A WEAK-SCALING RELATION AMONG CRITICAL EXPONENTS†

by

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ABSTRACT

We derive a relationship involving the exponents δ, η, and an exponent Q that measures the deviation from homogeneity of the direct correlation function.

In previous works[1,2], herein referred to as I and II, we derived a relationship between the critical exponents δ and η. In the usual notation, it is

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

This was derived assuming that long-range correlations satisfy a certain homogeneity (scaling) condition described below. Recently Ferer, Moore, and Wortis[3] concluded, on the basis of numerical analysis of Ising expansions, that such homogeneity is probably not satisfied in 3 dimensions. They considered the 2-point correlation function [our $\hat{h}(\underset{\sim}{r})$ in the notation of I and II] along the critical isochore [i.e. for number density ρ equal the critical density ρ_c, in the lattice-gas language used in I and II] when the temperature T is above the critical temperature T_c. In I and II we worked at $T=T_c$ for small $|\rho-\rho_c|$, but if $\hat{h}(\underset{\sim}{r})$ does not satisfy a homogeneity condition for large $|\underset{\sim}{r}|$ along the critical isochore, there is no reason to expect it to do so along the critical isotherm; the purpose of this note is to reassess our derivation of (1) assuming a weakened form of homogeneity of the direct correlation function $c(\underset{\sim}{r})$ that is suggested by the findings of ref. [3]. [It is the off-critical behavior of $c(\underset{\sim}{r})$ rather than of $\hat{h}(\underset{\sim}{r})$ that enters crucially into our derivation of (1).]

Our main result is a demonstration that a weakening in homogeneity of $c(\underset{\sim}{r})$ for large $r=|\underset{\sim}{r}|$ and small κr (κ^{-1} = the correlation length) of the form and magnitude suggested by the work of Ferer et. al. can indeed lead to a deviation from (1) of the order of magnitude that appears to be found in 3 dimensions. Specifically, we derive a new relationship [eq. (13)] among η, δ, d, and an exponent Q that measures the deviation of $c(\underset{\sim}{r})$ from its strong-scaling form at $T=T_c$. If Q is taken to be of the same sign and magnitude as the corresponding exponent q associated with $\hat{h}(\underset{\sim}{r})$ at $\rho=\rho_c$, then we find that the value of $q \approx 1/7$ arrived at[4] in ref. [3] yields $\eta \approx 1/21$. We have no a priori reason for identifying Q and q, but we suspect that any weak-scaling theory in which a single parameter must bear the full burden of expressing the departure from strong scaling will make this identification. A study of $c(\underset{\sim}{r})$ at $T=T_c$ comparable in accuracy to the study of $\hat{h}(\underset{\sim}{r})$ at $\rho=\rho_c$ made in ref. [3] would do much to clarify the feasibility of such a theory.

We use the notation of I except as otherwise indicated, writing a function of $\underset{\sim}{r}_{12}$ sometimes as f(12) and sometimes as $f(\underset{\sim}{r}_{12})$ as convenience dictates, and sometimes writing $\underset{\sim}{r}_2-\underset{\sim}{r}_1$ simply as $\underset{\sim}{r}$. We write $|\underset{\sim}{r}|$ as r. As in I, the subscript c refers to a critical value and the subscript o to evaluation at number density $\rho g(12)$ rather than ρ. We shall work mainly with $\hat{c}(\underset{\sim}{r}) = c(\underset{\sim}{r})-\delta(\underset{\sim}{r})n(\underset{\sim}{r})$, $\hat{c}_2(\underset{\sim}{r}) = \hat{c}(\underset{\sim}{r})-\hat{c}_c(\underset{\sim}{r})$, and $h(\underset{\sim}{r}) = \hat{h}(\underset{\sim}{r})-\delta(\underset{\sim}{r})n(\underset{\sim}{r})$, rather than $c(\underset{\sim}{r})$ and $\hat{h}(\underset{\sim}{r})$ themselves, where $\delta(\underset{\sim}{r})$ is the delta function [Kronecker for a lattice system, Dirac for a fluid] and $n(\underset{\sim}{r})$ is the 1-point density function, which is just ρ in a uniform system.

