Weak-Scaling Theory*

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ABSTRACT

Relations among critical exponents are derived. They are based upon a consideration of two correlation lengths, not necessarily equal, that arise in our analysis.

that when (1) is assumed,

$$2-\eta = \min[2, d(\delta-1)/(\delta+1)] \qquad (2)$$

if $2 \neq d(\delta-1)/(\delta+1)$, with the form of $\hat{h}(\underset{\sim}{r})$ complicated by logarithmic terms if $2 = d(\delta-1)/(\delta+1)$. On the other hand although a scaling relation between d, δ, and η did not appear in the original scaling-theory papers, it was shown by Fisher[8] that from scaling theory one gets, instead of (2),

$$2-\eta = d(\delta-1)/(\delta+1), \qquad (3)$$

regardless of the relative size of 2 and $d(\delta-1)/(\delta+1)$. It appears that in the 3-dimensional Ising model, the special case described by $2=d(\delta-1)/(\delta+1)$ may in fact occur. However, despite the resulting possibility that it is therefore only the occurrence of a logarithmic term in $\hat{h}(\underset{\sim}{r})$ that is responsible for the apparent violation of (2), as we have previously suggested[5,9], we conclude in this note that the violation is instead due to the breakdown of homogeneity in the functional forms of $\hat{h}(\underset{\sim}{r})$, $\hat{c}(\underset{\sim}{r})$ and related correlation functions.

To examine the way in which (1) might be expected to fail we find it useful to subtract from $\hat{h}(\underset{\sim}{r})$ its value, $\hat{h}_c(\underset{\sim}{r})$, at the critical point. (The subscript c will refer to critical values throughout this note). As in previous work we shall provisionally assume that

$$\hat{h}_c(\underset{\sim}{r}) \simeq \text{const}/r^{d-2} \text{ for } r \gg a \qquad (4)$$

for lack of any direct evidence against this functional form. In fact, Eq. (4) can serve as our definition of t. We now introduce a function $q(\underset{\sim}{r},\kappa)$ by writing instead of (1),

$$\hat{h}(\underset{\sim}{r})-\hat{h}_c(\underset{\sim}{r})=f_2(\kappa r)/r^{d-t-\tilde{q}(\underset{\sim}{r},\kappa)}, \qquad (5)$$

where (5) reduces to (1) if we assume that $\tilde{q}(r,\kappa)\approx 0$ for r>>a and set $f(x)=\text{const}+f_2(x)$. In (5) it is very natural to choose $f_2(x)=0(x^p)$ as $x\to 0$ (or $f_2(x)\sim x^p$, using the notation of Fisher[8]) and so to write for $r\to 0$ and small κ,

$$\hat{h}(r)-\hat{h}_c(r)\sim\kappa^p r^{p-d+t+\tilde{q}(\underset{\sim}{r},\kappa)} \qquad (6)$$

Even where $\tilde{q}(\underset{\sim}{r},\kappa)$ appears to be zero for r>>a, as in the case of the 2-dimensional Ising model, one can not <u>a priori</u> expect $\tilde{q}(\underset{\sim}{r},\kappa)$ to remain zero as $r\to 0$. In particular, we now argue that along the coexistence curve we must expect to find that when d=2 or 3 and r and κ are small $\tilde{q}(\underset{\sim}{r},\kappa)$ is essentially independent of r and given by

$$\tilde{q}(\underset{\sim}{r},\kappa)\approx d-t-2/\epsilon,\ (r\ \text{small}), \qquad (7)$$

where ε is the exponent defined by the expression $\kappa\sim|\rho-\rho_c|^{\epsilon}$ for points along the coexistence curve; $|\rho-\rho_c|\sim|T-T_c|^{\beta}$. Our expectation of (7) follows from the expectation that for small fixed r, the T-dependence of $\partial(\hat{h}-\hat{h}_c)/\partial T$ at $\rho=\rho_c$ must be like that of the specific heat

Weak-Scaling Theory

For the three-dimensional Ising model, neither the set of scaling relations that follow from the work of Widom[1,2], Kadanoff[3], and others[4] nor a modified scaling-type relation independently proposed by ourselves[5] appears to be exactly satisfied[6]. In both the scaling-theory approach of Kadanoff[3] and others[4] and in our own previous work[5] a single correlation length $\xi = \kappa^{-1}$ is postulated to appear in various correlation functions. In particular, the density-density or spin-spin correlation function that we denote[5] as $\hat{h}(\underset{\sim}{r})$ is assumed to have the functional form first proposed by Fisher[7]

$$\hat{h}(\underset{\sim}{r}) \approx f(\kappa r)/r^{d-t} = \kappa^{d-t} F(\kappa r) \text{ for } r >> a \qquad (1)$$

where d is dimensionality, $r = |\underset{\sim}{r}|$, and a is a molecular diameter or lattice spacing. The exponent we write as t is usually denoted as $2-\eta$.

