Phase Transitions in Finite Systems: Influence of Geometry on Approach Toward Bulk Critical Behavior

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We predict the manner in which a physical system, of size $L^{d-d'} \times \infty^{d'}$, subject to periodic boundary conditions, approaches bulk critical behavior as $L \to \infty$. While for $T > T_c(\infty)$ the approach is exponential, for $T < T_c(\infty)$ it is generally governed by power laws whose indices are determined by the *bulk* exponents for the corresponding d- and d'-dimensional systems. Specific predictions on the spherical model of ferromagnetism and the relativistic Bose gas with pair production are verified by analytical results.

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Phase transitions in finite-size systems have been studied extensively over the past fifteen years or so.[1] Although the critical region has been the main focus of interest, the question of the approach of the system toward bulk behavior at temperatures away from $T = T_c(\infty)$ has also drawn some attention. Until recently it had been a common belief that, under periodic boundary conditions, this approach was exponential in nature—a result supported by exact calculations on certain examples of the Ising model,[2] the spherical model,[3] and the Bose gas[4-6]—so much so that the power-law behavior found for the free energy of a spherical-model film, for $T < T_c(\infty)$, was termed as "anomalous."[1] Lately, however, it has begun to emerge that, while for $T > T_c(\infty)$ the approach is indeed exponential, that for $T < T_c(\infty)$ may well be through power laws instead. For instance, the recent work of Privman and Fisher on finite-size effects in Ising-type models[7] of size $L^{d-d'} \times \infty^{d'}$ shows that, for $T < T_c(\infty)$, the low-field susceptibility of these systems, while exponential for a "cylindrical" geometry $(d'=1)$, varies as L^d for a "block" geometry $(d'=0)$. The same authors have further shown[8] that, for models with O(n) symmetry $(n > 1)$, the approach is algebraic even in the cylindrical case:

$$\chi_0 = \begin{cases} L^{2(d-1)} & (d'=1), \quad \text{(1a)} \\ L^d & (d'=0). \quad \text{(1b)} \end{cases}$$

The aim of the present Letter is threefold. First, we shall show that, for systems with continuous symmetries where the Mermin-Wagner theorem holds (and hence the lower critical dimension, $d_<$, is 2), the approach for $T < T_c(\infty)$ depends strongly on the geometry of the system and more commonly (in fact, for all $d' < 2$) turns out to be algebraic in nature; only for $d'=2$ does one encounter an exponential approach. Second, we shall demonstrate how one can predict, from the *bulk* behavior of the system in d dimensions near $T = T_c(\infty)$ and in d' dimensions near $T=0$, the various indices relevant to the question of approach. Third, we shall verify, with the help of analytical results, a set of predictions made on the spherical model of ferromagnetism and the relativistic Bose gas with pair production.

We consider a system of size $L^{d-d'} \times \infty^{d'}$, d being less than the upper (and greater than the lower) critical dimension of the system; for $d=3$, $d'=0$, 1, and 2 represent the geometry of a cube, a cylinder, and a film, respectively. The system is supposed to be subject to periodic boundary conditions and hence to obey the Privman-Fisher hypothesis[9] on the singular part of the free-energy density, viz.,

$$f^{(s)}(T,H;L) \approx TL^{-d} Y(x_1,x_2), \tag{2}$$

where $Y(x_1,x_2)$ is a universal function of the reduced variables x_1 $(=C_1 L^{1/\nu} t)$ and x_2 $(=C_2 L^{\Delta/\nu} H/T)$, $t = [T - T_c(\infty)]/T_c(\infty)$, ν and Δ being the usual d-dimensional bulk indices, while C_1 and C_2 are nonuniversal scale factors characteristic of the given system. Now, while the bulk system is critical at $T = T_c(\infty)$, the finite-size system, in the universality class under consideration, is critical at a shifted temperature $T_c(L) > 0$ if $d' > 2$ and only at $T=0$ if $d' \leq 2$. The crossover in the former case has been studied previously[3,5]; we shall, therefore, concentrate on the latter case alone.

