Universal size dependence of the free energy of finite systems near criticality

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A scaling framework is developed for the emergence of the universal finite-size correction $(u\ln L)/L^2$, recently found by Cardy and Peschel in the free-energy density of the two-dimensional (2D) conformally invariant models at T_c. Our approach applies in the critical region $T \simeq T_c$, and accounts for the universality of u, but not its value. We predict a similar universal term, $(u\ln L)/L^3$, in 3D. We also find that the "corner" free energy in the bulk ($L=\infty$) has the leading singular behavior $(-vu\ln|t|)$.

Effects of system size L and boundaries on critical behavior have been subject to active investigations in recent years. The finite-size scaling theory,[1-6] introduced by Fisher,[1] finds extensive applications in the analysis of experimental, Monte Carlo, and transfer-matrix data,[2-5] as well as in recent theoretical developments related to conformal invariance.[6] For systems with periodic boundary conditions, the finite-size scaling is now well understood both in the phenomenological scaling theory[1,5] and the field-theoretical (FT) ε-expansion formulation.[7,8] For other boundary conditions, the progress has been more limited. In particular, for an important case of *free boundary conditions*,[9-11] corresponding to the Dirichlet boundary conditions in the continuum FT description,[9] the ε-expansion approach[10] needs further development especially for $T<T_c$. The scaling formulations[1,5,10,11] and general renormalization-group (RG) considerations[12] have been proposed and tested.[1-4]

However, some unexplored questions remain unanswered for systems with free boundaries, especially in connection with the precise form and definition[5,10] of the "nonsingular background" contribution $f_{\rm ns}$ corresponding to the additive FT counterterms. Thus, for the *free-energy density* f measured in units of k_BT, we expect

$$f(t,L)=f_s(t,L)+f_{\rm ns}(t,L), \tag{1}$$

for small $t\equiv(T-T_c)/T_c$. Here the "singular" (as $L\to\infty$) part f_s develops the thermodynamic singularities in the $L\to\infty$ limit.

Recently, Cardy and Peschel[13] discovered that the critical-point free energy $f(0,L)$ of the two-dimensional (2D) conformally invariant models with free boundaries that are curved or have corners, contains the term $(u\ln L)/L^2$, with a *universal* coefficient u. Note that in the finite-size systems, the universal amplitudes generally depend on the sample shape and boundary conditions[5,14] but not on the microscopic lattice structure and interaction details within a given RG universality class. In this work, we propose a scaling mechanism which accounts for the universality of u. We will mostly use the 2D notation. However, a discussion of the possible universal term $(u\ln L)/L^3$ in 3D can be formulated along similar lines.

We consider systems with critical points with no logarithmic bulk singularities, i.e., α noninteger,[15] and below their upper critical dimension which is, e.g., $D=4$ for the ferromagnetic Ising spin model, etc.[16] Then the singular part of the free energy can be described by the hyperuniversal scaling form[5]

$$f_s(t,L)=L^{-D}Y[t(L/\lambda)^{1/\nu}]+\cdots, \tag{2}$$

where λ is the only nonuniversal constant entering (it can be assumed positive without loss of generality). This length scale (λ) is comparable to the microscopic lattice spacing (inverse momentum cutoff). Corrections to scaling in (2) are proportional to higher negative powers of L.[5,17] As long as the dimensionality D can be regarded as a *continuous variable*, e.g., in the framework of the ε expansion,[10] it is natural to assume that for general D, the nonsingular part of the free energy can be expanded in the inverse powers of L.[5,9,10,12] For D near 2, we consider terms to order L^{-2},

$$f_{\rm ns}(t,L)=\psi_0(t)+\psi_1(t)/L+\psi_2(t)/L^2+o(L^{-2}). \tag{3}$$

Here, the successive terms can be associated with the bulk (interior), surfaces, corners and/or surface-curvature contributions.[9,10] Similar decomposition of the full free energy $f(t,L)$ away from T_c, is well established[1] (see below). The functions $Y(\tau)$, with

$$\tau\equiv t(L/\lambda)^{1/\nu}, \tag{4}$$

and $\psi_0(t),\psi_1(t),\psi_2(t)$ are regular at the origin and can be expanded in the Taylor series in τ or t, respectively. All these functions depend implicitly on D.

When the dimensionality passes through an integer value, $D=2$ here, the singular ($\sim L^{-D}$) and nonsingular ($\sim L^{-2}$) terms in the free energy may have divergent amplitudes yielding additional logarithmic factors. A familiar example of this effect is the emergence of the bulk logarithmic specific-heat singularity[15,18] as $\alpha\to 0$. Such a mechanism arises naturally in the RG framework for the bulk[18,19] and finite-size[12,20] properties. Thus, we assume the D dependence