In scaling theory it is acknowledged that $\hat{h}(\underset{\sim}{r})$ does not in general have the form given by (1) for all r, including $r \gtrsim a$, but the scaling theory arguments[3] are nevertheless developed as though it did; in our approach[5] explicit provision was made for the fact that neither $\hat{h}(\underset{\sim}{r})$ nor $\hat{c}(\underset{\sim}{r})$, the modified direct correlation function, will in general be a homogeneous function of r and ξ except for large r/a and large ξ/a. This difference between the two approaches accounts for the difference in the relation among dimensionality d and the critical exponents δ and η (in the usual notation[8]) predicted by each approach. We previously concluded[5]

$c_v \sim |T-T_c|^{-\alpha'}$. But for $T<T_c$ and $\rho=\rho_c$, $\hat{h}(\underset{\sim}{r})$ is the sum of a term that looks like the one-phase $\hat{h}(\underset{\sim}{r})$ along the coexistence curve plus a "long-range order" term $\sim M^2$ for each M on that curve (where $M=|\rho-\rho_c|$) and independent of r. Unless for small r there were a compensating term in the expression for the one-phase $\hat{h}(\underset{\sim}{r})$ to cancel the M^2-term in the sum that makes up the two-phase $\hat{h}(\underset{\sim}{r})$ at $\rho=\rho_c, T<T_c$, the M^2-term would yield a $|\Delta T|^{2\beta-1}$ contribution (where $\Delta T=T-T_c$) to the specific heat singularity for $\rho=\rho_c$, $\Delta T<0$, and would thus force the inequality $\alpha' \geq 1-2\beta$. Therefore, we conclude that in any model in which $\alpha' < 1-2\beta$, as in the Ising model for d=2 and d=3, the dominant contribution to $\hat{h}-\hat{h}_c$ along the coexistence curve for small r is independent of r and is proportional to M^2, so that

$$\hat{h}-\hat{h}_c \sim M^2, \quad (r \to 0). \tag{8}$$

Comparing (6) and (8), we see that $P=2/\varepsilon$, and (7) follows. Looking ahead for a moment we note that we shall find nothing in our argument that necessitates or even suggests the breakdown of the homogeneity of K in $M^{1/\beta}$ and ΔT or the associated breakdown of homogeneity of thermodynamic quantities in these variables. If we assume the simplest form of such homogeneity[10], then $\alpha'=\alpha$.

We are now in a position to introduce the second length Λ, which we define as the r at which the small-r expression for $\hat{h}-\hat{h}_c$ given by (8) is of the same order of magnitude as the large -r expression given by

$$\hat{h}-\hat{h}_c \sim \mathrm{const}/r^{d-t}, \tag{9}$$

which we expect to hold for all r sufficiently large for $\hat{h}$ to be negligible compared to $\hat{h}_c$. In the case of the nearest-neighbor Ising model, $\hat{h}$ is surely exponentially damped for large r, so that (4) guarantees that (9) will hold for large enough r. From (8) and (9), it then follows that $\kappa^{2/\epsilon} \sim \Lambda^{-d+t}$, or letting $\Lambda \sim \kappa^{-\theta}$, that

$$\theta\,(d-t) = 2/\epsilon\,, \tag{10}$$

and from (10) and (7), that

$$d-t-q = 2/\epsilon\,, \tag{11}$$

where q is the value approached by $\tilde{q}$ as $r/a \rightarrow 1$ and $\kappa a \rightarrow 0$. Thus θ and q are related by

$$\theta(d-t) = d-t-q\,. \tag{12}$$

We can give a physical interpretation to θ and to Λ by comparing (10) with the identical Eq. (16) of reference [11] In that reference we discuss a length $\Lambda \sim \kappa^{-\theta}$ that characterizes the mean size of micro-domains of conjugate phase. This length was postulated by Widom[1] to be equal to $\xi = \kappa^{-1}$; indeed this was a basic hypothesis of Widom's paper, from which follows the relation $d-t = 2/\epsilon$. In ref.[11] we argued instead that $\Lambda \lesssim \xi$ or $0 \lesssim \theta \leq 1$, and that for high d, $\theta < 1$. From the argument it follows that the length $\kappa^{-\theta}$

introduced in ref.[11] can be identified with the Λ we have introduced here. Widom further identified Λ as a measure of the thickness of an interface between a phase and its conjugate in the bulk (in the presence of an infinitisimal external field). If we retain this identification and allow $\theta < 1$ but otherwise follow Widom's arguments[1,10] we find $\mu + (2-\theta)\nu = 2\beta + \gamma$ instead of Widom's $\mu + \nu = 2\beta + \gamma$, where μ, γ, and ν are the critical exponents describing the temperature dependence of the surface tension σ, compressibility K_T, and κ, respectively, along the coexistence curve: $\sigma \sim |\Delta T|^{\mu}$, $K_T \sim |\Delta T|^{\gamma}$, $\kappa \sim |\Delta T|^{\nu}$.

