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The Fully Finite Spherical Model

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A lattice sum technique is applied to the constraint equation of the finite size mean spherical model. It is shown that this allows the investigation of the model over a wide range of temperatures, for a wide range of system sizes. Correlation lengths and susceptibilities are shown to obey crossover scaling around $T=0$ below the lower critical dimension, and finite size scaling between the lower and upper critical dimensions. Universal scaling forms are suggested for the lower critical dimension. At and above the upper critical dimension, the behavior is identical to that of finite sized mean field theory. The scaling at and above the upper critical dimension is shown to be modified by the existence of a dangerous irrelevant variable which also governs the failure of hyperscaling. Implications for phenomenological renormalization experiments are discussed. Numerical results of scaling are displayed.

KEY WORDS: Finite size scaling; spherical models; phenomenological renormalization.

1. INTRODUCTION

Finite size scaling, proposed a number of years ago by Fisher[1] has been widely used to extract the thermodynamic limit from finite systems of small size. In regard to a fully finite system of length scale L (for example, a system of cubic geometry) the theory can be summarized as follows. Let $\chi(t)$ be a response function behaving as $\chi \sim t^{-\gamma}$ in the thermodynamic limit. For finite L, χ_L will be rounded, and scale in the form[1-3]

$$\chi_L(T) \sim L^{\gamma/\nu} X(L^{1/\nu}\tilde{t}) \tag{1}$$

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Here ν is, as usual, the exponent measuring the divergence of the correlation length ξ, and

$$\tilde{t} \equiv \frac{T - T_c}{T_c} + \varepsilon(L) \tag{2}$$

where $\varepsilon(L)$ is a shift obeying $\lim_{L \to \infty} \varepsilon(L) = 0$, and $X(x)$ is the rounding function. It has been argued[2,3] that corrections to Eq. (1) should be governed by corrections to scaling of the infinite system.

Finite size scaling can be derived from simple renormalization group (RG) scaling arguments.[3,24] Consider the RG transformation for the susceptibility. It will scale like

$$\chi_\infty(t, u) = b^{\gamma/\nu} X(tb^{1/\nu}, ub^{y}) \tag{3}$$

where b is the RG rescaling factor, t is the temperature like scaling field, u is the most important irrelevant scaling field, and $y < 0$. (We are neglecting other relevant fields, such as the applied magnetic field in the case of a magnetic critical point). This scaling form implies a power law divergence

$$\chi_\infty(t, u) \sim t^{-\gamma} X(1, 0) + t^{-(\gamma + y\nu)} u X_u(1, 0) + \cdots \tag{4}$$

where the second term is the correction to scaling of the infinite system.

For a finite system of length L, Brezin[2] has argued that the RG rescaling factor b can be taken proportional to L, and a modified form of (3) holds (L is not rescaled). The finite size scaling form is

$$\chi_L(t, u) = L^{\gamma/\nu} X(\tilde{t} L^{1/\nu}, \tilde{u} L^{y}) \tag{5}$$

(We have included the possibility of finite size shifts in the scaling fields, which are often ignored). Expanding this form for small u yields the correction to scaling. If the infinite system behaves as

$$\chi_\infty(t) \sim t^{-\gamma}(1 + t^{p}) \tag{6}$$

then the finite system will scale as

$$\chi_L(t) = L^{\gamma/\nu} X(\tilde{t} L^{1/\nu}) + L^{(\gamma - p)/\nu} u X_u(\tilde{t} L^{1/\nu}) \tag{7}$$

The second term is the correction to finite size scaling, and will govern convergence to the scaling form of Eq. (1).

An important application of (1) is the phenomenological renormalization (PR) transformation introduced by Nightingale[4] (see Ref. 5 for a more recent review). Noting that the finite size scaling equation for the correlation length takes the form

$$\xi_L(T) = LY(L^{1/\nu}\tilde{t}) \tag{8}$$

one can define a rescaling transformation, $L \to L'$, $t \to t'$ via the constraint

$$\xi_L(t)/L = \xi_{L'}(t')/L' \tag{9}$$

which has $t = 0$ as a fixed point. It is possible to develop approximates to t_c as the intersection between ξ_L/I and $\xi_{L'}/L'$. By Eq. (2) above, $t_{c,L}$ defined by

$$\xi_L(t_{c,L})/L = \xi_{L'}(t_{c,L})/L' \tag{10}$$

(often $L' = L + 1$ is taken) will converge to $t = 0$ as

$$t_{c,L} \sim \varepsilon(L) \tag{11}$$

with corrections to Eq. (10) occurring from bulk ($L = \infty$) corrections to scaling. The critical exponent ν may be recovered via the equation

$$1/\nu_L = \ln\left[\frac{1}{L}\frac{\partial \xi_L}{\partial T}(t_{c,L})\left(\frac{1}{L'}\frac{\partial \xi_{L'}}{\partial T}(t_{c,L})\right)^{-1}\right]\Big/\ln(L/L') \tag{12}$$

which also will have corrections originating from the bulk (for discussions of Eqs. (4) and (6) and methods of increasing convergence rates, see Refs. 3 and 6 and references contained therein).

