SOME IMPLICATIONS OF WEAK-SCALING THEORY*

by

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Abstract

The weak-scaling theory we have developed is extended to facilitate contact with the numerical results of Ferer et. al. Our conclusions are consistent with their results, and certain specific extensions of their numerical work are suggested by our analysis.

January, 1970
Report No. 156

* This work was supported in part by the Research Foundation of State University of New York

In a previous note[1], we outlined the derivation of a set of weak-scaling relations based upon the appearance of two correlation lengths, Λ and ξ. Our analysis rested upon an investigation of the form of the density - density correlation function $\hat{h}(\mathbf{r})$ along the coexistence curve. In order to make contact with the results of Ferer, Moore, and Wortis[2] that hold along the critical isochore, as well as our own techniques[3,4] that involve $\hat{h}(\mathbf{r})$ along the critical isotherm, we extend here the discussion given in ref. [1].

We use the notation of ref.[1], where we introduced the function $\tilde{q}(\mathbf{r},\kappa)$ by writing

$$\hat{h}(\mathbf{r}) - \hat{h}(\mathbf{r})_c = f(\kappa r) / r^{d-t-\tilde{q}(\mathbf{r},\kappa)}, \tag{1}$$

$\kappa = \xi^{-1} \sim |T-T_c|^{\nu}$ for $M=0, T \geq T_c$, and $\kappa \sim M^{2/\epsilon}$ along the coexistence curve; and $\tilde{q}(\mathbf{r},\kappa) \to 0$ for $r \to \infty$. Here $M = |\rho - \rho_c|$, where ρ is the density in fluid language, so that M is proportional to magnetization in spin language. As usual T is temperature, and the subscript c will refer to critical values throughout this note. We argued in [1] that for the Ising model, and also for simple fluids, we might further expect to find along the coexistence curve, for small κ,

$$\hat{h}(\mathbf{r}) - \hat{h}(\mathbf{r})_c \sim M^2 \quad \text{for} \quad r < \Lambda, \tag{2}$$

as well as

$$\tilde{q}(\mathbf{r},\kappa) \simeq q \quad \text{for} \quad r < \Lambda, \tag{3a}$$

$$\tilde{q}(\mathbf{r},\kappa) \approx 0 \quad \text{for} \quad r > \Lambda, \tag{3b}$$

where

$$q = d - t - 2/\epsilon, \tag{4}$$

$$\Lambda = \kappa^{-\theta}, \tag{5}$$

$$d - t - q = \theta(d-t) \leq d - t. \tag{6}$$

It is worth noting that in the case of the spherical model[5] one has instead of (3)

$$\tilde{g}(r,\kappa) \to g \text{ for } r/a \to 1, \tag{7a}$$

$$\tilde{g}(r,\kappa) \approx 0 \text{ for } r \gg a, \tag{7b}$$

where a is a lattice spacing. More generally, we anticipate (7) instead of (3) for any systems[6] that satisfy the Ornstein-Zernike hypothesis that the direct correlation function looks like the pair potential $V(r)$ times $-(kT)^{-1}$ for $V(r)/kT \ll 1$.

Off the coexistence curve the argument that we used to establish (2) in the Ising case is no longer available, but it is reasonable to hypothesize that the dominant contribution to $\hat{k}-\hat{k}_c$ for small r is still a term proportional to M^2 as one approaches the critical point along any straight line in the one-phase region of the ($M^{1/\beta}$, ΔT) - plane. Once we accept the assumption, together with the homogeneity of κ in $M^{1/\beta}$ and ΔT, we are directly led by the argument of [1] to (4) and (6) along the critical isotherm as well as along the coexistence curve. Support for the assumption has been obtained as follows: Using functional-expansion techniques that we have previously developed[3], and assuming $\tilde{g}(r,k)$ to be given by (3), we again find (6), but this time for $T=T_c$. Details of this derivation will be given elsewhere[4]; the important point to make here is that these details are independent of the arguments of [1] that lead to (6) along the coexistence curve. Taken alone, this result for $T=T_c$ does not guarantee that either θ or g (which conceivably could be functions of M and ΔT) will remain fixed as we pass from the coexistence curve to the critical isotherm, but guarantees only that if one of them is fixed, the other remains fixed also. However, from the significance of $\xi^{d\theta}$ as the characteristic fluctuation volume discussed in ref. [7] we would expect θ to remain fixed, and hence (4) to remain valid on the critical isotherm. This is consistent with the validity of (2) on the critical isotherm and, more generally, on any straight line in the single-phase part of the $(M^{1/\beta}, \Delta T)$-plane that passes through the origin. The form of (2) implies that the critical isochore for $T \geq T_c$ may well be a very special line in this connection, upon which the otherwise dominant term in $\hat{h}-\hat{h}_c$ for $\tau \approx a$ could vanish (simply because M^2 vanishes) leaving as the most dominant term another term, presumably still of the form

$$\hat{h}-\hat{h}_c \sim K^P \tau^{P-d+t+\tilde{g}_0(\tau,K)} \tag{8}$$

but not necessarily with $P = 2/\epsilon$ and $\tilde{g}_0(\tau,K) = \tilde{g}(\tau,K)$. In fact, there is direct evidence for $P \neq 2/\epsilon$ since in order for $\partial\hat{h}/\partial T|_{\tau \approx a}$ to behave like the specific heat C_v, as we would expect it to do, we must have $P = (1-\alpha)/\nu$ for $\tau \approx a$. In general, however, $(1-\alpha)/\nu \neq 2/\epsilon$.