To effect a crossover over a finite range of temperatures, from $T = T_c(\infty)$ down to $T=0$, we generalize the Privman-Fisher hypothesis by writing x_1 and x_2 as

$$x_1 = \tilde{C}_1 L^{1/\nu} \tilde{t}, \quad x_2 = \tilde{C}_2 L^{\Delta/\nu} H/T, \tag{3}$$

where $\tilde{C}_1$, $\tilde{C}_2$, and $\tilde{t}$ are so defined that the validity of the hypothesis is extended as desired; at the same time, they reduce to the original C_1, C_2, and t as $T \to T_c(\infty)$. Following Fisher,[10] we postulate that the temperature dependence of x_1 conforms to the requirement that

$$x_1 = \tilde{C}_1 L^{1/\nu}\tilde{t} = b[L/\xi(T)]^{1/\nu}, \quad (4)$$

where $\xi(T)$ is the bulk correlation length while b is a universal number. Clearly, if we throw all the temperature dependence arising from $\xi(T)$ into $\tilde{t}$, then $\tilde{C}_1$ can be made temperature independent. The scaling forms for the zero-field susceptibility and the (singular part of the) specific heat of the system are then given by

$$\chi_0(T,0;L) = -\left(\frac{\partial^2 f^{(s)}}{\partial H^2}\right)_{H=0} = -\frac{\tilde{C}_2^2 L^{2\Delta/\nu}}{T^2}\left(\frac{\partial^2 f^{(s)}}{\partial x_2^2}\right)_{x_2=0} \approx (\tilde{C}_2^2 L^{\gamma/\nu}/T) Z(x_1,0) \quad (5)$$

and

$$c^{(s)}(T,0;L) = -T\left(\frac{\partial^2 f^{(s)}}{\partial T^2}\right)_{H=0} \simeq -T\tilde{C}_1^2 L^{2/\nu}\left(\frac{\partial\tilde{t}}{\partial T}\right)^2\left(\frac{\partial^2 f^{(s)}}{\partial x_1^2}\right)_{x_2=0} \approx \tilde{C}_1^2 (T\,\partial\tilde{t}/\partial T)^2 L^{\alpha/\nu} Z^*(x_1,0), \quad (6)$$

where Z and Z^* are appropriate derivatives of $Y(x_1,x_2)$. Specializing to the spherical model, we compare the known bulk behavior[3,11] of ξ, χ_0, and $c^{(s)}$ for $T \gtrsim T_c(\infty)$ with the corresponding results emerging from Eqs. (4)–(6) for $x_1 \to +\infty$ and find that, for $2<d<4$,

$$\tilde{t} = \frac{K_c - K}{K_c} = \frac{T - T_c(\infty)}{T}, \qquad \tilde{C}_1 = K_c a^{2-d}, \quad \tilde{C}_2 = (Ka^{d+2})^{-1/2}, \quad (7)$$

where $K = J/T$, $K_c = J/T_c(\infty)$, J and a being the exchange energy and the lattice constant, respectively.

We now propose that for $\tilde{t}<0$ and $L\to\infty$, χ_0 approaches its bulk behavior as $L^{\zeta}|\tilde{t}|^{\theta}$, where ζ and θ are as yet undetermined exponents. This obviously requires that

$$Z(x_1,0) \to Z_-|x_1|^{\theta} \quad (x_1 \to -\infty), \quad (8)$$

with Z_- universal; it readily follows that $\zeta = (\gamma+\theta)/\nu$. At this point we observe that the asymptotic condition $x_1 \to -\infty$ corresponds equally well to the situation where L stays fixed but $\tilde{t} \to -\infty$, which happens as $T\to 0$; see Eq. (7). But then we should be encountering the bulk critical behavior of the d'-dimensional system, viz., $\chi_0 \propto T^{-\dot{\gamma}} \propto |\tilde{t}|^{\dot{\gamma}}$, where $\dot{\gamma}$ has its obvious meaning. Comparison of the two situations demands that, for consistency,

$$\theta = \dot{\gamma}, \quad \zeta = (\gamma + \dot{\gamma})/\nu, \quad (9)$$

the corresponding amplitude being

$$X = \tilde{C}_2^2 T^{-1} Z_- \tilde{C}_1^{\dot{\gamma}} = Z_- J^{-1} K_c^{\dot{\gamma}} a^{(2-d)\dot{\gamma}-(d+2)}. \quad (10)$$

