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Value of η for Long-Range Interactions*

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The relationship $2 - \eta = m$ is derived for the Ising model with a potential of the large- r form $v(\vec{r}) \propto -r^{-d-\sigma}$, when $m/d < 1/2$ [and for continuum fluids with such a $v(\vec{r})$ when $m/d < 1/3$], where η has its usual meaning as a critical exponent and $m = \min[\sigma, 2]$. On the basis of this result, it is argued that the numerical estimates of Nagle and Bonner indicate a breakdown of strong scaling in the Ising chain with long-range potential.

This paper has three main objectives. The first is to give the formally exact result

$$2 - \eta = m, \quad (1)$$

which we find for the Ising model (i. e., the lattice gas) if $m/d < \frac{1}{2}$ and the pair potential is of the form

$$v(\vec{r}) \sim -A r^{-d-\sigma} \quad \text{for } r \rightarrow \infty. \quad (2)$$

Here $A > 0$, d is dimensionality, $\sigma < 0$, $r = |\vec{r}|$, $m = \min[2, \sigma]$, and η has its usual meaning as a critical exponent. For continuum fluids we show that a sufficient condition for (1) is $m/d < \frac{1}{3}$. The weaker $m/d < \frac{1}{2}$ appears to be sufficient for fluids, too, but we defer discussion of this point until a later publication. Our results here extend our own previous discussion¹ of (1), based on simple homogeneity assumptions, as well as a more recent derivation² of (1) for the case of a special spin system especially tailored to a renormalization-group³ and Feynman-diagrammatic^{4,5} approach. (That system is Ising-like when $n = 1$, where n is the spin dimensionality.)

A second purpose is to point out in passing an alternative to the functional-integral form of the partition function as a starting point for any such diagrammatic analysis. It is a cluster-integral formalism developed earlier⁶⁻⁸; its chief advantage is that it is immediately applicable to continuum fluids⁶ and to the Ising model⁷ as well as to the fluidlike or Ising-like models that have been constructed to lend themselves to special types of analyses.

Our third main purpose here is to show that (1), taken together with the numerical results of Nagle and Bonner⁹ for the Ising chain, yields a relation that is inconsistent with the usual scaling laws as given, e. g., in Kadanoff's¹⁰ scaling theory. This

appears to be strong evidence in favor of the contention—argued by us at length elsewhere from several different standpoints^{11,12}—that for $d \rightarrow 0$ and fixed σ , or for $\sigma \rightarrow 0$ and fixed d , one would expect the breakdown of any of the usual scaling laws explicitly involving d for both the Ising model and continuum fluids.

We shall denote as $F(\vec{r})$ the density-density correlation function [the $\hat{F}(\vec{r})$ of some of our earlier references] or the spin-spin correlation function. The η of (1) can be defined by the assumption

$$[F(\vec{r})]_c \sim -r^{-d+2-\eta}, \quad r \rightarrow \infty$$

where the subscript c refers to a critical value. Using the cluster-expansion techniques that we have developed and discussed elsewhere,⁶⁻⁸ we obtain Eq. (1) (independent of any scaling assumptions) by comparing the spatial decay as $r \rightarrow \infty$ of the "chain-graph" contribution $\mathcal{C}(\vec{r})$ with the decay of all the other graphs that contribute to the \mathcal{C} -bond expansion of $F(\vec{r})$. For simplicity we consider first the case of the Ising model or lattice gas in which the "hypervertex function" [the \hat{F}_2^s of Ref. 6 and the $\nu_2\sigma(1-2)$ of Ref. 7] depends upon temperature T and field H (or density ρ , in lattice-gas language) but has no spatial extension and hence has a Fourier transform ν_2 that is \vec{k} independent. We see that $\mathcal{C}(\vec{r})$ is longest ranged at a distinguished value $\nu_{2,d}$ of ν_2 , at which value $\mathcal{C}(\vec{r}) \sim -r^{-d+m}$ for $r \rightarrow \infty$,¹³ while all other graphs contributing to $F(\vec{r})$ fall off more rapidly than $\mathcal{C}(\vec{r})$ for every ν_2 including $\nu_{2,d}$, as long as $m/d < \frac{1}{2}$. The $\frac{1}{2}$ here arises as follows: It is only where $m/d < \frac{1}{2}$ that one can be sure that for $\nu_2 = \nu_{2,d}$ none of the other \mathcal{C} -bond ν_m -hypervertex graphs contributing to $F(\vec{r})$ will dominate the single \mathcal{C} -bond graph.