In I and II we showed the way in which (1) followed from the result $c_c(\underset{\sim}{r}) \sim [\hat{h}_c(r)]^p$, for $r \to \infty$, which yielded

$$2-\eta = \min[2, d(p-1)/(p+1)], \tag{2}$$

with p equal to δ, the exponent that measures the shape of the critical isotherm; $|\mu-\mu_c| \sim |\rho-\rho_c|^\delta$ at $T=T_c$ (μ = chemical potential). Our work was based on the postulate that $\hat{h}$ can be written as $\hat{h} = \hat{h}^S+\hat{h}^L$, where for $\kappa a \ll 1$ and $r/a \gg 1$, we have $\hat{h} = \hat{h}^L$ with

$$\hat{h}_c^L \sim r^{t-d}, \tag{3.a}$$

$$\hat{h}^L-\hat{h}_c^L \simeq f(\kappa r)\, r^{t-d} = e(\kappa r)\, \kappa^{d-t}. \tag{3.b}$$

Here t is used to denote what is usually written as $2-\eta$. In the same spirit, we postulated that $\hat{c} = \hat{c}^S+\hat{c}^L$, where for $\kappa a \ll 1$ and $r/a \gg 1$, we have $\hat{c} = \hat{c}^L$, with $\hat{c}^L$ such that

$$\hat{c}_c^L \sim r^{-s-d}, \tag{4.a}$$

$$\hat{c}^L-\hat{c}_c^L \simeq F(\kappa r)\, r^{-s-d} = \kappa^{s+d} E(\kappa r). \tag{4.b}$$

As argued in I and II, we expect $t = \min[s,2]$. In [3] it was pointed out that if one assumes (3) then one also expects the Ising-model $f(x)$ in (3) to be given by

$$f(x) \sim x^{(1-\alpha)/\nu} \text{ for } x \to 0, \rho=\rho_c, T \geq T_c, \quad (3.c)$$

because only then does the κ dependence for $x \to o$ merge smoothly into a κ dependence of $\hat{h}(\underset{\sim}{r})$ at $r \sim a$ that is consistent with having the specific heat at $\rho=\rho_c$, $T \geq T_c$, given by $C_v \sim \partial\hat{h}(\underset{\sim}{r})/\partial T$ at $r=a$. Similarly when (4) is assumed, it is natural to postulate that $F(x)$ in (4) is such that

$$F(x) \longrightarrow x^m \text{ as } x \to 0, \quad m \geq t, \quad (4.c)$$

on the following basis: We have

$$\int \hat{C}_2^L \, d\underset{\sim}{r} \sim \kappa^s \quad (5)$$

from (4.b). From (3.b), the expectation that $\int \hat{h}^S d\underset{\sim}{r}$ will remain bounded as $\kappa \to o$, and the Fourier-transform relation,

$$-\rho\,\hat{C}(\underset{\sim}{k}) = [\rho\,\hat{H}(\underset{\sim}{k})]^{-1}, \quad (6)$$

we have $\int \hat{c}_2 d\underset{\sim}{r} \sim \kappa^t$. Thus by subtraction, since $s \geq t$,

$$\int \hat{C}_2^S \, d\underset{\sim}{r} \sim \kappa^m, \; m \geq t. \quad (7)$$

But since $\hat{c}_2^{\,S}$ is a short-range object, loaded at the origin, Eq. (7) is consistent with $\hat{c}_2^{\,S} \sim (\kappa^m$ times a function of r that is essentially independent of $\kappa)$, and if the κ-dependence of $\hat{c}_2^{\,L}$ is to smoothly merge into that of $\hat{c}_2^{\,S}$, we expect (4.c).

