Hyperuniversality and the renormalization group for finite systems

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The structure of finite-size scaling within the framework of the field-theoretic renormalization-group approach is examined. New size-dependent ultraviolet divergences are introduced into the theory. It is shown, nonetheless, that "two-scale-factor" universality reflects itself in the finite-size free energy and produces a scaling form such as that discussed by Privman and Fisher. A consequence is that the singular part of the finite-system free energy *at the bulk critical point* is universal. Extensions to surface and interfacial free energies, first proposed from the results of Ising simulations, are supported qualitatively.

I. INTRODUCTION

Finite-size scaling, formulated several years ago by Fisher and co-workers[1] has been used in a variety of ways to extrapolate results obtained from a finite system to obtain information appropriate to an infinite system. In its traditional and simplest form the statement of finite-size scaling asserts that all lengths diverging at bulk criticality are proportional to, say, the disordered-phase bulk correlation length $\xi_\infty = C_0 t^{-\nu}$, and the singular part of the free-energy density near bulk criticality may be expressed (in zero ordering field) as

$$(k_B T_c)^{-1} f_s(t,L) \approx A_1 |t|^{2-\alpha} W^{(\pm)}\left[\frac{L}{\xi_\infty}\right], \quad t \gtrless 0 . \tag{1}$$

Here α and ν are the standard critical exponents for the specific heat and correlation length, L is the linear size of the system, and t is the reduced temperature $t=(T-T_c)/T_c$. A_1 and C_0 are system-dependent constants, and the function $W^{(\pm)}$ is expected to be a universal function of its arguments. No additional metrical factor appears in the argument of $W^{(\pm)}$ in (1) as heuristic arguments[2] (and, indeed, the renormalization-group structure discussed below) on the form of correlations indicate.

In a recent paper Privman and Fisher[2] argued that the asymptotic free-energy density given in (1) can, in fact, be expressed in the following form

$$(k_B T_c)^{-1} f_s(t,L) \approx L^{-d} Y(C_1 t L^{1/\nu}) , \tag{2}$$

where d is the spatial dimensionality of the system assumed less than the upper critical dimension d_u, and $Y(x)$ is a universal function common to all systems in the universality class of the given system. The new hypothesis eliminates one of the nonuniversal amplitudes by assuming a relationship between the constants of (1) of the form $A_1 C_0^d = U$, where U is universal. This last relationship is recognized as the condition for "two-scale-factor" or hyperuniversality[3–5] which holds that for the bulk system $(k_B T)^{-1} f_s \xi^d$ is asymptotically universal. This form of universality should hold in (1) in the limit $L \to \infty$, so that (2) may be viewed as the expression of two-scale-factor universality within the framework of finite-size scaling.

Evidence has been accumulating that the reduced form (2), with only one nonuniversal constant, holds. Singh and Pathria[6,7] have verified (2) within the context of the ideal, relativistic Bose gas and the spherical model of ferromagnetism. Mon[8] has found that Monte Carlo data on the three-dimensional Ising model are in accord with (2) in that the *total* singular part of the free energy (in units of $k_B T_c$) is universal at bulk criticality. Mon and Jasnow[9] also found, again from Monte Carlo simulations, that the *total* interfacial free energy for two coexisting phases in a finite system *at bulk criticality* is universal, which would be consistent with an "interfacial version of (2). For the surface tension (interfacial free energy per unit "area") $\sigma(t,L)$, one would conjecture

$$(k_B T_c)^{-1} \sigma(t,L) \approx L^{-(d-1)} \Sigma(C_1 t L^{1/\nu}) , \tag{3}$$

where the scaling function Σ is presumed to be universal. Finally, Mon and Nightingale[10] have found that Monte Carlo simulations for the incremental free energy of an Ising *free surface* show that the total surface free energy is a universal number at bulk criticality. The last relation (3) and the analog for free surfaces would be extensions of the Privman-Fisher form of finite-size scaling.

