2] in the neighborhood of the critical temperature $T = T_c$ of a second-order phase transition in a system of size L, finite-size effects are controlled by the ratio L/ξ_∞, where ξ_∞ is the bulk correlation length, diverging as $|t|^{-\nu}$ when $t = (T - T_c)/T_c \to 0$. It has been found, however, that the above hypothesis fails at space dimensionalities d above the upper critical dimensionality d_u.[3-6] Renormalization group analysis reveals that the violation of finite-size scaling, as well as the breakdown of hyperscaling, is a consequence of the appearance in the theory of a "dangerous irrelevant variable" at $d > d_u$. In the derivation of scaling laws for the thermodynamic functions one essentially relies upon the assumption of analytical dependence of these functions on the irrelevant variables, which is not the case at $d > d_u$.[7,8] It

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has been suggested that if hyperscaling is not valid, finite-size effects are controlled by a different ratio, namely L/l_∞, where l_∞ is the so-called thermodynamic length.[9,10] For systems of fully finite block geometry this length diverges as

$$l_\infty \sim |t|^{-(2\beta+\gamma)/d} \tag{1}$$

when $t \to 0$. It is evident from (1) that when the hyperscaling relation $d\nu = 2\beta + \gamma$ holds, then the thermodynamic length coincides with the correlation length.

The investigation of finite-size scaling in the mean-field regime is of special interest for systems with long-range interactions decaying at large distances r as $r^{-d-\sigma}$, with $0 < \sigma < 2$, since then $d_u = 2\sigma$ may become less than the physically attainable dimensionalities $d = 1, 2, 3$, provided σ is small enough.

The aim of the present work is the formulation of a general hypothesis of modified finite-size scaling for systems with long-range interactions of dimensionalities above the upper critical one. The ideas suggested in ref. 9 for systems with short-range interactions ($\sigma = 2$) and fully finite geometry ($d' = 0$) will be extended to the case of arbitrary $\sigma \in (0, 2)$ and general geometry of the form $L^{d-d'} \times \infty^{d'}$. Periodic boundary conditions will be assumed in the $d - d'$ directions along which the system is finite.

From a methodological point of view it is convenient to use the exactly solvable mean spherical model as a basis for further generalizations.

2. FINITE-SIZE SCALING FOR THE SPHERICAL MODEL WITH LONG-RANGE INTERACTIONS

A new analytical technique for the evaluation of the free energy density of the mean spherical model with inverse power law interaction was suggested in ref. 11. A pair interaction potential $J(r)$, decaying at large distances r as $r^{-d-\sigma}$ with $\sigma > 0$ a parameter, has been considered in the case of a finite lattice $\Lambda = \otimes_{k=1}^{d} \{1, \ldots, L_k\}$ with periodic boundary conditions. The Fourier transform

$$\hat{J}(\mathbf{q}) = \sum_{\boldsymbol{l} \in \Lambda} \tilde{J}_\Lambda(\boldsymbol{l}) \exp(-i\boldsymbol{l} \cdot \mathbf{q}) \tag{2}$$

of the effective potential $\tilde{J}_\Lambda(\boldsymbol{l})$ which takes into account interactions with repeated images of the system,[12]

$$\tilde{J}_\Lambda(\boldsymbol{l}) = \sum_{\mathbf{t} \in \mathbb{Z}^d} J\left(\left[\sum_{k=1}^{d} (l_k - L_k t_k)^2\right]^{1/2}\right)$$

has the long-wavelength asymptotic form ($0<\sigma<2$, $\rho_\sigma>0$)

$$\hat{J}(\mathbf{q}) \simeq \hat{J}(\mathbf{0})(1-\rho_\sigma |\mathbf{q}|^\sigma), \qquad |\mathbf{q}| \to 0 \tag{3}$$

The free energy density $f_L(t, h)$, depending on a magnetic field $H \in \mathbb{R}^1$, $h = H/k_B T$, has been evaluated in the case of a system of hypercubic shape, $L_k = L$, $k = 1,..., d$. Extending the method suggested in ref. 11 to the case of an $L^{d-d'} \times \infty^{d'}$ geometry, for the singular part of the free energy density in the neighborhood of the critical point we obtain, at $d > 2\sigma$,

$$\begin{aligned}(k_B T)^{-1} f_L^{(s)}(t, h) \\ &\simeq \frac{1}{2}\rho_\sigma(K_c - K)\tilde{\phi} - \frac{1}{4}\rho_\sigma^2 |W'_{d,\sigma}(0)| \tilde{\phi}^2 \\ &- \frac{h^2}{2\rho_\sigma K\tilde{\phi}} - \frac{1}{2}\sigma \frac{\Gamma((d+1)/2)}{\pi^{(d+1)/2}} L^{-d} \sum_{\boldsymbol{l}(d-d')}' |\boldsymbol{l}|^{-d} u_{d,\sigma}(L|\boldsymbol{l}|\tilde{\phi}^{1/\sigma})\end{aligned} \tag{4}$$