In [3] a deviation from (3.b) was found that suggests the form, if $x=\kappa r$,

$$r^{d-t}(\hat{h}^L-\hat{h}_c^L) = f(x)r^q \text{ as } x \to 0, \tag{3.b'}$$
$$= f_2(x) \quad \text{otherwise,}$$

instead of (3.b), with $f(x)$ still given by (3.c) and q on the order of[4] 1/7. The condition $x \to 0$ in (3.b') can be made more specific. Moore, Jasnow, and Wortis[5] found that

$$\int \hat{h}(\underset{\sim}{r})\,d\underset{\sim}{r} \sim \kappa^{-t} \text{ for } \rho=\rho_c \tag{8}$$

despite their evidence that (3.b) breaks down when $x \to 0$. This implies that $x \to 0$ cannot simply be taken to mean x less than some fixed small number (which would lead to $\int \hat{h}(\underset{\sim}{r})d\underset{\sim}{r} \sim \kappa^{-t-q}$ for $q > 0$) but instead suggests the introduction of a second length $\sim \kappa^{-\theta}$, $0 < \theta < 1$, such that $x \to 0$ is taken to mean $x < \kappa^{\theta}$. If (3.b') holds with this interpretation of $x \to 0$ it is again possible for (8) to be satisfied. The deviation from (4.b) that is then more-or-less obviously suggested by (3.b') is of the form, for $\kappa a >> 1$ and $r >> a$,

$$r^{d+s}(\hat{C}-\hat{C}_c) \simeq F(x)r^{Q} \text{ for } x < \kappa^{\theta} \tag{4.b'}$$
$$\simeq F_2(x) \quad \text{otherwise,}$$

with $x = \kappa r$ and $F(x)$ given by a power of x,

$$F(x) \sim x^{\tau}. \tag{4.c'}$$

We shall conclude below that $\tau = t-Q$. The quantity θ will be left undetermined, as will Q, although we should expect the latter to be of the same order of magnitude as the q in (3.b'). We shall assume $s=t$ in (4.b') for simplicity because we wish to investigate the possibility that $t < 2$, and for such t there is no reason to postulate a separate exponent for $\hat{c}$, as pointed out in I and II.

We showed in II that if (3.a), (3.b), (4.a) and (4.b) are assumed, then the terms in our expansion of c_c that contain the functional derivatives of $\hat{c}$ with respect to n [i.e. contributions involving certain ℓ-point correlation effects for $\ell > 2$] do not dominate the contributions to c_c that are wholly expressible in terms of $\hat{c}$ and $\hat{h}$. In this note we shall continue to neglect the ℓ-point effects for $\ell > 2$. Ignoring these higher derivatives of $\hat{c}$ and assuming that the pair potential is short ranged, we are left at the critical point for large r_{12} with

$$c_c(12) \cong \text{const}\,[h_c(12)]^{\delta} + S_1 ,$$

$$S_1 \simeq \rho\int[\hat{C}_2^S(13)]_0\, h_c(23)\, d(3) + \rho\int[\hat{C}_2^L(13)]_0\, h_c(23)\, d(3) - \rho h_c(12)\int[\hat{C}_c(12)]_0\, d(2) .$$

Since
$$\int[\hat{C}_2^S(13)]_0\, h_c(23)\, d(3) \sim h_c(12)\int[\hat{C}_2^S(12)]_0\, d(2) \tag{9}$$

for $r_{12} \to \infty$, we have

$$S_1 \simeq -\rho h_c(12)\int[\hat{C}_2^L(12)]_0\, d(2) + \rho\int[\hat{C}_2^L(13)]_0\, h_c(23)\, d(3) \tag{10}$$

for $r_{12} \to \infty$. In II, the first integral of (10) was found to be of order $h_c\kappa_0^s$ from (5), and the second of order $h_c^{\delta+1}$. We shall not concern ourselves further with the second integral since $O(h_c^{\delta+1})$ is not likely to be increased beyond $O(h_c^{\delta})$ by a small departure from (4.b). It is no longer true however that we can expect (5) to hold. In fact, letting

$$\int \hat{C}_2^L\, d\underset{\sim}{r} = \int_{x<\kappa^\theta} \hat{C}_2^L\, d\underset{\sim}{r} + \int_{x\geq\kappa^\theta} \hat{C}_2^L\, d\underset{\sim}{r} , \tag{11}$$

we find from (4.b') and (4.c') that if $\tau-t+Q > 0$, then $\int_{x<\kappa^\Theta}\hat{c}_2^L d\underset{\sim}{r} \sim \kappa^{\tau-(1-\Theta)(Q+\tau-t)}$, while a reasonable $F_2(x)$ (for example $F_2(x) \sim x^t$ for $\kappa^\Theta < x < 1$ and $F_2(x) \sim x^{\text{const}}e^{-\text{const}\,x}$ for $x > 1$)

still yields $O(\kappa^t)$ for the second integral in (11)[6].