In this paper we shall discuss the mean spherical model with periodic boundary conditions in a cubic geometry (finite in all directions). Although finite size effects in the spherical model have been considered in some detail for certain geometries[2,7-9], we believe that the technique discussed herein, which involves the Ewald sum technique to perform a sum over the Brillouin zone, is of interest for a variety of reasons. It allows us to study the system numerically over the complete range of values of the parameters L, T, and H, not just in the asymptotic regime. It also allows us to generate expansions for the thermodynamics, both in the finite size scaling regime, and in the regime which approaches the thermodynamic limit exponentally. This makes it possible to see the expected features of finite size scaling emerge in a simple way, including corrections to scaling. Finally, we believe the technique to be applicable to other systems[10].

The paper is divided as follows. In Section 2 we present a brief review of the thermodynamics of the model. In Section 3 we describe our method of defining the correlation length in a finite system and of solving the model for $H=0$. Section 4 is a lengthy discussion of finite size scaling of the model in all dimensions less than $d=6$. Results of phenomenological renormalization experiments are shown to exhibit proper behavior for d between 2 and 4, and for d less than 2. Failure of the usual scaling form at the lower critical dimension, $d=2$, is discussed in some detail. Presence of a dangerous irrelevant scaling variable is proposed as the mechanism for the structure of scaling when $d>4$.

For readers who wish to skip the calculational details, we summarize the results obtained in Section 4. Those readers may also want to consult the figures of that section which illustrate the results with numerical graphs of ξ_L.

$d \leqslant 2$

Since finite size scaling is often used to determine whether or not a given finite system undergoes a transition in the thermodynamic limit, the behavior of finite systems at and below their lower critical dimension (two for the spherical model) is of interest. Both the finite and the infinite spherical models have a critical point at $T=0$, but with different critical exponents. One expects the system to show crossover from infinite to finite behavior as $T=0$ is approached. For $d<2$, crossover scaling (see Refs. 1, 11) is obeyed, with dominant corrections governed by bulk corrections, as expected. For $d=2$, however, the infinite system has essential singularities in thermodynamic functions. These contribute logarithmic terms which prevent the usual scaling form from being realized. The following general scaling forms hold

$$\xi_L/L = X(\xi_\infty/L) \tag{13}$$

and

$$\chi_L(T) = \chi_\infty(T)\; Y(\xi_\infty/L) \tag{14}$$

The possible generality of this result is suggested by the fact that it holds for both the Ising model and the spherical model at their respective lower critical dimensions. We find, in addition, that (1) Eq. (13) implies that a PR experiment will show an apparent collapse of the functions ξ/L as $T=0$ is approached, and (2) Eq. (14) is not very useful in analyzing data, because the relationship between χ_∞ and ξ_∞ must be known in order to get a useful scaling form.

$2<d<4$

In this regime, finite size scaling was shown to hold for the spherical model by Brezin.[2] In a recent work, Luck[12] has shown that the corrections to finite size scaling are dominated by the corrections to scaling in the thermodynamic limit, as predicted.[3] Our results agree with those of these authors. They have also shown the scaling functions are singular in the limits $d \to 2+$ and $d \to 4-$. We show that the dominant corrections are also singular, but in such a way as to keep the overall functions nonsingular.

$d \geq 4$

This case was studied in detail by Brezin.[2] In his paper, he raises three issues which we reconsider here. (1) He asserts that the behavior of a finite system is inconsistent with mean field theory, which predicts a phase transition even for a finite system. (2) He argues that finite size scaling fails at and above four dimensions, because the thermodynamic functions do not fall in the expected form (Eq. (1)). (3) On the basis of (1) and (2) above the fact that the limit $d \to 4$ is singular, and in fact that the limiting critical theory in a bulk four-dimensional system is mean field theory, he concludes that an ε expansion is not useful in studying a finite system.

Our conclusions are as follows. (1) In more than four dimensions, the theory which predicts the behavior of a finite system is a version of the Wilson–Ginzburg–Landau theory for a zero-dimensional system which yields the free energy

$$F(t, h, u) = L^{-d} \ln \left\{ \int d\psi \exp[-L^d(t\psi^2 - h\psi + u\psi^4)] \right\} \tag{15}$$

This free energy can be thought of as describing the behavior of an isolated, "giant" moment. We note that a modified form of (15) can be shown to correctly describe finite size rounding at a first order phase transition in a fully finite system.[13] We call this theory "rounded mean field theory," because it exhibits finite size rounding for finite L. In more than four dimensions, the finite spherical model and rounded mean field theory yield identical predictions near T_c. In four dimensions, parameters in Eq. (16) must be renormalized to yield the correct behavior. With that renormalization the results of this theory and the finite spherical model are identical. (2) In more than four dimensions, there is in the scaling form of the spherical model a dangerous irrelevant variable, which causes hyperscaling to fail. Finite size scaling holds, however, in the sense that (5) holds. However, Eq. (7) does not follow, because the scaling function is singular at $u = 0$. This is also the case in mean field theory. (3) Taking these results into account, one is led to reconsider the possibility of investigating a finite system via the ε expansion. In Fact the ε expansion has already been applied to the case of a finite Ising model in 4-ε dimensions, yielding scaling functions of the expected form for thermodynamic quantities.[10]

2. THE INFINITE SYSTEM

In this section we will review the thermodynamics of the mean spherical model. Although the results discussed here are well known, we present them in order to introduce notation and methods which will be useful later. For a review which includes a more complete discussion and references to the model, see Ref. 14.