It has recently been shown that conventional finite-size scaling (1) is contained within the structure of the field-theoretic renormalization-group approach.[11] Brézin[11] commented that counter terms appropriate to the infinite system should be sufficient to renormalize the theory for systems of finite size. This is reasonable since ultraviolet divergences are handled by the renormalization procedure, and these ought to be unmodified (see, however, below). Furthermore, correlations in the finite system satisfy the same renormalization-group equations as in the corresponding infinite system. Rudnick *et al.*[12] showed that the practical calculations could be extended to $4-\varepsilon$ dimensions and, using a combination of Poisson and Ewald sum techniques,[13] evaluated universal finite-size scaling functions to one-loop order. Brézin and Zinn-Justin[14] also arrived at the conclusion that ε-expansion techniques could, in principle, be used in finite-size scaling analyses. It has also been appreciated that two-scale-factor universality holds within the renormalization-group approach, at least as far as bulk properties are concerned.[15]

The work of Rudnick *et al.*[12] and Brézin and Zinn-Justin[14] provides a practical means of obtaining the finite-size free energy. In this paper, following Rudnick *et al.*, we show that explicit calculations in $d=4-\varepsilon$ indeed yield a free energy in agreement with the "two-scale-factor" form given in (2). We sketch how a general argument to all orders in perturbation theory would proceed; explicit calculations to two-loop order are reported. In $d=4$ there is a breakdown of hyperscaling, and, as discussed previously,[12] finite-size scaling does not hold in its simplest form. Singh and Pathria have recently investigated the possible extension of (2) when hyperscaling breaks down in the context of $O(n)$ models;[16] see, however, related comments by Shapiro.[17]

The outline of this short article is as follows. In the next section we sketch the renormalization-group calculation of the finite-size system free energy. Concluding remarks are given in Sec. III, and some further details are included in the Appendix.

II. RENORMALIZATION-GROUP APPROACH TO FINITE-SIZE FREE ENERGY

One begins, as usual, with a Landau-Ginzburg-Wilson description of the system in which case the Hamiltonian divided by $k_B T$ is taken to be

$$H=\int_\Omega d^dx\left[\tfrac{1}{2}(\nabla s)^2+\tfrac{1}{2}rs^2+(1/4!)us^4\right] \qquad (4)$$

in "box" domain Ω with volume $V(\Omega)=L^d$. Periodic boundary conditions are assumed throughout. The Hamiltonian (4) is for an Ising-like system, but the analysis is easily extended to the case of an n-component order parameter. As usual $r\propto T-T_0$, where T_0 is a reference temperature. The partition function takes the form[12]

$$Z=\int_{-\infty}^{\infty} dm\,\exp[-L^dH_{mf}(m)]\exp[-L^d\Gamma_1(m)]\ , \qquad (5)$$

where $H_{mf}\equiv rm^2/2+um^4/4!$ and

$$\exp[-L^d\Gamma_1(m)]=\int \mathscr{D}\sigma\,\exp[-H_1(\sigma;m)]\ . \qquad (6)$$