From the argument used to deduce that the power appearing in (4.c) is at least t, we can now estimate τ in (4.c'), using $\tau-(1-\Theta)(Q+\tau-t)$ in (5) instead of $s \geqslant t$. If $\tau-(1-\Theta)(Q+\tau-t) \leqslant t$, the argument leads to the conclusion that $\tau-(1-\Theta)(Q+\tau-t) = \tau$, which is satisfied if $\tau = t-Q$, and we thus concluded that $S_1 \sim h_c \kappa_o^{t-q}$, with $Q \geqslant 0$. [$\tau-(1-\Theta)(Q+\tau-t) > t$ implies $Q < 0$ and $S_1 \sim \kappa_c \kappa_o^t$.] But $\kappa^t \sim |\rho-\rho_c|^{\delta-1}$, coming from (8) and $|\mu-\mu_c| \sim |\rho-\rho_c|^{\delta}$, implies $\kappa_o^t \sim h_c^{\delta-1}$. Hence if $Q \geqslant 0$, then $S_1 \sim h^{\delta-[Q(\delta-1)/t]}$, and in (2) we have

$$p = \delta - [Q(\delta-1)/t] \tag{12}$$

instead of δ, yielding the restriction , if $t < 2$:

$$t = d[\delta-1-Qt^{-1}(\delta-1)]/[\delta+1-Qt^{-1}(\delta-1)] . \tag{13}$$

As an equation for t this has two solutions, one of which approaches $d(\delta-1)/(\delta+1)$ as $Q \to 0$. This is the one we should expect to find realized. The deviation of p from δ in (12) is of the right order of magnitude to give reasonable values of η if[7] $Q \not\approx q$. To see this we note that if $d=3$ and $\delta=5$, then the solution of (13) that approaches 2 as $Q \to 0$ goes like $t \approx 2-(Q/3)$ for small Q so that if Q were equal to $q \approx 1/7$, then η would be $\approx 1/21$.

References

1. G. Stell, Phys. Rev. Letters **20**, 533 (1968).

2. G. Stell, "Extension of the Ornstein-Zernike Theory II" (to appear).

3. M. Ferer, M.A. Moore, and M. Wortis, Phys. Rev. Letters **22**, 1382 (1969).

4. In ref. [3] it is actually the combination $[(1-\alpha)/\nu]+t-d+Q$ that is assessed. It is found to be 0.47 ± 0.06 while $[(1-\alpha)/\nu]+t-d$ is estimated in [3] to be 0.33 ± 0.01. Hence the resulting estimate of Q, obtained by subtraction, already depends on estimates of α, ν, and t.

5. M.A. Moore, D. Jasnow, and M. Wortis, Phys. Rev. Letters **22**, 940 (1969).

6. The case $\tau-t+Q < 0$ cannot be adequately handled within the framework of our assumptions. It gives rise to a small - x divergence in the first integral as a result of the simple functional form we postulate for $\hat{c}_2^L$ and, strictly speaking, is untenable under our postulate. We therefore ignore this case here.

7. Our work provides only a hint that one should set $Q=q$. If one treats (4.b') and (4.c') as globally (rather than asymptotically) valid, one finds directly through (6) that for $\kappa \to 0$, $Q=q$. Also implied is $\tau = (1-\alpha)/\nu$, giving rise to the divergence difficulties noted in footnote 6. It is to be expected that ignoring the asymptotic nature of (4) will lead to such difficulties; the question is whether a more sophisticated treatment of $\hat{c}^L$ can justify retaining $Q=q$ while bypassing the divergences.