Here $K = \hat{J}(\mathbf{0})/k_B T$, $K_c = 1$, the symbol $\boldsymbol{l}(d-d')$ means that the summation is over $\boldsymbol{l} \in \mathbb{Z}^{d-d'}$ and the primed summation sign that the term with $|\boldsymbol{l}| = 0$ is omitted; the function $u_{d,\sigma}(z)$ is defined as

$$u_{d,\sigma}(z) = \int_0^\infty dx\, (1+x^2)^{-(d+1)/2} E_{\sigma,1}(-x^\sigma z^\sigma) \tag{5}$$

where

$$E_{\alpha,\beta}(z) = \sum_{k=0}^\infty \frac{z^k}{\Gamma(\alpha k + \beta)}, \qquad \alpha > 0 \tag{6}$$

is the Mittag–Leffler function (for more details see ref. 11). The parameter $\tilde{\phi} = \phi/\rho_\sigma$, and $\phi = 2s/K - 1$ is a linear function of the spherical field s and obeys the mean spherical constraint. When $d > 2\sigma$, $d' < \sigma$, the mean spherical constraint in the neighborhood of the critical point takes the form[13]

$$\begin{aligned}|W'_{d,\sigma}(\sigma)|\, \tilde{\phi} L^{d-\sigma} - D^{(0)}_{d',\sigma}(\tilde{\phi} L^\sigma)^{(d'-\sigma)/\sigma} + D^{(I)}_{d,\sigma}(\tilde{\phi} L^\sigma)^{(d-\sigma)/\sigma} \\ + 2Y^{(s)}_{d,d',\sigma}(\tilde{\phi} L^\sigma) = \rho_\sigma t L^{d-\sigma} + \rho_\sigma^{-1} h^2 L^{d-\sigma} \tilde{\phi}^{-2}\end{aligned} \tag{7}$$

This equation is valid for all dimensionalities d such that $\sigma I < d < \sigma(I+1)$ with some integer $I \geqslant 2$; $W'_{d,\sigma}(0)$ is the derivative at $\tilde{\phi} = 0$ of the Watson-type integral

$$W_{d,\sigma}(\tilde{\phi}) = (2\pi)^{-d} \int_{[-\pi,\pi]^d} d^d q\, (\tilde{\phi} + |\mathbf{q}|^\sigma)^{-1} \tag{8}$$

$Y^{(s)}_{d,d',\sigma}(\cdot)$ is the spin-wave scaling function introduced at $d'=1$ by Fisher and Privman[12]; the constant $D^{(l)}_{d,\sigma}$ is given by the explicit expression

$$D^{(l)}_{d,\sigma}=2\pi(-1)^{l}\left[(4\pi)^{d/2}\,\Gamma\left(\frac{d}{2}\right)\sigma\sin\frac{(d-\sigma l)\pi}{\sigma}\right]^{-1} \tag{9}$$

The study[14] of the pair spin–spin correlation function $G_L(\mathbf{R};t,h)$ in a system with geometry $L^{d-d'}\times\infty^{d'}$ has shown that its leading asymptotic form as $\tilde{\phi}\to 0$ and $|\mathbf{R}|\gg 1$ is

$$G_L(\mathbf{R};t,h)\simeq D(T)\,|\mathbf{R}|^{-d+\sigma}X(\tilde{\phi}^{1/\sigma}\mathbf{R},\tilde{\phi}^{1/\sigma}L) \tag{10}$$

where $\tilde{\phi}$ obeys Eq. (7). The above result indicates that at any space dimensionality d the role of an effective correlation length is played by the quantity

$$\xi_L(t,h)=[\tilde{\phi}_L(t,h)]^{-1/\sigma} \tag{11}$$

When $d>2\sigma$ and $L\to\infty$, the solution $\tilde{\phi}_L$ of the spherical constraint (7) is such that $\tilde{\phi}_L L^{\sigma}\to 0$. Then, by neglecting terms of $\mathcal{O}(\tilde{\phi}_L L^{\sigma})$ in (7) and taking into account definition (11), we obtain the following equation for ξ_L:

