Phase Transitions in Finite Systems

In their Letter,[1] Singh and Pathria make three claims which require further evaluation. They pertain to a d-dimensional system, infinite in d' dimensions, which exhibits a critical phase transition in the thermodynamic limit, and are as follows: (1) The free energy takes a geometry-dependent but otherwise universal form from $T \approx T_c(\infty)$ down to $T=0$; (2) the approach to bulk behavior for $T < T_c(\infty)$ is governed by bulk exponents of the d- and d'-dimensional systems; and (3) specific predictions about the exponents governing the approach to bulk behavior are made. These will each be discussed below.

Starting with statement (3), the authors predict that if X is a thermodynamic function such that the d-dimensional bulk behavior is $X \sim T^{-\gamma}$ and the d'-dimensional bulk behavior is $X \sim T^{-\dot{\gamma}}$, then in the finite system $X \sim L^{\zeta} T^{-\dot{\gamma}}$, with

$$\zeta = (\gamma + \dot{\gamma})/\nu. \tag{1}$$

The authors do not make clear how general they expect this result to be, but this result only holds for the spherical model. To see this, take the fully finite case ($d'=0$) and let X be the susceptibility χ. For any fully finite O(n) model the susceptibility obeys $\chi \sim L^d/T$ in the low-temperature phase, as can be easily shown from the fluctuation-response relation. Thus, (1) implies that $d\nu = \gamma + 1$. Comparison with the hyperscaling relation $d\nu = \gamma + 2\beta$ shows that Eq. (1) can only be satisfied if $\beta = \frac{1}{2}$, i.e., only if $n = \infty$ or $d \geq 4$ in the O(n) model.

It is possible to generalize the authors' arguments to the O(n) model. They start by extending the Privman-Fisher hypothesis[2] to the low-temperature phase; the singular part of the free energy density is assumed given by $f^{(s)}(T,H,L) = TL^{-d}Y(x_1,x_2)$ where Y is geometry dependent but universal, $x_1 = \tilde{C}_1 L^{1/\nu}\tilde{t}$, $x_2 = \tilde{C}_2 L^{\Delta/\nu} H/T$, and $\tilde{t}$ and $\tilde{C}_2$ are functions of T defined to make this work down to $T=0$. The low-temperature behavior of these two functions is crucial to their analysis, and thus the natural generalization is to define two new exponents, p and q, such that as $T \to 0$, $\tilde{C}_2 \to \hat{C}_2 T^p$ and $\tilde{t} \to \hat{C}_1 t T^{-q}$, where $\hat{C}_1$ and $\hat{C}_2$ are nonuniversal scale factors (note that $p = \frac{1}{2}$ and $q=1$ were used in the Letter, but these hold only for the spherical model). The generalization of Eq. (1) is

$$\zeta = [\gamma + (\dot{\gamma} + 2p - 1)q^{-1}]/\nu. \tag{2}$$

However, the determination of p and q is nontrivial. There is the condition that in the fully finite case $\zeta = d$. This and hyperscaling implies that $p/q = \beta$. Another condition suggested by the authors is the finite-size scaling *Ansatz*, namely $\tilde{t} \sim \xi_\infty^{-1/\nu}$. However, use of this relation for $n \geq 2$ is hindered by the fact that $\xi_\infty = \infty$ for $T \leq T_c$.[3] Thus, the predictive value of this approach is questionable without further study.

The question of the approach to bulk behavior for $T < T_c(\infty)$ has been extensively studied.[4] Low-temperature analysis indicates that the exponent governing the approach (ζ) can be determined from the behavior of the d'-dimensional system. This is because below $T_c(\infty)$ all correlation lengths in the finite dimensions are pinned at L, so that all degrees of freedom in these dimensions are essentially frozen out. The only fluctuations are in the infinite dimensions. Thus, ζ is governed by d and the exponents of the d'-dimensional system. In light of this, the conclusion of the authors summarized in statement (2) of my opening paragraph is too weak; the bulk exponents of the d-dimensional system are not required.

The starting assumption of the paper, statement (1), predicts a universal crossover from the $T_c(\infty)$ finite-size scaling regime to the low-temperature regime. This is plausible. One expects the low-temperature phase to have the universality of the d'-dimensional transition at $T=0$, which is critical and has L as an irrelevant variable. On the assumption that the bulk system has only one critical transition temperature, all correlation lengths in the finite dimensions are equal to L at and below $T_c(\infty)$. Thus, as long as all irrelevant variables are small compared to L, the free energy is essentially universal even for T as large as $T_c(\infty)$. All systems in the same d'-dimensional $T=0$ universality class collapse onto a universal, low-temperature function for L sufficiently large at $T_c(\infty)$. Likewise, at $T_c(\infty)$, the free energy is of the universality class of the bulk transition. If the universality class of the low-temperature phase includes that of the bulk transition, a universal function will describe both regimes, as envisioned by these authors. Perhaps this is the condition for $\tilde{t}$ and $\tilde{C}_2$ to be universal.

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[1] S. Singh and R. K. Pathria, Phys. Rev. Lett. **55**, 347 (1985).

[2] V. Privman and M. E. Fisher, Phys. Rev. B **30**, 322 (1984).

[3] The method suggested by the authors to find $\tilde{t}$ and $\tilde{C}_2$ is to ". . . compare the known bulk behavior of [thermodynamic functions] for $T \geq T_c(\infty)$ . . ." [see p. 348 of Ref. 1, just after Eq. (6)]. The possibility of determining the behavior of these functions at $T \approx 0$ from the behavior for $T \geq T_c(\infty)$ is highly impractical, because to do so requires infinite precision, i.e., an exactly solvable model.

[4] V. Privman and M. E. Fisher, J. Stat. Phys. **33**, 385 (1983), and Phys. Rev. B **32**, 447 (1985).

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