We are interested in the mean spherical model in a cubic, $L \times L \times \cdots \times L = L^d$, geometry, with periodic boundary conditions.[2] This model is essentially a Gaussian model with a constraint. The energy of interaction is

$$E\{\sigma\} = -\frac{1}{2}\sum_{l,l'} J(l-l')\,\sigma_l\sigma_{l'} - H\sum_l \sigma_l + \mu\sum_l \sigma_l^2 \tag{16}$$

and the constraint is

$$L^d = -\frac{1}{\beta}\frac{\partial}{\partial\mu}\ln Z \tag{17}$$

Equation (17) is equivalent to the constraint

$$\sum_l \langle\sigma_l^2\rangle = L^d \tag{18}$$

which was originally intended as an approximation to the constraint of the Ising system, namely

$$\sigma_l^2 = 1 \qquad (1 \leqslant l \leqslant N) \tag{19}$$

The constraint equation is essential in developing the thermodynamics. With nearest neighbor interactions (which we will assume throughout this paper) $J(l+l') = J\delta_{l,l+1}$, and Eq. (17) takes the form

$$\beta = \left\{\frac{1}{L^d}\sum_{n_1,\ldots,n=1}^{L}\left[\alpha + J\sum_{i=1}^{d}\left(1-\cos\frac{2\pi n_i}{L}\right)\right]^{-1}\right\}\Bigg/\left(1-\frac{H^2}{\alpha^2}\right) \tag{20}$$

[2] The connection between the n-vector model in the $n \to \infty$ limit and the spherical model still holds with periodic boundary conditions.[11]

where

$$\alpha \equiv \mu - Jd \tag{21}$$

This equation defines $\alpha(T)$ implicitly, from which the thermodynamics can be obtained. For example

$$\begin{aligned}
&\text{Susceptibility} \qquad \chi(H=0) = 1/\alpha(T) \\
&\text{Correlation length} \qquad \xi(H=0) = 1/\sqrt{\alpha(T)} \\
&k\text{-space correlation function} \qquad \tilde{G}(k) = \beta^{-1}\left[\alpha + J\sum_1^d (1-\cos k_i)\right]^{-1}
\end{aligned} \tag{22}$$

all depend upon T through $\alpha(T)$.

In the infinite system, the sums in Eq. (20) are replaced by integrals. With $H=0$, Eq. (20) can be shown to be equivalent to[15]

$$\beta = \int_0^\infty e^{-\mu t}[I_0(Jt)]^d\, dt \tag{23}$$

by writing

$$\left[\alpha + J\sum_1^d\left(1-\cos\frac{2\pi n_i}{L}\right)\right]^{-1} = \int_0^\infty dt \exp\left\{-\left[\alpha + J\sum_1^d\left(1-\cos\frac{2\pi n_i}{L}\right)\right]t\right\} \tag{24}$$

The quantity $I_0(Jt)$ appearing in (23) is a modified Bessel function. A continuous phase transition occurs where $\alpha = 0$. Thus, T_c is defined by

$$\alpha(T_c) = 0 \tag{25}$$

Equation (23) can be expanded about the point $\alpha = 0$ in the following way. Write

$$\int_0^\infty e^{-\mu t}[I_0(Jt)]^d\, dt = \int_0^{K_0} e^{-\mu t} I_0^d(Jt)\, dt + \int_{K_0}^\infty e^{-\mu t} I_0^d(Jt)\, dt \tag{26}$$

where K_0 is large enough to use the asymptotic expansion[16] for $I_0(x)$

$$I_0(x) \sim e^x(2\pi x)^{-1/2} \qquad \text{as} \quad x \to \infty \tag{27}$$

Thus we can write

$$\beta = F(\alpha, K_0) + \left(\frac{1}{2\pi J}\right)^{d/2} \int_{K_0}^{\infty} e^{-\alpha t} t^{-d/2}\, dt \tag{28}$$

which defines $F(\alpha, k_0)$ as an analytic function of α. An asymptotic expansion for the second term of Eq. (28) can be derived by repeated integration by parts. Thus, for d in the range $2 < d < 4$, for example,

$$\int_{K_0}^{\infty} e^{-\alpha t} t^{-d/2}\, dt = \frac{2}{d-2} K_0^{(d-2)/2} - \frac{2}{d-2} \Gamma\left(\frac{4-d}{2}\right) \alpha^{(d-2)/2} + \text{taylor series in } \alpha \tag{29}$$

The only contribution to the integral that goes as a nonintegral power of α is the second term in the r.h.s. of Eq. (29). For small α, the constraint equation is, then

$$\beta = \beta_c - a\alpha^{(d-2)/2} + b\alpha + O(\alpha^2) \tag{30}$$

Inverting

$$\alpha \sim t^{-2/(d-2)} \tag{31}$$

From (31) the thermodynamics at $H = 0$ are

$$\begin{aligned} &\text{Susceptibility} && \chi \sim t^{-2/(d-2)} \\ &\text{Correlation function} && G(\mathbf{l}) = f(l^2)\, e^{-l^2 t^{1/(d-2)}} \\ &\text{Correlation length} && \xi \sim t^{-1/(d-2)} \end{aligned} \tag{32}$$

and the various critical exponents follow straightforwardly

$$\left(\nu = \frac{1}{d-2} \qquad \gamma = \frac{2}{d-2} \qquad \alpha = \frac{d-4}{d-2} \cdots\right)$$

