

yields $g(0) = -0.22$ and without screening $g(0) = -0.07$. This appears to be completely unjustified, however. We further note that Singwi's¹⁴ "self-consistent" dielectric function yields a $g(r)$ much better than ϵ_{KL} [i.e., less negative $g(0)$]. On the other hand, in what Singwi calls the Hartree-Fock limit his ϵ reduces to ϵ_H . Because Langreth² has proven ϵ_H is incorrect [see discussion following Eq. (11)], Singwi's ϵ must be incorrect as well. If Singwi's self-consistency procedure could be

corrected to yield ϵ_{KL} in the Hartree-Fock limit, it would undoubtedly yield an ϵ far superior to anything yet derived.¹⁵ Finally, we wish to emphasize that just because the Kleinman-Langreth and Hubbard $g(r)$ contain similar corrections to the RPA $g(r)$ does not mean they will give similar corrections to other quantities. In fact, we have found that for a given ionic pseudopotential they yield corrections of opposite sign to the phonon frequencies of magnesium calculated¹⁶ with ϵ_{RPA} .

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¹L. Kleinman, Phys. Rev. **172**, 383 (1968).

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⁴The screening constant K_S does not appear in Ref. 3. It was added at Hubbard's suggestion by L. M. Falicov and V. Heine, Advan. Phys. **10**, 57 (1961), and by many other workers.

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⁷R. W. Shaw, Jr., J. Phys. C **3**, 1140 (1970).

⁸R. W. Shaw, Jr. (private communication).

⁹To facilitate comparison between ϵ_H and ϵ_{KL} we used the same α in both. Hubbard himself chose $\alpha = \frac{1}{2}$ for all κ .

¹⁰J. Hubbard [Phys. Letters **25A**, 709 (1967)] obtained $g_{\text{RPA}}(0) = -0.50$ for $r_s = 2$.

¹¹We have not recalculated $g(r)$ using the dielectric function ϵ_{STLS} of Singwi *et al.* (Ref. 6), since ϵ_{STLS} is not given in closed form. It is possible that the self-consistent nature of ϵ_{STLS} [i.e., its dependence on $g(r)$] will reduce the error made in $g_{\text{STLS}}(r)$ by taking $\eta = 10$ as the upper limit of integration relative to the error in $g_{\text{RPA}}(r)$.

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¹⁵Dr. Shaw informs me that he and Dr. Langreth are currently working on this problem.

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Some Implications of Weak-Scaling Theory*

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

In a previous paper,¹ the author outlined the derivation of a set of weak-scaling relations based upon the appearance of two correlation lengths, Λ and ξ . The analysis rested upon an investigation of the form of the density-density correlation function $\hat{F}(\vec{r})$ along the coexistence curve. In order to make contact with the results of Ferer, Moore, and Wortis² that hold along the critical isochore, as well as our own techniques^{3,4} that involve $\hat{F}(\vec{r})$ 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 $\tilde{q}(\vec{r}, \kappa)$ by assuming that along the coexistence curve

$$\hat{F}(\vec{r}) - \hat{F}(\vec{r})_c = f(\kappa r) / r^{d-t-\tilde{q}(\vec{r}, \kappa)} \quad (1)$$

Here $\hat{F} = \rho^2 \hat{h}$, where \hat{h} is the correlation function discussed in our earlier work and ρ is the number density. Letting $M = |\rho - \rho_c|$, so that M is proportional (in spin language) to magnetization, we assume that $\kappa = \xi^{-1} \sim M^\epsilon$ along the coexistence curve and that $\kappa \sim |T - T_c|^\nu$ when $M = 0$ and $T > T_c$. As

usual T is temperature, and the subscript c will refer to critical values throughout this paper. We argued in Ref. 1 that for the Ising model, and also for simple fluids, we might further expect to find along the coexistence curve, for small κ ,

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

as well as

$$\tilde{q}(\vec{r}, \kappa) \approx q \quad \text{for } r < \Lambda, \quad (3a)$$

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

where

$$q = d - t - 2/\epsilon, \quad (4)$$

$$\Lambda = \kappa^{-\theta}, \quad (5)$$

$$d - t - q = \theta(d - t) \leq d - t. \quad (6)$$

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

$$\tilde{q}(\vec{r}, \kappa) \rightarrow q \quad \text{for } r \rightarrow 1, \quad (7a)$$

$$\tilde{q}(\vec{r}, \kappa) \approx 0 \quad \text{for } r \gg 1, \quad (7b)$$

where the lattice spacing has been taken as unity. More generally, we anticipate (7) instead of (3) for any systems⁶ that satisfy the Ornstein-Zernike hypothesis that the direct correlation function looks like the pair potential $V(\vec{r})$ times $(\kappa T)^{-1}$ for $V(\vec{r})/\kappa T \ll 1$.