All such graphs with ν unlabeled vertices and b bonds satisfy the relation $2(b+1) \geq 2\nu$, and there will be among them ones that give rise to terms—for example, $\gamma^{-b(d-m) + \nu d}$ terms—that will dominate $\mathcal{C}(\vec{r})$ unless $m/d < \frac{1}{2}$. The dominance of $\mathcal{C}(\vec{r})$ as $r \rightarrow \infty$ causes critical-point behavior of $F(\vec{r})$ at $\nu_{2,d}$ [at which the transform $\bar{F}(\vec{k})$ is ∞ for $\vec{k}=0$], which identifies $\nu_{2,d}$ as the critical $\nu_{2,c}$.

The analysis for the continuum fluid is identical in all fundamental respects. The main differences are that in Fourier space the hypervertex functions $\nu_n(\{\vec{k}_i\})$ (the \bar{F}_n^s of Ref. 6) are no longer \vec{k}_i -independent functions of ρ and T , that are even or odd in $\rho - \rho_c$ as n is even or odd. Instead they will go as $\nu_n(\{\vec{k}_i\}) = \nu_{n,0} + \sum_{i,j} \nu_{n,i,j} \vec{k}_i \vec{k}_j + \dots$, and graphs containing at least one odd-ordered ν_n are no longer guaranteed to vanish when $\rho = \rho_c$, as they are in the simple lattice-gas case. For $m/d < \frac{1}{3}$, however, the $\mathcal{C}(\vec{r})$ is still guaranteed to dominate all other graphs contributing to $F(\vec{r})$ for all $\nu_{2,0}$, including the particular $\nu_{2,0}$ at which $\bar{F}(0) = \infty$, regardless of whether the $\nu_{n,0}$ for odd n turn out to vanish at the critical point or not. (This is because $b+1 \geq 2\nu$ for all the graphs whether $\rho = \rho_c$ or not.) The behavior of the fluid $\nu_n(\{\vec{k}_i\})$ at $\nu_{2,0,c}$ would require further study in order to weaken the sufficiency condition $m/d < \frac{1}{3}$ to $m/d < \frac{1}{2}$ using this approach.

A comparison of the graphs introduced in Refs. 6 and 7 with those recently used by various authors to gain information concerning critical behavior of certain special systems via diagrammatic analysis shows that such analysis can be made directly for the Ising model via the former graphs. The “renormalized” r of Ref. 5 relates directly to the ν_2 of Ref. 7 or \bar{F}_2^s of Ref. 6, the u_0 of Ref. 5 corresponds to the ν_4 of Ref. 7 or \bar{F}_4^s of Ref. 6, etc. For the Ising-like ($n=1$) systems of Refs. 2–5, our \mathcal{C} -bond ν_n -hypervertex representation reduces to the diagrammatic expansion used there; the chief difference between the diagrams for the Ising-like systems and the Ising-model graphs of Ref. 7 is the presence of hypervertices of arbitrarily high order in the Ising case. The chief difference between diagrams for the Ising-like systems and a continuum fluid has already been noted here: The hypervertices in the latter case carry a \vec{k} dependence, and odd-order hypervertices do not vanish at the critical point. Thus, a diagrammatic evaluation as per Ref. 5 will permit a precise and explicit assessment of the effects, if any, of the absence of hole-particle symmetry in the fluid case on

TABLE I. Evaluation of the z of Eq. (8) and the η of Eq. (7) by means of the Nagle-Bonner estimates of γ and β .

σ	0.20	0.30	0.40	0.50	0.60	0.70	0.80	0.90
z from (8)	0.40	0.59	0.74	0.85	0.94	0.98	0.99	1.00
z_{sm}	0.40	0.60	0.80	1.00	1.00	1.00	1.00	1.00
$2-\eta$ from (7)	0.50	0.51	0.54	0.59	0.64	0.71	0.81	0.90

the numerical values of the critical indices.

It is convenient to discuss the way the status of the scaling laws hinges upon the validity of (1) in the context of our weak-scaling relations,¹¹ which are the same relations given by previous scaling theories¹⁰ but with d replaced by a new exponent z , where $z \leq d$. Relations that do not explicitly involve d are unchanged. Thus we retain, for example,