$$\begin{aligned}|W'_{d,\sigma}(0)|\,(L/\xi_L)^{\sigma}L^{d-2\sigma}-D^{(0)}_{d',\sigma}(L/\xi_L)^{-\sigma+d'}\\ =\rho_\sigma\tilde{t}L^{d-\sigma}+\rho_\sigma^{-1}h^2L^{d+\sigma}(\xi_L/L)^{2\sigma}\end{aligned} \tag{12}$$

where the variable

$$\tilde{t}=t-2Y^{(s)}_{d,d',\sigma}(0)/\rho_\sigma L^{d-\sigma} \tag{13}$$

allows for the finite-size shift in the critical temperature.[7,15] Obviously, the solution of Eq. (12) may be written in the form

$$\xi_L=L\xi(\tilde{t}L^{y_T},hL^{y_H},L^{y_u}) \tag{14}$$

where, at $d>d_u=2\sigma$,

$$y_T=1/\nu=\sigma,\qquad y_H=\Delta/\nu=3\sigma/2,\qquad y_u=2\sigma-d \tag{15}$$

On the other hand, by introducing the new variables

$$\xi_L^*=\xi_L L^{-1-q_1y_u},\qquad t^*=\tilde{t}L^{y_T+q_2y_u},\qquad h^*=hL^{y_H+q_3y_u} \tag{16}$$

with

$$q_1=-(2\sigma-d')^{-1},\qquad q_2=q_1y_T,\qquad q_3=q_1y_H \tag{17}$$

we see that the solution of Eq. (12) may be written in the equivalent form

$$\xi_L = L^{1+q_1 y_u} \bar{\xi}(\tilde{t} L^{y_T + q_2 y_u}, h L^{y_H + q_3 y_u}) \tag{18}$$

Note that there $q_1 y_u > 0$, in apparent contradiction with the assumption of Binder *et al.*[9] The explanation of this fact is the following: the inequality $q_1 y_u \leqslant 0$ adopted in ref. 9 holds only in the case when the effective correlation length may be defined in terms of the second moment of the pair correlation function. In the case of long-range interactions ($0 < \sigma < 2$) or near the critical point, the role of an effective correlation length which scales long distances in the pair correlation function [see Eq. (10)] is played by the quantity $\tilde{\phi}^{-1/\sigma}$.[14] It is known that at the critical point the latter quantity increases faster than linearly in L when $L \to \infty$ if $d > d_u$.[3,5,6,16]

Consider now expression (4) for the singular part of the free energy density. Since, in view of (18), $L\bar{\phi}_L^{1/\sigma} \to 0$ when $L \to \infty$ at fixed t^*, h^*, the sum on the right-hand side of Eq. (4) may be approximated at $0 < d' < \sigma$, $d > 2\sigma$, as follows:

$$\begin{aligned}
&\sum_{l(d-d')}' |l|^{-d} u_{d,\sigma}(L\,|l|\,\tilde{\phi}^{1/\sigma}) \\
&\quad \simeq u_{d,\sigma}(0) \sum_{l(d-d')}' |l|^{-d} \\
&\qquad - (L^\sigma \tilde{\phi})^{d'/\sigma} \frac{2\pi^{(d-d')/2}}{\Gamma((d-d')/2)} \int_0^\infty dr\, r^{-d'-1} [u_{d,\sigma}(0) - u_{d,\sigma}(r)] \\
&\quad = u_{d,\sigma}(0) \sum_{l(d-d')}' |l|^{-d} - \frac{\pi^{(d+1)/2}}{d'\Gamma((d+1)/2)} |D_{d',\sigma}^{(0)}|\, (L^\sigma \tilde{\phi})^{d'/\sigma}
\end{aligned} \tag{19}$$

Now, by taking into account Eqs. (14) and (18), we can cast the free energy density (4) into two equivalent forms:

$$(k_B T)^{-1} f_L(t, h) \simeq L^{-d} f(\tilde{t} L^{y_T}, h L^{y_H}, L^{y_u}) \tag{20}$$

and

$$(k_B T)^{-1} f_L(t, h) \simeq L^{-d^*} \bar{f}(\tilde{t} L^{y_T + q_2 y_u}, h L^{y_H + q_3 y_u}) \tag{21}$$

where the exponent d^*,

$$d^* = d + d' q_1 y_u \tag{22}$$

is related to Fisher's anomalous dimension.[17]