3. THE FINITE SYSTEM

In a finite system, there are two complications to the picture described above. First, the position space correlation function $G(l)$ no longer decays monotonically. In fact, $G(l)$ has the periodicity of the lattice. Thus, $\sqrt{\alpha}$ is no longer a reasonable inverse correlation length. Consequently,

$$\xi^2 \equiv \frac{\sum_{\mathbf{l}} l^2 G(\mathbf{l})}{\sum_l G(\mathbf{l})} \tag{33}$$

is the expected definition of correlation length.

The above sum can be calculated. However, on a periodic lattice, l^2 should be replaced with a length function having the periodicity of the lattice. We propose replacing l^2 with

$$\frac{L^2}{2\pi^2}\left\{d-\left[\cos\left(\frac{2\pi l_1}{L}\right)+\cdots+\cos\left(\frac{2\pi l_d}{L}\right)\right]\right\} \tag{34}$$

in Eq. (33). This reduces to l^2 for $L \gg l$. Using this definition and Eq. (22) for the correlation function, an elementary calculation (see Appendix A for details) yields

$$\begin{aligned}\xi_L^2 &= \frac{dL^2}{2\pi^2}\left\{1-\frac{\alpha}{\alpha+J\left(1-\cos\dfrac{2\pi}{L}\right)}\right\}\\ &\sim \frac{dL^2 J}{\alpha L^2+2\pi^2 J} \quad \text{as} \quad L\to\infty\end{aligned} \tag{35}$$

for the mean spherical model.

The second complication is that the constraint equation (20) which must be inverted to obtain $\alpha(T)$ involves a sum rather than an integral. The sum in Eq. (20) cannot be performed analytically, as far as we know (except in one dimension). For small values of L it can be summed explicitly on a computer. For moderately large values of L the computation becomes prohibitive, because of the slow convergence of the sum; the terms decay only as fast as $1/k^2$ near the edge of the Brillouin zone. In fact, the sum is reminiscent of the slowly converging sums encountered in computing ionic crystal binding energies (Madelung constants). A variety of techniques have been developed to speed convergence of these sums, the technique developed by Ewald[17] being a highly successful one (see Ref. 18 for a general discussion of the method). In what follows we apply the Ewald technique to Eq. (20).

First, we write the sum as

$$\beta=\frac{1}{L^d}\sum_{n_1,\ldots,n_d}\int_0^\infty dt\,\exp\left\{-\left[\alpha+J\sum_1^d\left(1-\cos\frac{2\pi n_i}{L}\right)\right]t\right\} \tag{36}$$

Then we divide the integral over t into

$$\int_0^K dt+\int_K^\infty dt \tag{37}$$

where K is to be determined. Consider first the second term of Eq. (37).

For K sufficiently large, the sum over n_i converges rapidly, and so we can approximate the cos with its second order approximation, which yields

$$\frac{1}{L^d}\sum_{n_1,\ldots,n_d}\int_K^\infty dt\exp\left\{-\left[\alpha+\frac{J}{2}\sum_1^d\left(\frac{2\pi}{L}n_i\right)^2\right]t\right\} \tag{38}$$

Let $K=qL^2$, with q to be determined, and let

$$S(x)\equiv\sum_{n=-L/2}^{L/2}\exp(-n^2x) \tag{39}$$

Changing the variable of integration from t to $x=t/qL^2$

$$\frac{q}{L^{d-2}}\int_1^\infty dx\,e^{-\alpha qL^2x}\{[S(2\pi^2Jqx)]^d-1\}+\frac{e^{-\alpha qL^2}}{\alpha L^2} \tag{40}$$

where we have separated out the $n_i=n_2=\cdots=n_d=0$ term.

The remaining term in Eq. (37) can be handled with the Poisson sum formula[2]

$$\begin{aligned}\frac{1}{L^d}&\sum_{n_1,\ldots,n_d}\int_0^K\exp\left\{-\left[\alpha+J\sum_1^d\left(1-\cos\frac{2\pi n_i}{L}\right)\right]t\right\}dt\\&=\sum_{m_1,\ldots,m_d=-\infty}^{\infty}\left(\frac{1}{2\pi}\right)^d\int_{\substack{\text{Brillouin}\\ \text{zone}}}d^dk\\&\quad\times\int_0^K\exp\left\{-\left[\alpha+J\sum_1^d\left(1-\cos\frac{2\pi n_i}{L}\right)\right]t\right\}e^{i\mathbf{m}\cdot\mathbf{k}L}\,dt\end{aligned}$$