As in Ref. 12, one sets $s=\sigma+m$, where σ has no $k=0$ part, and finds $H(s)=H_{mf}(m)+H_1(\sigma;m)$, so that H_1 is the σ-dependent part of $H(s)$. In Ref. 12 Γ_1 is evaluated via a loop expansion for the *finite system;* the reader is referred to that article for details. In the diagram expansion of Γ_1 appearing in (6), the analogous momentum integrations in the bulk calculation are now replaced by discrete sums over $q_i=2\pi n_i/L$, where $n_i=0,\pm1,\pm2,\ldots$, and $i=1,2,\ldots,d$. (The single terms with all the $n_i=0$ are, of course, discarded.) The Poisson sum technique is then used to transform the sums into the corresponding infinite-system contributions plus some finite-size corrections. In Refs. 12 and 14 only one-loop graphs were considered, and the finite-size corrections to that order are all finite as the ultraviolet cutoff is removed to infinity. However, at higher-loop level, the finite-size corrections introduce *new* ultraviolet divergences in addition to the usual bulk ones. But as one might expect, these new size-dependent divergences have to be canceled exactly without introducing any new renormalization constants, because essential features of the renormalized theory should not depend on the short wavelength behavior. As a check on this point, we carried out a two-loop calculation of the free energy explicitly. It is shown, indeed, that the usual infinite-system renormalization constants are enough to renormalize the theory, and the size-dependent ultraviolet divergences do cancel exactly with each other. As an example of this point, a two-loop graph calculation is sketched in the Appendix. Another important fact to notice is that every term of the diagram expansion of (6) (after counter terms remove divergences) will be a function of the dimensionless variables κL, L^2T, $\kappa^{4-d}u$, and $L^{d-2}m^2$, where κ is an inverse length which is introduced in the renormalization process and sets the scale of the renormalized theory. Here $T=t+\kappa^{4-d}um^2/2$ is the "mass" appearing in the propagator, with $t\propto T-T_c$ (see below). In the Appendix some terms of the diagram expansion are considered in further detail.

The essential features of the calculation are illustrated as follows. The renormalized form of the full exponential in (5), $\Gamma=H_{mf}+\Gamma_1$, takes the form

$$\Gamma_R(t,m,u,\kappa;L)=\Gamma_B(r,m,u,\Lambda;L)-a_1^\infty-a_2^\infty r-a_3^\infty r^2\ , \qquad (7)$$

where the additive renormalizations are introduced in the usual way and are the same as for the infinite system, as indicated by the superscript. The subscript B indicates the bare function. The bare, original, parameters r,m,u on the right-hand side are replaced as usual by

$$r\Longrightarrow Z_{\phi^2}t+\delta t,\quad u\Longrightarrow\kappa^{-\varepsilon}Z_u u,\quad m\Longrightarrow Z_\phi^{1/2}m\ , \qquad (8)$$

where, as confirmed explicitly to two-loop order, the Z's are the same as for the infinite system. The renormalization-group equation for Γ_R is

$$\left[\kappa\frac{\partial}{\partial\kappa}+\beta(u)\frac{\partial}{\partial u}-\tfrac{1}{2}\eta(u)m\frac{\partial}{\partial m}+[-2+\gamma_{\phi^2}(u)]t\frac{\partial}{\partial t}\right]\Gamma_R =G(t,u,\kappa)\ , \qquad (9)$$

where the inhomogeneous term, which results from the additive renormalizations, is given by

$$G(t,u,\kappa)=-\kappa\frac{d}{d\kappa}(a_1^\infty+a_2^\infty r+a_3^\infty r^2)\Big|_{\text{bare}}\ , \qquad (10)$$

where bare quantities are held fixed. In our two-loop calculation, the additive renormalization constants are chosen as in Eq. (4.1) of Ref. 12. The inhomogeneous part is itself renormalized and is finite, containing no divergences as the cutoff is taken to infinity, or, equivalently, no poles in $\varepsilon=4-d$. As noted elsewhere[11,12] the system size plays the role of a parameter in (9).

The renormalization-group equation is solved in the usual fashion (see, e.g., Refs. 12, 18, and 19 and below) by introducing the flows (or running coupling constants) so that one replaces $t\to\rho^2t(\rho)$, $u\to u(\rho)$, $\kappa\to\kappa\rho$, and $m\to m(\rho)$. Then one has

$$\Gamma_R=\Gamma_R[\rho^2t(\rho),m(\rho),u(\rho),\kappa\rho;L]+\int_\rho^1\frac{d\lambda}{\lambda}G[\lambda^2t(\lambda),u(\lambda),\kappa\lambda]\ , \qquad (11)$$

where

$$\Gamma_R[\rho^2 t(\rho), m(\rho), u(\rho), \kappa\rho; L] = \tfrac{1}{2}\rho^2 t(\rho) m^2(\rho) + \frac{1}{4!}(\kappa\rho)^{\epsilon} u(\rho) m^4(\rho) + L^{-d}\tilde{\Gamma}_1[L^2 T(\rho), L^{d-2} m^2(\rho), u(\rho); \kappa\rho L] \ . \quad (12)$$