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 $\hat{F} - \hat{F}_c$ 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 $(M^{1/\beta}, \Delta T)$ plane. Once we accept this assumption, together with the homogeneity of κ in $M^{1/\beta}$ and ΔT , we are directly led by the argument of Ref. 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 $\tilde{q}(\vec{r}, \kappa)$ to be given by (3), we again find (6), but this time for $T = T_c$. Details of this derivation will be given elsewhere⁴; the important point to make here is that these details are independent of the arguments of Ref. 1 that lead to (6) along the coexistence curve. Taken alone, this result for $T = T_c$ does not guarantee that either θ or q (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 $\hat{F} - \hat{F}_c$ for $r \approx 1$ could vanish (simply because M^2 vanishes) leaving as the most dominant term another term, presumably still of the form

$$\hat{F} - \hat{F}_c \sim \kappa^p \gamma^{p-d+t+\tilde{q}_0(\vec{r}, \kappa)} \quad (8)$$

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

On the critical isochore, the power of r in (8) is not constrained by our arguments to be zero for small r , as it was along the phase boundary. It is precisely this power of r , $(1 - \alpha)/\nu - d + t + \tilde{q}_0(\vec{r}, \kappa)$, that Ferer *et al.* investigated for the 3- d Ising model for small κ and r . They found it to be 0.47 ± 0.06 , and using their value of $(1 - \alpha)/\nu - d + t$, we find that this yields $\tilde{q}_0 \approx 1/7 \pm 1/14$. Although they gave results only for $r < 3$, they argued that their results indicated that for small κ , $\tilde{q}_0(\vec{r}, \kappa)$ has an essentially constant value over a range of r that includes $r \gg 1$ as well as $r \approx 1$, but they were unable to deduce the distance Λ_0 beyond which $\tilde{q}_0(\vec{r}, \kappa)$ 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 Ref. 1 and of this paper support their conclusion that \tilde{q}_0 can be expected to be nonzero for a range of values over which $r \gg 1$, 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 Ref. 1 along the coexistence curve, one considers the Λ_0 at which the small- r and large- r form of $\hat{F} - \hat{F}_c$ 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

$$(1 - \theta_0)/\theta_0 = q_0 \nu / (1 - \alpha), \quad (9)$$

where q_0 is the value approached by \tilde{q}_0 as $r \rightarrow 1$ and $\kappa \rightarrow 0$.

Equation (9) defines the length Λ_0 in terms of q_0 , ν , α , and κ . Arguments were given in Ref. 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 $\tilde{q}_0(\vec{r}, \kappa)$ given by Eq. (8) behaves like a nonzero constant only for r near 1 with $\tilde{q}_0(\vec{r}, \kappa) \approx 0$ for $1 \ll r \ll \Lambda$. In this case Eq. (9) would no longer define a Λ_0 that would manifest itself in any tangible way in the structure of $\hat{F} - \hat{F}_c$. This is precisely the situation in the spherical-model case, where if $d \geq 4$, both $\tilde{q}(\vec{r}, \kappa)$ and $\tilde{q}_0(\vec{r}, \kappa)$ for small κ are $d - 4$ for $r \approx 1$ but zero for $r \gg 1$. 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 $r \gg 1$ but $\tilde{q}_0 \approx 1$ for $r \approx 1$. The question is: Will the numerical analysis reveal that strong scaling of $\hat{F}(\vec{r})$ for $r \gg 1$ is preserved, as one knows it is, or will the $\tilde{q}_0 \approx 1$ for $r \approx 1$ misleadingly suggest numerically that strong scaling has been violated?

A second question that the work of this paper

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 q with q_0 . If we do equate θ and θ_0 , we have from (9) and our earlier equations that

$$q_0 = q(1 - \alpha)/2\beta. \quad (10)$$

Taking $\alpha = 1/8$, $\beta = 5/16$, and using the values $q = 3/50$ and $q = 1/12$, which probably represent two extreme possibilities,¹ we find $q_0 = 21/250$ and $q_0 = 7/60$, respectively. These values are consistent with the $1/7 \pm 1/14$ from Ref. 2. Nevertheless, it would clearly be valuable to have some more-or-less direct numerical assessment of q that eliminates the necessity of our going through (10) in order to make contact with the rest of our scaling relations.

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²M. Ferer, M. A. Moore, and M. Wortis, Phys. Rev. Letters **22**, 1382 (1969).

³G. Stell, Phys. Rev. Letters **20**, 533 (1968); Phys. Rev. B **1**, 2265 (1970).

⁴G. Stell (to be published). In a preliminary study (State University of New York Engineering Report No. 144), we considered only the case in which a certain inequality (which we have subsequently found to be essentially $2/\epsilon - t + q > 0$) 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 $d - t - q = \theta(d - t)$ follows.

⁵In the spherical model, the argument used in Ref. 1 to obtain Eq. (2) for the Ising model is not applicable. Nevertheless $\hat{F} - \hat{F}_c \approx f_2(\vec{r}) M^2$ as $r \rightarrow 1$, with $f_2(\vec{r})$ depending on r like r^0 . Setting $q \approx 0$ for $r \gg 1$, 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 $r \approx 1$.

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Mean g Values of Rare-Earth Ions: Extension to Monoclinic Symmetries

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A previous calculation of the mathematical properties of a Kramers doublet for extrema of the mean g value is extended to monoclinic symmetries. The theory is applied to the paramagnetic resonance data for $\text{LaF}_3:\text{Yb}^{3+}$. These data are shown to be consistent with a Yb^{3+} site of C_{2v} point symmetry.

In a recent paper,¹ some mathematical properties of an isolated Kramers doublet were derived for the condition that the mean g value was an extremum. The doublet wave functions were expressed as linear combinations of free-ion states associated

with a single value of J ; i. e.,

$$\begin{aligned} |\alpha\rangle &= \sum_M a_M |J, M\rangle, \\ |\beta\rangle &= \sum_M (-1)^{(J-M)} a_M^* |J, -M\rangle, \end{aligned} \quad (1)$$