The $m\neq 0$ terms are damped in k by $e^{i\mathbf{m}\cdot\mathbf{k}L}$, so again the cos can be approximated. The $\mathbf{m}=0$ term can be integrated exactly. These two steps yield (again taking $K=qL^2$)

$$\begin{aligned}&\frac{1}{2^d}\left(\frac{1}{2\pi J}\right)^{d/2}q^{(2-d)/2}\frac{1}{L^{d-2}}\int_1^\infty e^{-\alpha qL^2/x}x^{(d-4)/2}\left\{\left[S\left(\frac{x}{2Jq}\right)\right]^d-1\right\}dx\\&\quad+\int_0^K I_0^d(Jt)\,e^{-\mu t}\,dt\end{aligned} \tag{42}$$

Putting this together

$$\beta=\int_0^K e^{-\mu t}I_0^d(Jt)\,dt+\frac{1}{L^{d-2}}f(\alpha L^2) \tag{43}$$

with

$$f(\alpha L^2) \equiv \frac{1}{\alpha L^2} e^{-\alpha L^2 q} + q \int_1^\infty e^{-\alpha L^2 qx} \{ [S(2\pi^2 Jqx)]^d - 1 \} \, dx$$
$$+ \frac{1}{2^d} \left(\frac{1}{2\pi J} \right)^{d/2} q^{(2-d)/2} \int_1^\infty e^{-\alpha L^2 q/x} x^{(d-4)/2} \left\{ \left[S\left(\frac{x}{2Jq} \right) \right]^d - 1 \right\} dx \tag{44}$$

The above equation was easily run on a computer (a VAX 780 at UCSC) and inverted to yield $\alpha_L(T)$. The sum $S(x)$ converges rapidly for q judiciously chosen, because x is no smaller than 1. Here q is chosen to be $(2\pi J)^{-1}$ to satisfy the balance between the convergence requirements of $S(2J\pi^2 qx)$ and $S(x/2Jq)$. Four terms of each sum were taken. The integrands are rapidly damped and so can be integrated easily using a Simpson's rule algorithm. The most difficult term computationally is

$$\int_0^K e^{-\mu t} I_0^d(Jt) \, dt \tag{45}$$

This was written

$$\int_0^{K_0} e^{-\mu t} I_0^d(Jt) \, dt + \int_{K_0}^K e^{-\mu t} I_0^d(Jt) \, dt \tag{46}$$

In the first integral, the approximation scheme of Abramowitz and Stegun was employed for the modified Bessel function (Ref. 16, p. 378, Eq. 9.8.1 and 9.8.2). The second term was treated analytically via the first term of the asymptotic expansion for $I_0(x)$, Eq. (27). Here K_0 was chosen to be 88 for somewhat machine dependent reasons. Since K must be greater than K_0, the minimum length is $L = (K/q)^{1/2}$, which is approximately 24. For $L < 24$ the sum in Eq. (20) was computed exactly.

The only approximation in Eq. (43) was in replacing the cosines in the integrals by a low order expansion in their arguments. Thus, the terms written there are only the leading terms in an asymptotic expansion. The next terms (or the leading corrections) can be derived in a standard manner. Both fall in the form

$$g(\alpha L^2)/L^d \tag{47}$$

4. IMPLICATIONS FOR FINITE SIZE SCALING

From Eq. (43) and (35) it is possible to see the expected features of finite size scaling emerge mathematically. The first can be written in the useful form

$$L^{d-2}[\beta - \beta_\infty(\alpha)] + L^{d-2} \int_K^\infty e^{-\mu t} I_0^d(Jt) \, dt = f(\alpha L^2) + \frac{g(\alpha L^2)}{L^2} \tag{48}$$

where β_∞ is the inverse temperature of the infinite system (Eq. (23)) and f and g are defined in Eq. (44) and (47). The scaling equation for the correlation length is found by expanding the cos in Eq. (35), yielding

$$\xi_L^2 = L^2 dJ\left[\frac{1}{\alpha L^2 + 2\pi^2 J}\right]\left[1 - O\left(\frac{1}{L^2}\right)\right] \tag{49}$$

To show that finite size scaling holds, it is sufficient to show that Eq. (48) takes the form

$$L^{d-2} t \equiv W(\alpha L^2) \tag{50}$$

with $W(x)$ some function. Then inverting will yield $1/\alpha$ equal to a function in the form $L^2 X(L^{1/\nu} t)$, and scaling of the susceptibility and correlation length will follow from their definitions (Eq. (22) and (49)).

To obtain the key result above, we use the methods of Section 2 to expand

$$\int_K^\infty e^{-\mu t} I_0^d(Jt)\, dt \tag{51}$$

the term in Eq. (48) which does not scale manifestly. We illustrate the method in detail for the case $2 < d < 4$; in all other dimensions one follows a similar procedure.