We thus see that, for $T<T_c(\infty)$, the approach of the given finite-size system $L^{d-d'}\times\infty^{d'}$ toward bulk critical behavior in d dimensions is determined jointly and completely by the *bulk* exponents appropriate to both d and d' dimensions. Since, for $2<d<4$, $\nu = 1/(d-2)$ and $\gamma = 2/(d-2)$ while, for $d'<2$, $\dot{\gamma} = 2/(2-d')$, our predictions take the form

$$\theta = \frac{2}{2-d'}, \quad \zeta = \frac{2(d-d')}{2-d'}, \qquad X = Z_- J^{-1} K_c^{\dot{\gamma}} a^{-d-\zeta}. \quad (11)$$

It follows that for a "block" geometry ($d'=0$), $\zeta = d$, and for a "cylindrical" geometry ($d'=1$), $\zeta = 2(d-1)$; cf. Eqs. (1). Similar remarks apply to other thermodynamic quantities; in particular, for the specific heat we predict that

$$\theta^* = \dot{\alpha} - 2 = -\frac{4-d'}{2-d'} = -(1+\theta), \qquad \zeta^* = \frac{\alpha+\dot{\alpha}-2}{\nu} = -\frac{2(d-d')}{2-d'} = -\zeta, \qquad X^* = \tilde{C}_1^{\dot{\alpha}} Z_-^* = Z_-^* K_c^{\dot{\alpha}} a^{-d-\zeta^*}, \quad (12)$$

where the various symbols have obvious meanings. The approach in question, therefore, takes place generally through a power law; it is only for $d'=2$ that the approach becomes exponential in nature. We shall now check our predictions against analytical results for the spherical model and the relativistic Bose gas.

In a recent study of finite-size effects in the field-free spherical model under periodic boundary conditions, we have shown[12] that, for $2<d<4$, the singular part of the free-energy density of the system is indeed in conformity with the scaling hypothesis (2) and that the scaling function $Y(x_1,0)$ is given by the parametric equations

$$Y(y) = \left(\frac{y}{\sqrt{\pi}}\right)^d\left[\frac{1}{d}\Gamma\left(\frac{4-d}{2}\right) - \mathscr{K}\left(\frac{d-2}{2}\middle| d^*;y\right) - \mathscr{K}\left(\frac{d}{2}\middle| d^*;y\right)\right] \quad (13)$$

and

$$x_1(y) = \frac{y^{d-2}}{8\pi^{d/2}}\left[\left|\Gamma\left(\frac{2-d}{2}\right)\right| - 2\mathscr{K}\left(\frac{d-2}{2}\middle| d^*;y\right)\right], \quad (14)$$

where y is the *thermogeometric parameter*[12,13] appropriate to the system,

$$y = \tfrac{1}{2}(L/a)\phi^{1/2} \quad [\phi = (\lambda/J) - 2d], \quad (15)$$

λ being the usual spherical field, d^* $(=d-d')$ is the number of dimensions in which the system is finite, while

$$\mathscr{K}(n|d^*;y)=\sum_{\mathbf{q}(d^*)}\frac{K_n(2yq)}{(yq)^n}\quad [q=(q_1^2+\ldots+q_{d^*}^2)^{1/2}>0], \tag{16}$$

$K_n(z)$ being the well-known modified Bessel functions. The scaling functions for χ_0 and $c^{(s)}$ turn out to be

$$Z(x_1,0)=\frac{1}{8y^2},\quad Z^*(x_1,0)=-\frac{32\pi^{d/2}y^{4-d}}{\Gamma(\frac{1}{2}(4-d))+2\mathscr{K}(\frac{1}{2}(d-4)|d^*;y)}. \tag{17}$$