$$\gamma = \nu(2 - \eta). \quad (3)$$

On the other hand, we have

$$\gamma + 2\beta = \nu z \quad (4)$$

instead of

$$\gamma + 2\beta = \nu d. \quad (5)$$

Here we use the customary notation of Fisher.¹⁴

Combining (3) and (4) we have

$$z = (\nu - 2\beta)(2 - \nu)/\gamma \quad (6)$$

instead of the scaling result

$$d = (\gamma + 2\beta)(2 - \eta)/\gamma. \quad (7)$$

Assuming (1), we find

$$z = (\gamma + 2\beta)\sigma/\gamma. \quad (8)$$

We give in Table I the right-hand side of (8) evaluated by means of the Nagle-Bonner estimates⁹ of γ and β , which were all obtained in the case $d = 1$. Since they show $z \neq 1$ unambiguously, these results are incompatible with (1) and (7) taken together. The resulting z from (8) is much like the spherical-model z , which was computed in Ref. 11 and is given by 2σ if $\sigma < \frac{1}{2}d$ and d if $\sigma > \frac{1}{2}d$. This z is shown as z_{sm} in Table I directly below the z from (8), and one can see that the two functions behave in a quite similar fashion, which seems reasonable. While formally exact, our derivation of Eq. (1) is obviously lacking in rigor because of the convergence questions raised by our use of the \mathcal{C} -bond expansion; similar remarks apply to most of the results of Refs. 1–8.

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Effect of Orbital Degeneracy on the Anderson Model of a Localized Moment in a Metal

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As conventionally written, the localized-center portion of the Anderson Hamiltonian suffers from the defect of lack of rotational invariance in real space (and possibly spin space also) when describing a center with $(2l+1)$ degenerate spatial orbitals. A simple modification is suggested which restores the rotational invariance in both spaces. The eigenvalues of this localized-center portion of the Hamiltonian can be determined by inspection, and are consistent with Hund's rule. The modification leads to nontrivial changes in the properties of the full Anderson Hamiltonian. Within the context of the Hartree-Fock approximation, the likelihood of orbital broken symmetry is reduced.

The Anderson Hamiltonian,¹ describing the interaction between the conduction electrons of a metal and a localized magnetic center, can be written

$$H = H_0 + H_1 + H_{01} + H_{\bullet\bullet}, \quad (1)$$

$$H_0 = \epsilon_0 \sum_s n_{ms}, \quad (2)$$

$$H_1 = \sum_{ks} \epsilon_k n_{ks}, \quad (3)$$

$$H_{01} = \sum_{ks} (V_k c_{ks}^\dagger c_{ms} + V_k^* c_{ms}^\dagger c_{ks}), \quad (4)$$

$$H_{\bullet\bullet} = \frac{1}{2} U \sum_s n_{ms} n_{m,-s}, \quad (5)$$

where

$$n_{ms} \equiv c_{ms}^\dagger c_{ms}, \quad n_{ks} \equiv c_{ks}^\dagger c_{ks} \quad (6)$$

are the number operators associated with the localized center and the conduction band, respectively. The one-electron energies ϵ_k (for the conduction band) and ϵ_0 (for the localized center) are measured with respect to the Fermi level. There is a single localized spatial orbital (denoted by m) on the localized center. The electron-electron interaction Hamiltonian $H_{\bullet\bullet}$ represents the Coulomb interaction between two opposite-spin electrons on the center. $H_0 + H_{\bullet\bullet}$ represents the center by itself, H_1 is the conduction band by itself, and H_{01} is the hopping of electrons of either spin between center and conduction band.

Anderson himself¹ first considered generalizing this Hamiltonian to the case where there are

$(2l+1)$ degenerate spatial orbitals associated with the center. H_0 and H_{01} are now augmented by sums over the magnetic quantum number m ,

$$H_0 = \epsilon_0 \sum_{ms} n_{ms}, \quad (7)$$

$$H_{01} = \sum_{kms} (V_k c_{ks}^\dagger c_{ms} + V_k^* c_{ms}^\dagger c_{ks}). \quad (8)$$

Anderson suggested replacing (5) by

$$H_{\bullet\bullet} = \frac{1}{2} U \sum_{mm's} n_{ms} n_{m',-s} + \frac{1}{2} (U - J) \sum_{mm's} (1 - \delta_{mm'}) n_{ms} n_{m's}. \quad (9)$$

However, Caroli *et al.*,² and Lucas and Mattis³ independently pointed out that such an $H_{\bullet\bullet}$ is not rotationally invariant in spin space, and therefore suggested replacing (9) by

$$H_{\bullet\bullet} = \frac{1}{2} U \sum_{mm's} n_{ms} n_{m',-s} + \frac{1}{2} (U - J) \sum_{mm's} (1 - \delta_{mm'}) n_{ms} n_{m's} - \frac{1}{2} J \sum_{mm's} (1 - \delta_{mm'}) c_{ms}^\dagger c_{m,-s} c_{m',-s}^\dagger c_{m's}. \quad (10)$$

Although (10) is rotationally invariant in spin space, it is *not* rotationally invariant in real space (a fact not realized by Caroli *et al.*²). It is the purpose of this paper to point out that there is a very simple generalization of (10) that is simultaneously invariant to rotations in both real and spin space.⁴

In the case of a $(2l+1)$ -fold orbital degeneracy,