Let $K = qL^2$ with $q = (2\pi J)^{-1}$ as above. Using the symptotic expansion for $I_0(x)$ (Eq. (27)) and integrating by parts yields

$$\begin{aligned}\int_K^\infty e^{-\mu t} I_0^d(Jt)\, dt = q^{d/2} \Bigg\{ & \frac{2}{d-2} e^{-\alpha q L^2} (qL^2)^{(2-d)/2} \\ & - \frac{2}{d-2} \Gamma\left(\frac{4-d}{2}\right) \alpha^{(d-2)/2} \\ & + \frac{2}{d-2} \sum_{n=0}^\infty \frac{2(-1)^n \alpha^{n+1}}{n!(2n+4-d)} (qL^2)^{n+2-d/2} \Bigg\}\end{aligned} \tag{52}$$

In Section 2 we saw that

$$\beta_\infty(\alpha) = \beta_c - a\alpha^{(d-2)/2} + b\alpha + \cdots \tag{53}$$

Note that the nonanalytic terms must cancel, since $\int_0^K e^{-\mu t} I_0^d(Jt)\, dt$ is an analytic function of α for finite L ($K \propto L^2$ which is finite). We find for the constraint equation

$$\begin{aligned}L^{d-2}(\beta - \beta_\infty) = {} & f(\alpha L^2) + \frac{1}{L^2} g(\alpha L^2) + h(\alpha L^2) \\ & + \frac{b\alpha L^2}{L^{4-d}} + \frac{c(\alpha L^2)^2}{L^{6-d}} + L^{d-2} O\left(\frac{\alpha L^2}{L^2}\right)^3\end{aligned} \tag{54}$$

with

$$h(\alpha L^2) = \frac{2}{d-2} q \left(\sum_{n=0}^{\infty} \frac{2(-1)^n}{n!} \frac{(\alpha L^2 q)^{n+1}}{2n+4-d} + e^{-\alpha L^2 q} \right) \tag{55}$$

Now, $f(\alpha L^2)$ (defined in Eq. (44)) has an expansion of the form

$$f(\alpha L^2) = \frac{1}{\alpha L^2} + A_1 + A_2 \alpha L^2 + A_3 (\alpha L^2)^2 + \cdots \tag{56}$$

With A_i's determined numerically through Eq. (44). The terms in Eq. (54) which are independent of (αL^2) will generate a temperature shift. Equation (50) is realized as

$$L^{d-2} \left\{ -\frac{1}{T} [t - \varepsilon(L)] \right\} = W(\alpha L^2) + \frac{b \alpha L^2}{L^{4-d}} + \frac{g(\alpha L^2)}{L^2} + \cdots \tag{57}$$

With

$$\varepsilon(L) = T \left(A_1 - \frac{2}{d-2} q \right) L^{2-d} \tag{58}$$

and

$$W(\alpha L^2) = h(\alpha L^2) + f(\alpha L^2) - L^{d-2} \varepsilon(L) \tag{59}$$

The shifted temperature is

$$\tilde{t} = t - \varepsilon(L) = t - T_c \left(A_1 - \frac{2}{d-2} q \right) L^{2-d} \tag{60}$$

where the shift goes like $L^{-1/\nu}$, in accord with standard finite size scaling conjectures. The dominant correction term is $b\, \alpha L^2 / L^{4-d}$, which is proportional to the parameter which multiples the bulk correction, b, and scales as predicted by corrections to finite size scaling (Eq. (7)).

Numerically, it is found that

$$f(\alpha L^2) \simeq \frac{e^{-\alpha L^2 q}}{\alpha L^2} \tag{61}$$

is a good approximation to the first few terms of the expansion of $f(\alpha L^2)$. Under this approximation

$$\varepsilon(L) \sim \frac{d}{d-2} \frac{T_c q}{L^{d-2}} \tag{62}$$

and

$$W(\alpha L^2) \cong \frac{1}{\alpha L^2} - \frac{1}{d-2}\left(\frac{4}{4-d}\right) q^2 \alpha L^2 + \cdots \tag{63}$$

Using similar methods it is possible to generate an expansion in the region where αL^2 is large. The result is

$$\beta_L = \beta_\infty + \frac{e^{-\alpha L^2 q}}{L^{d-2}} \left[\frac{1}{\alpha L^2} - \frac{2}{d-2} + O(\alpha L^2)\right] \tag{64}$$

In this region, the convergence to infinite behavior is exponentially fast, a well-known result.[11]

The discussion from here on will be divided into various dimensions.

(a) $2<d<4$

To see that Eq. (54) is the expected scaling form for the susceptibility, consider that in the infinite system Eq. (53) implies the following for the susceptibility

$$\chi_\infty \sim t^{-\gamma}[1 - O(t^p)] \tag{65}$$

with $\gamma = 2/(d-2)$, $p = (4-d)/(d-2)$, and $\nu = 1/(d-2)$. It follows from Eq. (7) that the expected from is

$$\chi_L = L^2 X(\tilde{t} L^{d-2}) + L^{d-2} Y(\tilde{t} L^{d-2}) \tag{66}$$

Indeed, inverting Eq. (54) yields precisely this, asymptotically.