For $\tilde{t}>0$ *and* $L\to\infty$ (which makes $x_1\to+\infty$), the parameter y diverges while the functions $\mathscr{K}(n|d^*;y)$ vanish exponentially. The finite-size effects in $f^{(s)}$, χ_0, and $c^{(s)}$ are then given by

$$\delta(f^{(s)})=\frac{f^{(s)}(L)-f^{(s)}(\infty)}{f^{(s)}(\infty)}\simeq-[dd^*\pi^{1/2}/\Gamma(\tfrac{1}{2}(4-d))]\left(\frac{2\xi}{L}\right)^{(d+1)/2}e^{-L/\xi}, \tag{18}$$

$$\delta(\chi_0)\simeq-[2d^*\pi^{1/2}/\Gamma(\tfrac{1}{2}(4-d))]\left(\frac{2\xi}{L}\right)^{(d-1)/2}e^{-L/\xi}, \tag{19}$$

and

$$\delta(c^{(s)})\simeq-[2d^*\pi^{1/2}/\Gamma(\tfrac{1}{2}(4-d))](2\xi/L)^{(d-3)/2}e^{-L/\xi}, \tag{20}$$

respectively. It is remarkable that the exponential factor governing the approach of all the three quantities studied here is the same; it also agrees with the factor obtained by Barber and Fisher[3] for the quantity $\delta(\chi_0)$ for a system with $d^*=1$. It seems worthwhile to point out here that, in his analysis of the quantity $\delta(\xi)\{=[\xi(L)-\xi(\infty)]/\xi(\infty)\}$ for the spherical model with $d'=1$, Luck[14] has also obtained precisely the same exponential factor; see, as well, Lüscher,[15] who has carried out a similar study for the scalar case $n=1$.

In the critical region, where $|\tilde{t}|=O(L^{-1/\nu})$ and hence $|x_1|=O(1)$, Eqs. (2), (5), and (6) give directly the well known results[9]: $f^{(s)}\propto L^{-d}$, $\chi_0\propto L^{\gamma/\nu}$, and $c^{(s)}\propto L^{\alpha/\nu}$.

To study the situation for $\tilde{t}<0$ *and* $L\to\infty$ (which makes $x_1\to-\infty$), we make use of the asymptotic behavior of the functions $\mathscr{K}(n|d^*;y)$ as $y\to0$; see Eqs. (79) and (80) of Ref. 12. If we substitute those results into (17) and then into Eqs. (5) and (6), we find that all the predictions made in Eqs. (11) and (12) are verified. In the process, universal amplitudes Z_- and Z_-^* are also determined and are seen to depend on d' alone:

$$Z_-=\frac{(8\pi)^{d'/(2-d')}}{[\Gamma(\frac{1}{2}(2-d'))]^{2/(2-d')}},\qquad Z_-^*=1/(2-d')Z_-. \tag{21}$$

Thus, for $d'<2$, the susceptibility χ_0 is governed by a power law, L^{ζ}, whose exponent depends strongly on the geometry of the system; for $d=3$, it goes as L^3 for a cube $(d'=0)$ and as L^4 for a cylinder $(d'=1)$. Only for $d'=2$, such as a film in three dimensions (the only case for $d=3$ where exact calculations were previously available[3]), is the approach exponential. Similar remarks apply to other thermodynamic quantities, including the specific heat.

Since the approach of the given (d,d') system toward bulk behavior is determined solely by the *bulk* exponents in d and d' dimensions, it is clear that for all systems in the same universality class the manner of approach will be the same. This is indeed vindicated by our separate calculations on the relativistic Bose gas with pair production,[16] where similar methods have been used to study the free energy, the specific heat, and the condensate fraction of the system in three dimensions; calculations for a d-dimensional system, including those on the isothermal compressibility of the system, will be reported in a separate communication. As expected, the various exponents, such as θ^* and ζ^*, turn out to be the same as in the case of the spherical model, while nonuniversal quantities, such as $\tilde{C}_1$, $\tilde{C}_2$, and $\tilde{t}$, are quite different.

Although we have presented calculations only for the exactly solvable models, the methods outlined here may have scope for wider application. For instance, consider the n-vector models in the cylindrical geometry, $L^2\times\infty^1$, in three dimensions. Since the behavior of the zero-field susceptibility for a bulk system with $d'=1$, as $K\to\infty$, is known to be[17]

$$\chi_0\propto\begin{cases}e^{2K} & (n=1,\ \text{Ising}), \quad (22a)\\ K^2 & (n\geqslant2), \quad (22b)\end{cases}$$

we would expect that, in this case, the approach toward bulk behavior for $T<T_c(\infty)$ will be exponential only in the Ising case and algebraic in all other cases. This expectation is indeed upheld in Refs. 7 and 8.

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