Here $L^{-d}\tilde{\Gamma}_1 = \Gamma_1$ is the loop correction containing all diagram contributions, and

$$T(\rho) = \rho^2 t(\rho) + \tfrac{1}{2}(\kappa\rho)^{\epsilon} u(\rho) m^2(\rho) \ . \quad (13)$$

A test of hyperuniversality requires much the same approach as for the bulk system. One should include the possibility of the coupling constant u differing from the fixed-point value to demonstrate system independence. Nonuniversal amplitudes may then depend explicitly on the value of u. In addition one should demonstrate that appropriate results are independent of renormalization scheme. This latter requirement cannot be met fully; we shall return to this point below.

The most explicit way to proceed is to linearize about the fixed point. One uses the scaling fields $g_t(\rho)$ and $g_u(\rho)$ which arise in the computation of ordinary bulk properties,

$$\begin{aligned} g_u(\rho) &= g_u \rho^{\omega} = \Delta u \rho^{\omega} \ , \\ g_t(\rho) &= t(\rho)\left[1 - \frac{\nu' g_u(\rho)}{\nu^2 \omega}\right] = g_t \rho^{-(1/\nu)} \end{aligned} \quad (14)$$

with $\Delta u = u - u^*$, u^* being the fixed-point value. The exponent $\omega = \epsilon + O(\epsilon^2)$ is the correction to scaling exponent,[20] and the function $\nu(u)$ enters the flow equation for $t(\rho)$ in the usual way. The correlation length exponent is $\nu = \nu(u^*)$, and $\nu' = (d\nu/du)_{u^*}$.[18] The starting value is $g_t = t[1 - (\nu'/\nu^2\omega)\Delta u]$, which reduces to t if the fixed-point value were chosen. Scaling variables x, y, and z may then be introduced as

$$x = \frac{g_t}{\kappa^2}(\kappa L)^{1/\nu}, \quad y = \frac{g_u}{(\kappa L)^{\omega}}, \quad z = \kappa\rho L \ . \quad (15)$$

Substituting back into (12) shows that $L^d \Gamma_R(t, m, u, \kappa; L)$ may be written as $L^d \Gamma_R = \tilde{\Gamma}_R[x, y, z; L^{d-2} m^2(\rho)]$. It is straightforward to show that the trajectory integral in (11) is also a function of x, y, and z. A change of integration variables allows one formally to perform the m integration in (5) and then conclude that the singular part of the reduced free energy is a function of the scaling variables x, y, and z. All system dependence has been included in the starting values g_t and g_u. A somewhat better job avoids linearization around the fixed point with the introduction of the metrical factors X and Y as in Refs. 15 and 19; it is emphasized that the same operations as for demonstrations of universality in bulk systems are required.

The ρ dependence has not yet been removed from the results. The theory is independent of this parameter, merely swapping the free energy between the fluctuations and the trajectory integral, but a consistent choice must be made. For computational reasons, to allow numerical analysis of the free energy from the critical to the finite-size regime, a cumbersome choice was made previously.[12] Here, since the formal structure is all that is required, the simpler choice $\rho\kappa L = 1$ will serve.[11] This choice of ρ, as discussed in Ref. 12, corresponds to the strongly finite-size regime in which the bulk correlation length ξ_∞ is large compared to the system size L, so the renormalization must end when the effective block spin size $[\sim(\kappa\rho)^{-1}]$ is on the order of L. This yields for the singular part of the system free energy the schematic form

$$(k_B T_c)^{-1} f_s(t, L) = L^{-d}[Y(x, y)]_{\text{singular}} \quad (16)$$

which indeed has the structure of the Privman-Fisher free energy, with the system dependences being contained in x and y. (The bracket indicates that the singular part needs to be extracted. For the trajectory integral contribution this corresponds to the piece scaling as $L^d t^{2-\alpha}$.) A detailed expression for the function $Y(x,y)$, suitable for numerical evaluation from the critical to the strongly finite-size regime, is only available to one-loop order.[12]