The correlation length also scales as predicted, with corrections occurring asymptotically from the bulk. A phenomenological renormalization experiment (PR) would find ξ_L/L as shown in Figs. 1 and 2. These functions cross for various L at $t = \varepsilon(L)$. It can be seen that for this system in this dimensional regime PR experiments provide good evidence for a phase transition and approximations to the exponents. We also add that expansion yields an approximate form for the scaling function

$$X(x) \cong \frac{q^2(8-d)}{(4-d)} \left[x + \left(x^2 + \frac{2q^2(8-d)}{4-d}\right)^{1/2}\right]^{-1} \tag{67}$$

This holds in the finite size region and in the low temperature phase, where

$$\chi_L \sim \frac{L^d}{T} [\varepsilon(L) + |t|] \tag{68}$$

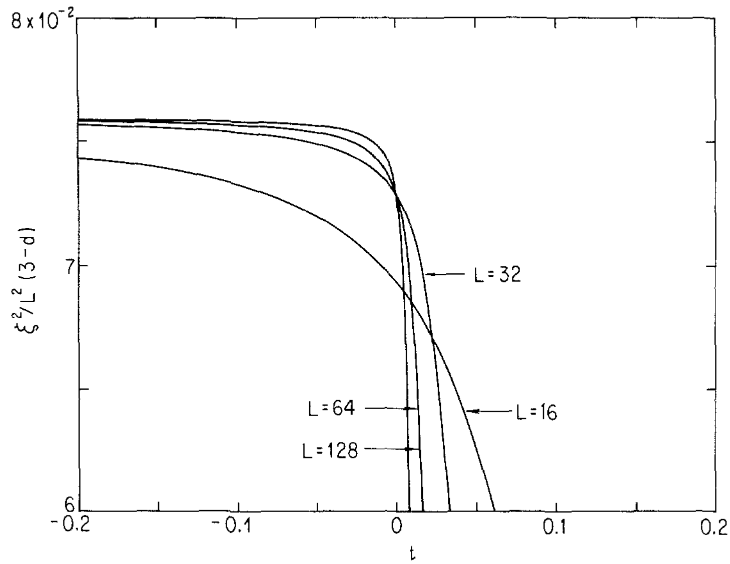


Fig. 1. Results of a PR experiment (ξ^2/L^2 vs. t) for $d=3$. Curves cross at $t=\varepsilon(L)$, which is indistinguishable from $t=0$ for $L \geqslant 32$. Curves are calculated as described in Section 3.

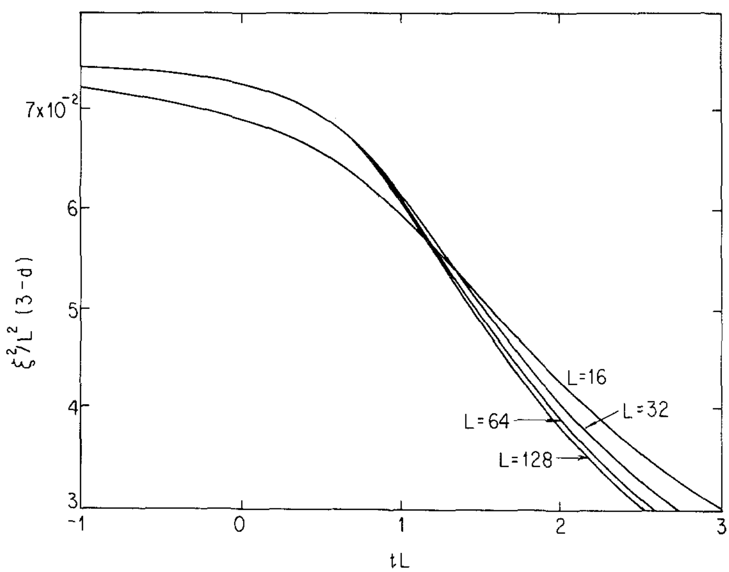


Fig. 2. ξ^2/L^2 vs. $tL^{1/\nu}$ for three-dimensional spherical model ($1/\nu=1$). Finite size scaling predicts that these curves collapse in the scaling region, which they do for $L \geqslant 32$.

As dimension four is approached, the scaling function diverges, as does the leading correction term. The reason can be seen in Eq. (54). As the upper critical dimension is crossed, the finite size scaling term and the dominant correction term exchange roles. At $d=4$ they have combined to produce logarithmic dependence.

$$L^{d-2}\tilde{t}=\frac{1}{\alpha L^2}-\frac{qd}{2(4-d)}\alpha L^2+\frac{qd}{2(4-d)}\alpha L_0^{4-d}L^{d-2}+\cdots$$

$$\rightarrow\frac{1}{\alpha L^2}-\frac{qd}{\alpha}L^2\ln(L/L_0)\qquad \text{as}\quad d\rightarrow 4 \tag{69}$$

(See Eq. (29) for origin of $L_0^2=K_0/q$).

Similarly as dimension two is approached, divergences occur in the shift, the scaling function, and corrections. The divergence of the shift combines with the divergence of β_c to produce logarithms. The scaling function and correction divergences combine to produce finite terms as well.

(b) $d\leqslant 2$

It is interesting to consider the above analysis for $d\leqslant 2$, the lower critical dimension. This is relevant to applications of finite size scaling to the question of whether a system undergoes a phase transition. In this region, there is a critical transition at $T=0$ in both the infinite and finite systems. The expected behavior is crossover from $\chi_L\sim L^dT^{-1}$ in the finite system, to $\chi\sim T^{-2/(d-2)}$ (or $\chi\sim e^{2/T}$ for $d=2$) in the infinite system. Crossover scaling has been discussed by Fisher,[1] see also Ref. 11. The correlation length diverges at $T=0$ in the infinite system, but is bounded by L in the finite system.