$$Y(\tau;D)=-\frac{u}{D-2}+y(\tau)+O(D-2), \tag{5}$$

$$\psi_2(t;D)=\frac{u\lambda^{2-D}}{D-2}+\bar{\psi}_2(t)+O(D-2). \tag{6}$$

The choice of the length scale factor λ in the singular term in (6), is arbitrary. Indeed, if we use $\bar{\lambda}$ instead, the difference is finite in the $D \to 2$ limit [it is $u\ln(\bar{\lambda}/\lambda) + O(D-2)$], and can be absorbed in the definition of $\bar{\psi}_2(t)$. [One can also replace λ in Eq. (6) by 1. This, however, obscures the units of the quantities involved.] The singular terms must have constant coefficients, of opposite signs, as shown in (5) and (6), because Y and ψ_2 depend on different variables. The key observation, however, is that since $Y(\tau;D)$ is universal, both u and $y(\tau)$ in (5) must be universal. Assuming that ψ_0 and ψ_1 in (3) have finite limits as $D \to 2$, we get[21]

$$f_{2\mathrm{D}}(t,L) = \psi_0(t) + \psi_1(t)/L + \bar{\psi}_2(t)/L^2 + y[t(L/\lambda)^{1/\nu}]/L^2 + u\ln(L/\lambda)/L^2 + \cdots . \quad (7)$$

Note that the choice of the identical factors u in the singular terms in (5) and (6) ensures that the free energy (7) is regular as $D \to 2$. Similar expression for the 3D case is

$$f_{3\mathrm{D}}(t,L) = \psi_0(t) + \psi_1(t)/L + \psi_2(t)/L^2 + \bar{\psi}_3(t)/L^3 + y[t(L/\lambda)^{1/\nu}]/L^3 + u\ln(L/\lambda)/L^3 + \cdots , \quad (8)$$

where the notation is self-explanatory. Obviously, the scaling considerations alone cannot predict the *values* of the universal and nonuniversal quantities in (7) and (8). For example, for the periodic boundary conditions, we have $\psi_{k>0} \equiv 0$ and $u \equiv 0$. For further results in 2D, including the values of the universal critical point coefficients $Y(0)$ and u in some geometries, consult literature on conformal invariance.[6,13,22,23]

Consider now the behavior away from critically.[1] To simplify the notation, we assume $D=2$ and $t>0$ (i.e., $T>T_c$). The bulk, surface, corner/curvature decomposition of the free energy (and other thermodynamic functions, which can be accommodated in the present formulation, e.g., by adding a magnetic field in a standard manner[5]) applies, in the form[1]

$$f(t,L) = f_0(t) + f_1(t)/L + f_2(t)/L^2 + \cdots , \quad (9)$$

where one may conjecture[1] exponentially small corrections for the case of the straight line boundaries with sharp corners. For curved boundaries, L^{-3}, etc., terms cannot be excluded. The expansion (9) is defined for $L \to \infty$ at *fixed* $t>0$. However, one can consider the t dependence of the functions $f_k(t)$ as $t \to 0^+$, and the way it matches[1,10] with the asymptotic form of (7) for $L/\lambda \gg t^{-\nu}$, i.e., for $\tau \gg 1$.

There is no reason to expect a contribution $\sim \ln L/L^D$ away from criticality.[24] Following the standard line of argument,[1,10] the large-τ behavior of the scaling function $y(\tau>0)$ in (7) must, therefore, take the form

$$y_{2\mathrm{D}}(\tau) = y_2\tau^{2\nu} + y_1\tau^{\nu} - \nu u \ln\tau + y_0 + \cdots , \quad (10)$$

where all the coefficients are universal. A similar result in 3D reads

$$y_{3\mathrm{D}}(\tau \gg 1) = y_3\tau^{3\nu} + y_2\tau^{2\nu} + y_1\tau^{\nu} - \nu u \ln\tau + y_0 + \cdots . \quad (11)$$

By using relations (7) and (10), we can identify the leading $t \to 0^+$ *singular behavior* of the 2D free-energy contributions in (9),

$$f_{0,s}(t) \approx y_2 t^{2\nu}/\lambda^2, \quad (12)$$

$$f_{1,s}(t) \approx y_1 t^{\nu}/\lambda, \quad (13)$$

$$f_{2,s}(t) \approx -\nu u \ln t . \quad (14)$$

Extension to 3D is straightforward. Relation $f_{1,s} \sim t^{\nu(D-1)}$ has been considered, e.g., in Ref. 1. Note that λ is the only nonuniversal parameter entering; it can be conveniently normalized via the coefficient of the $t^{2\nu} = t^{2-\alpha}$ bulk-free energy singularity (12), for $t \to 0^+$. While the universal coefficients y_k in (10) and (11) will generally change for $t<0$, the leading "corner" free-energy singularity will remain $-\nu u \ln|t|$. Note that for systems with sharp corners (no curvature), the universal coefficient u in (7), (8), and (14) can be represented as a sum of individual corner contributions. In 2D, these are known exactly.[13]

In summary, we have developed a scaling description of the finite-size effects for systems with free boundaries,[25] with corners (and/or curvature). The "corner" terms in the free energy are particularly interesting, involving logarithmic factors and a universal constant u.

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[25]Note that the conformal-invariance formalism (Ref. 13) for the "corner" free-energy correction in 2D, applies also for the Gaussian models. Our formulation, however, *does not incorporate* the Gaussian models because the hyperuniversal finite-size scaling form (2) breaks down (Ref. 11). Detailed studies of finite-size corrections at criticality, for Gaussian-type interfacial models in general D, have been reported by M. P. Gelfand and M. E. Fisher, Int. J. Thermophys. (to be published).