To complete the picture one would like to demonstrate independence of the renormalization scheme. For example, if the scheme were changed, the fixed-point value would, in general, change and so would various critical amplitudes. To compare results for, say, regularization via hard cutoff versus dimensional methods requires explicit calculation just as for bulk demonstrations of universality. One can show formally that the final scaling functions [e.g., $Y(x,y)$] are independent of scheme at least in a limited sense. Within the framework of calculating all counter terms in the symmetric theory at $T = T_c$, one can vary the normalization conditions (for example the definition of the renormalized coupling u) and show the independence of the scaling functions. The system dependence of the scaling variables x and y changes. Alternatively one can imagine computing the counter terms at two different reference temperatures. These forms of scheme independence are of the type one can easily demonstrate (without explicit loop calculations) for bulk properties. We have confirmed explicit independence between hard cutoff and minimal subtraction methods at the one-loop level.

III. CONCLUDING REMARKS

The arguments presented here indicate how the Privman-Fisher form of the singular part of the free energy is contained within the structure of the field-theoretic renormalization group. A few additional insights are obtained as well. One notices that L, while entering the scaled combinations, does not mix in the formation of the scaling fields, g_u and g_t. It is clear from the outset that in the construction of the renormalization-group equations for the vertices,[11] L is not renormalized. No "new" counter term is required. It (L) is a "parameter" much the same as the wave number and, within these schemes, does not enter the construction of scaling fields.

Surface and interfacial properties can be computed within the renormalization-group approach as well.[21] In the latter case specifically, one may imagine computing the interfacial free energy by considering the free-energy difference in a "slab" of infinite extent in $(d-1)$ directions and of "thickness" L subjected to antiperiodic or periodic boundary conditions.[21] This free-energy difference may be computed within the framework of the field-theoretic renormalization group, and it should explain the apparent universality of the total interfacial free energy at the bulk T_c as observed in Monte Carlo simulations.[9] The reasoning is as follows. We have already demonstrated that the finite-size free-energy density in "box" geometry with periodic boundary conditions has the form given by Privman and Fisher, as in Eq. (2). For slab geometry, with the system of finite extent in, say, the z direction, one expects a similar form with scaling function Y^{per} for the periodic case. Likewise, we expect in the case of antiperiodic boundary conditions, the finite-size free-energy density will again have the form (2), with a different universal function Y^{anti} having the same argument as that of Y^{per}, because both Y^{per} and Y^{anti} give the same bulk free energy as $L\to\infty$. Singh and Pathria have recently investigated the antiperiodic boundary condition case in the context of the spherical model;[22] they indeed found the free energy to have the form (2). To obtain the interfacial free energy per unit "area" or the surface tension for the finite system, the difference of the free-energy densities is merely multiplied by L.[21] The result indeed has the form conjectured in (3). We hope to report the explicit results of such a renormalization-group calculation in a future publication.

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APPENDIX

Some technical details are given in this Appendix. To two-loop order, the exponent of (5) is

$$\Gamma(m)=\tfrac{1}{2}rm^2+(1/4!)um^4+\tfrac{1}{2}\left[\frac{2\pi}{L}\right]^d\sum_{\mathbf{q}}{}'\ln(q^2+T_0)$$
$$+\tfrac{1}{8}u\left[\left[\frac{2\pi}{L}\right]^d\sum_{\mathbf{q}}{}'\frac{1}{q^2+T_0}\right]^2-\tfrac{1}{12}(um)^2\left[\frac{2\pi}{L}\right]^{2d}\sum_{\mathbf{q}_1,\mathbf{q}_2}{}'\frac{1}{(q_1^2+T_0)(q_2^2+T_0)[(\mathbf{q}_1+\mathbf{q}_2)^2+T_0]}\,, \tag{A1}$$