It is important to note that we have as yet said nothing that implies the failure of (1), even if $\theta < 1$ so that $2/\epsilon < d - t$, since as long as (7) is assumed to hold only when r is not large compared to a, the length Λ will not appear in (1) in any tangible way, despite our having introduced Λ in terms of $\hat{h} - \hat{h}_c$. On the other hand, if we assume that "r small" in (7) means $r \ll \Lambda$ rather than $r \lesssim a$, then (1) is no longer true when $d - t \neq 2/\varepsilon$, and our definition of Λ implies that $\hat{h} - \hat{h}_c$ actually changes its functional form at $r \sim \Lambda$. At first it might appear that assuming (7) for $r < \Lambda$ would imply that q would appear in lattice sums or volume integrals over $\hat{h}(\underset{\sim}{r})$, i.e. in the expression for K_T, along with d,t, and κ. Under any plausible assumptions about the way $\tilde{q}(\underset{\sim}{r}, \kappa) \to 0$ as $r/\Lambda \to \infty$, however, it turns out that we have

$$\delta - 1 = \epsilon t, \quad \gamma = \nu t \tag{13a}$$

instead of

$$\delta - 1 = \epsilon (t + q), \quad \gamma = \nu (t + q) \tag{13b}$$

as long as $\theta < 1$. To see this, we note that we would expect, letting $x = \kappa r$:

$$K_T \sim \int_{x>1} \hat{h}(\underset{\sim}{r}) d\underset{\sim}{r} + \int_{x<1} r^{d-t} d\underset{\sim}{r} + \int x^{2/\epsilon} r^{t-d+q} d\underset{\sim}{r} .$$

The q should not affect the anticipation $O(\kappa^{-t})$ contribution of the first two integrals, but the third integral can be expected to yield, from the $x < \kappa^{1-\theta}$ region, a term $O(\kappa^{2/\epsilon - \theta(2/\epsilon + t + q)})$ as well as an additional κ^{-t} term from the $\kappa^{1-\theta} < x < 1$ region. Thus we must have $2/\epsilon - \theta(2/\epsilon + t + q) \geq -t$ to recover (13a), but from (10) and (11), this is just the condition $\theta < 1$. (If $\theta = 1$, we have (13b) instead, but from (12), $\theta = 1 \Rightarrow q = 0$ and we are back to the scaling-theory assumption). Eqs. (13a) and (10) yield $\theta(d-t) = 2\, t/(\delta-1)$.

Since the widely accepted values of $\delta \gtrsim 5$ and $\eta \gtrsim 0$ for the 3-d Ising model are inconsistent with our previous results[5] based upon the assumption that $\tilde{q}(\underset{\sim}{r}, \kappa) \approx 0$ for a<<r, we surmise that $\tilde{q}(\underset{\sim}{r}, \kappa)$ is instead given by (7) for a<<r<<Λ while $\tilde{q}(\underset{\sim}{r}, \kappa) \approx 0$ for r>>Λ in the 3-d Ising case. (For the 2-d Ising model, $\tilde{q}$ appears to be 0 for <u>both</u> $r \approx a$ and r>>a, since the rhs of (7) is 0, while for the spherical model, a direct computation shows that (1) always holds, while (7) always holds for $r \approx a$, with $\tilde{q}=0$ for d=3 and 4 but $\tilde{q}=d-4$ for d≥5 for $r \approx a$. For a<<r<<Λ, $\tilde{q} \approx 0$ for all d.)

The fact that q does not appear in K_T as long as $\tilde{q} \approx 0$ when r>Λ indicates that the homogeneity of thermodynamic functions in $M^{1/\beta}$ and ΔT is as consistent with (5) as with (1), since one way[8] of deriving such homogeneity from scaling-theory arguments is by integrating over $\hat{h}(\underset{\sim}{r})$ after establishing the scaling form of that function. This suggests that we can append the results that follow from thermodynamic homogeneity to the results we have already derived, to obtain new relations involving exponents. In particular, from (11), (13a) and the thermodynamic homogeneity relations[2] $2\beta+\gamma = 2-\alpha$ (for $1 < \gamma+2\beta \leq 2$) and $\beta = \nu/\epsilon$ we find easily that, if $1<\gamma+2\beta\leq 2$, then $\delta\nu - 2+\alpha = \nu q$. If we use the sensible values $\alpha = 1/8$, $\beta = 5/16$, with the values $\delta = 5$, $\nu = 125/196$, $\eta = 1/25$, our equations yield q = 3/50 and θ = 49/52. These values of ν and η are perhaps on the low side; ν = 9/14 and η = 1/18, which are probably on the high side, yield q= 1/12 and θ = 35/38 instead.

In summary we make the following two points:

(i) For both the Ising and spherical models, as well as fluid models, we believe a second length, less than ξ, will appear in the sense discussed in ref. [11] for sufficiently high d, but the d appears to be model dependent. For the spherical model, d=5, while for the Ising model, d appears to be 3; for continuum fluids d may be 3 or it may be higher. Moreover, whether this appearance of a Λ less than ξ, which is associated with the failure of Eq. (3), also makes itself felt in the failure of (1) again depends on the particular model being considered. In the spherical model, for example, (1) persists, but in the Ising model, (1) appears to be violated as soon as Λ differs from ξ.

(ii) There is no evidence that the breakdown of homogeneity of thermodynamic quantities accompanies the breakdown of homogeneity of correlation. In particular, the non-appearance of q in $\int h \, d\underline{r}$ argues against the former breakdown.

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