3. THE GENERAL HYPOTHESIS

The exact results obtained in the preceding section for the mean spherical model admit a simple interpretation in terms of finite-size scaling functions depending on a dangerous irrelevant variable[17] u with exponent $y_u = d_u - d < 0$ at $d > d_u$:

$$\begin{aligned} f_L &= L^{-d} f(tL^{y_T}, hL^{y_H}, uL^{y_u}) \\ \xi_L &= L\xi(tL^{y_T}, hL^{y_H}, uL^{y_u}) \end{aligned} \tag{23}$$

where

$$\begin{aligned} f(x, y, z) &= z^{d' q_1} \bar{f}(xz^{q_2}, yz^{q_3}) \\ \xi(x, y, z) &= z^{q_1} \bar{\xi}(xz^{q_2}, yz^{q_3}) \end{aligned} \tag{24}$$

We may conjecture that the exponents q_1, q_2, and q_3 for $O(n)$ models at $d > d_u$ take the value (17) with $y_T = 1/\nu = \sigma$, $y_H = \Delta/\nu = 3\sigma/2$.

First, we should emphasize that the variable u is dangerous for the free energy density only when $d' > 0$. In this case the normalization coefficient of the free energy density [see Eqs. (21), (22)] has the meaning of a correlated volume:

$$L^{d-d'} \xi_L^{d'} \sim L^{d + d' q_1 y_u} = L^{d*} \tag{25}$$

In ref. 9 three arguments are given in favor of $d^* = d$. All of these arguments, however, are based on the assumption that the system is fully finite, i.e., that $d' = 0$.

Second, note that, as follows from (23) and (24),

$$\xi_L(t, h, u) = L^{1 + q_1 y_u} \bar{\xi}(tL^{y_T^*}, hL^{y_H^*}) \tag{26}$$

where

$$y_T^* = y_T + q_2 y_u, \qquad y_H^* = y_H + q_3 y_u \tag{27}$$

The existence of the thermodynamic limit ξ_∞ of ξ_L implies that at fixed $t > 0$ and $ht^{-\Delta}$

$$\xi_\infty(t, h, u) \sim t^{-\nu} X(ht^{-\Delta}) \tag{28}$$

where

$$\Delta = y_H^*/y_T^*, \qquad 1 + q_1 y_u = \nu y_T^* \tag{29}$$

and $X(\cdot)$ is a universal function. In view of (29), Eq. (26) may be rewritten in the form

$$l_L = Lg(tL^{y_T^*}, hL^{y_H^*}), \qquad l_L = \xi_L^{1/\nu y_T^*} \tag{30}$$

where a new characteristic length l_L of the finite system has been introduced and $g(x, y) = [\bar{\xi}(x, y)]^{1/\nu y_T^*}$. Next, from the existence of the thermodynamic limit l_∞ of l_L we obtain

$$l_\infty(t, h, u) \sim t^{-1/y_T^*} \tilde{X}(ht^{-\Delta}) \tag{31}$$

By differentiation of the finite-size scaling relationship for the free energy density with respect to the magnetic field, one may show that[9]

$$y_T^* = d^*/(\gamma + 2\beta), \qquad y_H^* = d^*(\gamma + \beta)/(\gamma + 2\beta) \tag{32}$$

Therefore, the characteristic length l_∞ introduced here [see Eq. (31)] coincides at $d' = 0$, when $d^* = d$, with the thermodynamic length defined by Binder *et al.*[9] [see Eq. (1)]. In the case of a general geometry $L^{d-d'} \times \infty^{d'}$, by Eqs. (17), (27), and (32), the dimensionality d^* may be written as

$$d^* = d - d'(d\nu - \gamma - 2\beta)/(d'\nu - \gamma - 2\beta) \tag{33}$$

Obviously, $d^* = d$ in the case when $d' = 0$, d being arbitrary, as well as in the case when $d < d_u$, and the hyperscaling relation $d\nu = \gamma + 2\beta$ holds, $d' < d_l = \sigma$ being arbitrary. However, only in the latter case does the characteristic length l_L coincide with the correlation length ξ_L. In any case, either when $d < d_u$ or when $d > d_u$, the length l_L obeys the universal finite-size scaling relation (30) with exponents y_T^* and y_H^* given by Eqs. (32) and (33).

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