where $q_i=2\pi n_i/L$, $n_i=0,\pm1,\pm2,\ldots$, the prime on the summation means no $\mathbf{q}=0$ mode, and $T_0=r+um^2/2$. As in the bulk renormalization calculation, we replace the "bare" quantities by the renormalized ones using (8) of the paper, where the renormalization constants, the Z's, are the same as in the infinite system calculation.[23] Since in the perturbation expansion (A1) the two-loop terms are $O(u)$ [keeping in mind that m^2 is of $O(1/u)$], when we expand Z's and compute Γ, we keep terms up to $O(u)$.

Each sum of (A1) is now transformed by Poisson transformation into the corresponding infinite-system term plus size-dependent correction terms. For example, Ref. 12 shows how to transform $\sum'\ln(q^2+T_0)$. Other terms are transformed similarly. To see how the Poisson transformation of the sums introduces size-dependent ultraviolet divergences, consider the last term of (A1). Applying the Poisson summation technique, one finds

$$\left[\frac{2\pi}{L}\right]^{2d}\sum_{\mathbf{q}_1,\mathbf{q}_2}{}'\frac{1}{(q_1^2+T_0)(q_2^2+T_0)[(\mathbf{q}_1+\mathbf{q}_2)^2+T_0]}=\int\frac{d^dq_1d^dq_2}{(q_1^2+T_0)(q_2^2+T_0)[(\mathbf{q}_1+\mathbf{q}_2)^2+T_0]}$$
$$+3\sum_{\mathbf{n}}{}'\int\frac{e^{i\mathbf{q}_1\cdot\mathbf{n}L}d^dq_1d^dq_2}{(q_1^2+T_0)(q_2^2+T_0)[(\mathbf{q}_1+\mathbf{q}_2)^2+T_0]}$$
$$-\frac{3}{T_0}\left[\frac{2\pi}{L}\right]^3\int\frac{d^dq}{(q^2+T_0)^2}$$
$$-\frac{3}{T_0}\left[\frac{2\pi}{L}\right]^d\sum_{\mathbf{n}}{}'\int\frac{e^{i\mathbf{q}\cdot\mathbf{n}L}}{(q^2+T_0)^2}d^dq+\frac{2}{T_0^3}\left[\frac{2\pi}{L}\right]^{2d}. \tag{A2}$$

The components of **n** are integers and the prime indicates $\mathbf{n}=0$ is absent. It is immediately seen that the first term on the right-hand side of (A2) is the usual bulk contribution; the second and the third terms depend on L and are logarithmically divergent at $d=4$. These kinds of L-dependent ultraviolet divergences are absent in one-loop calculations, as performed in Refs. 12 and 14.

After each sum of (A1) is transformed to a bulk term plus finite-size corrections, one introduces the renormalization constants into it. As noted, the Z's are taken to be the same as for the infinite system; they can be determined, say, by a minimal subtraction scheme.[24] Through tedious but straightforward analysis one can show that all ε poles do get canceled exactly, including those L-dependent divergences mentioned above, provided an L-dependent "mass shift" δt is introduced in (8). The mass shift δt starts to have L dependence at $O(u^2)$.

After multiplication through (A1) by L^d, it is easy to see that the variables on the right-hand side will be κL, $L^2 t$, and $L^{d-2}m^2$, i.e., after the explicit calculation of (A1), these will be the variables of $\Gamma(m)$. The required *additive* renormalizations are the same ones as needed in the bulk calculation, i.e, of the form of $a_1^\infty + a_2^\infty r + a_3^\infty r^2$. So after multiplication by L^d, the piece that will ultimately contribute to the singular part of the free energy involves only $L^2 t$. Thus the natural variables of our theory are κL, $L^2 t$, and $L^{d-2}m^2$.

In solving the renormalization equations, we change the variables t, u, m, and κ into the corresponding "running" ones, as above, which leads to the variables x, y, and z defined in (15).

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