On the critical isochore, the power of τ in (8) is not constrained by our arguments to be zero for small τ, as it was along the phase boundary. It is precisely this power of τ, $(1-\alpha)/\nu - d + t + \tilde{g}_0(\tau,K)$ that Ferer et.al. investigated for the 3-d Ising model for small K and τ. They found it to be 4.7 ± 0.06, and using their values of $(1-\alpha)/\nu - d + t$, we find that this yields $\tilde{g}_0 \approx 1/7 \pm 1/14$. Although they gave results only for $\tau/a < 3$, they argued that their results indicated that for small K, $\tilde{g}_0(\tau,K)$ has an essentially constant value over a range of τ that includes $\tau \gg a$ as well as $\tau \approx a$, but they were unable to deduce the distance Λ_0 beyond which $\tilde{g}_0(\tau,K)$ no longer has this value. More generally, they were unable to confirm the existence of any second correlation length from their findings. The arguments of [1] and of this note support their conclusion that $\tilde{g}_0$ can be expected to be nonzero for a range of values over which $\tau \gg a$, and further suggests the following way in which the length Λ_0 can be extracted from their results:

Mimicking the way Λ was introduced in [1] along the coexistence curve, one considers the Λ_0 at which the small-r and large-r form of $\hat{h}-\hat{h}_c$ are of the same order of magnitude. Thus one sets $\kappa^{(1-\alpha)/\nu}\Lambda_0^{(1-\alpha)/\nu-d+t+q_0} \approx \Lambda_0^{t-d}$ to get

$$(1-\theta_0)/\theta_0 = q_0\nu/(1-\alpha), \tag{9}$$

where q_0 is the value approached by $\tilde{q}_0$ as $r/a \to 1$ and $\kappa a \to 0$. Eq.(9) defines the length Λ_0 in terms of q_0, ν, α and κ. Arguments were given in [1] using Eq. (6) to show that along the coexistence curve, (3a) and $\gamma = t\nu$ are compatible only if $\theta < 1$. The same arguments can be used for $T>T_c, M=0$ here along with Eq. (9) to show that $\gamma = t\nu$ only if $\theta_0 < 1$, and that $\theta_0 = 1$ implies $\gamma = (t+q_0)\nu$. The possibility remains, however, that in the Ising model the $\tilde{q}_0(r,\kappa)$ given by Eq. (8) behaves like a nonzero constant only for r near a, with $\tilde{q}_0(r,\kappa) \approx 0$ for $a \ll r \ll \Lambda$. In this case Eq. (9) would no longer define a Λ_0 that would manifest itself in any tangible way in the structure of $\hat{h}-\hat{h}_c$. This is precisely the situation in the spherical-model case, where if $d \geq 4$, both $\tilde{q}(r,\kappa)$ and $\tilde{q}_0(r,\kappa)$ for small κ are d-4 for $r \approx a$ but zero for $r \gg a$. Although we do not believe that the situation is similar in the 3-d Ising case, there is surely room for further clarification on this point. What is strongly suggested to us by our analysis is the application of the numerical methods of ref.[2] to the 5-d spherical model, for which one knows that $\tilde{q}_0 \approx 0$ for $r \gg a$ but $\tilde{q}_0 \approx 1$ for $r \approx a$. The question is: Will the numerical analysis reveal that strong scaling of $\hat{h}(r)$ for $r \gg a$ is preserved, as one knows it is, or will the $\tilde{q}_0 \approx 1$ for $r \approx a$ misleadingly suggest numerically that strong scaling has been violated?

A second question that the work of this note raises is whether we can safely identify the Λ_0 and Θ_0 of the critical isochore with Λ and Θ, respectively. The physical significance of Θ discussed in ref. [7] suggests the identification, despite the fact that we cannot safely identify γ with γ_0. If we do equate Θ and Θ_0, we have from (9) and our earlier equations that

$$\gamma_0 = \gamma(1-\alpha)/2\beta . \tag{10}$$

Taking $\alpha = 1/8$, $\beta = 5/16$, and using the values $\gamma = 3/50$ and $\gamma = 1/12$, which probably represent two extreme possibilities,[1] we find $\gamma_0 = 21/250$ and $\gamma_0 = 7/60$, respectively. These values are consistent with the 1/7 ± 1/14 from ref. [2]. Nevertheless it would clearly be valuable to have some more-or-less direct numerical assessment of γ that eliminates the necessity of our going through (10) in order to make contact with the rest of our scaling relations.

We are indebted to D. Jasnow and M.A. Moore for helpful conversations and correspondence.

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4. G. Stell, "Extension of the Ornstein-Zernike Theory, III" (to appear). In a preliminary study (S.U.N.Y. Engineering Report No. 144), we considered only the case in which a certain inequality (which we have subsequently found to be essentially equivalent to $2/\varepsilon - t + q > 0$) is satisfied. Since this inequality is not realized in cases of interest, the relations that follow from it are not realized either. When the realizable case is considered the relation $d-t-\sigma=\theta(d-t)$ follows.

5. In the spherical model, the argument used in [1] to obtain Eq.(2) for the Ising model is not applicable. Nevertheless $\hat{h} - \hat{h}_c \approx F(\underset{\sim}{r})M^2$ as $r \to a$, with $F(\underset{\sim}{r})$ depending on r like r^0. Setting $q \approx 0$ for $r \gg a$, we find the $f(x)$ of Eq.(1) for the spherical model to be $x^{2/\epsilon}$, and (7a) follows with q still given by (4), although strictly speaking some orientational dependence of $\tilde{q}$ on r must be expected for $r \approx a$.

6. G. Stell, Phys, Rev. 184, 135 (1969).

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