We first consider d strictly less than 2. In this case

$$\beta_\infty(\alpha)\sim a\alpha^{(d-2)/2}+\beta_0+b\alpha+\cdots \tag{70}$$

Similar analysis to the above yields the scaling equation

$$\frac{L^{2-d}}{T}=f(\alpha L^2)+h(\alpha L^2)+\frac{\beta_0}{L^{2-d}}+\frac{g(\alpha L^2)}{L^2} \tag{71}$$

where

$$h(\alpha L^2)=-q\sum_{n=0}^{\infty}\frac{(-1)^n q^{n+1}(\alpha L^2)^n}{n!(2n-d+2)} \tag{72}$$

Evidently, $\varepsilon(L)=0$ and the corrections are $g(\alpha L^2)/L^2$ from the RHS of

(71), and β_0/L^{2-d} from corrections to bulk scaling. Again, the bulk correction dominates. Thus, the susceptibility takes the crossover scaling form

$$\chi_L = L^2 X(TL^{2-d}) + L^d Y(TL^{2-d}) \tag{73}$$

This is as predicted because the infinite susceptibility takes the form

$$\chi_\infty \sim \left(\frac{1}{T}\right)^{2/(d-2)} [1 + O(T)] \tag{74}$$

Expanding $f(\alpha L^2)$ to get the scaling functions yields

$$\xi^2/L^2 \sim \frac{d}{2\pi^2}\left[1 - \frac{L^{2-d}T}{2J\pi^2}\right] \tag{75}$$

Thus, PR experiments would show clearly the transition at $T=0$ (the only intersection point of Eq. (75) for varying L) and converge to the correct exponent. This is shown in Fig. 3.

Two is the lower critical dimensionality. Here the infinite model exhibits essential singularities in the thermodynamics at $T=0$

$$\xi_\infty \sim e^{1/T} \tag{76}$$

$$\chi_\infty \sim e^{2/T} \tag{77}$$

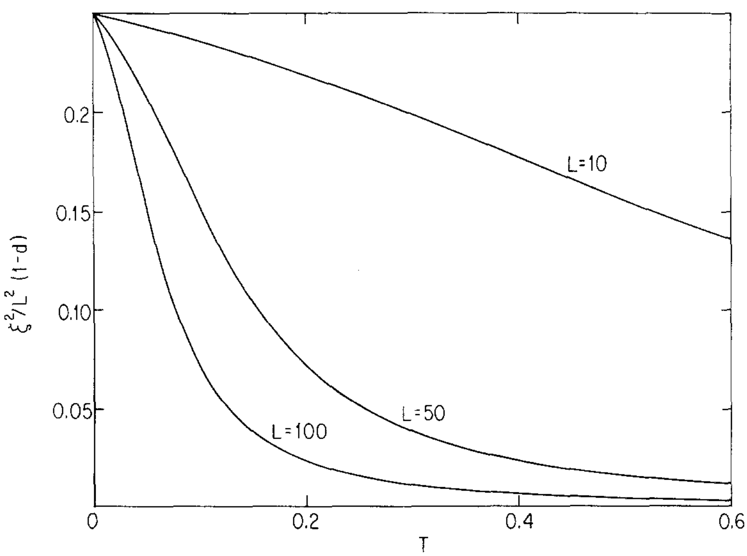


Fig. 3. Results of a PR experiment for $d=1$ spherical model. The transition at $T=0$ is clearly shown by the intersection of these curves at that point.

The finite model constraint equation takes the form

$$\frac{1}{T} - q\ln(qL^2) + b + c\alpha + O(d^2) = h(\alpha L^2) + f(\alpha L^2) + \frac{g(\alpha L^2)}{L^2} \tag{78}$$

with

$$h(\alpha L^2) = \sum_{n=1}^{\infty} \frac{(-1)^n (\alpha L^2 q)^n}{n \cdot n!} \tag{79}$$

We see that a logarithmic term makes reduction to the pure power law scaling form like Eq. (73) impossible. This can be seen clearly by inverting Eq. (78) to yield

$$\chi_L(T) = L^2 X\left(\frac{T}{1 - AT\ln L^2}\right) \tag{80}$$

and

$$\xi_L^2/L^2 = Y\left(\frac{T}{1 - AT\ln L^2}\right) \tag{81}$$

with ξ_L as defined in (35), and A a constant. Expanding $f(\alpha L^2)$ yields, in the low-temperature limit

$$L^2\alpha \simeq \frac{T}{1 - AT\ln L^2} \tag{82}$$

and

$$\xi_L^2/L^2 \sim \frac{1}{\pi^2}\left[1 - \frac{1}{\pi^2}(T + AT^2 \ln L^2)\right] \tag{83}$$

The functions ξ^2/L^2 do not cross; they collapse (Fig. 4). The scaling function is $1 - T$, which is consistent with $\nu = \infty$. The width of the finite size scaling region is also consistent with $\nu = \infty$, but the combination makes reduction to Eq. (75) impossible.

The reason for our failure to achieve the scaling form is clear. Derivation of this form assumes power law singularities, whereas the 2-d spherical model exhibits essential singularities. It is possible to generalize finite size scaling to include both types of singularities. The expected general scaling forms are[12,8]

$$\xi_L/L = Y(\xi_\infty/L) \tag{84}$$

$$\chi_L = \chi_\infty(T)\, Z(\xi_\infty/L) \tag{85}$$

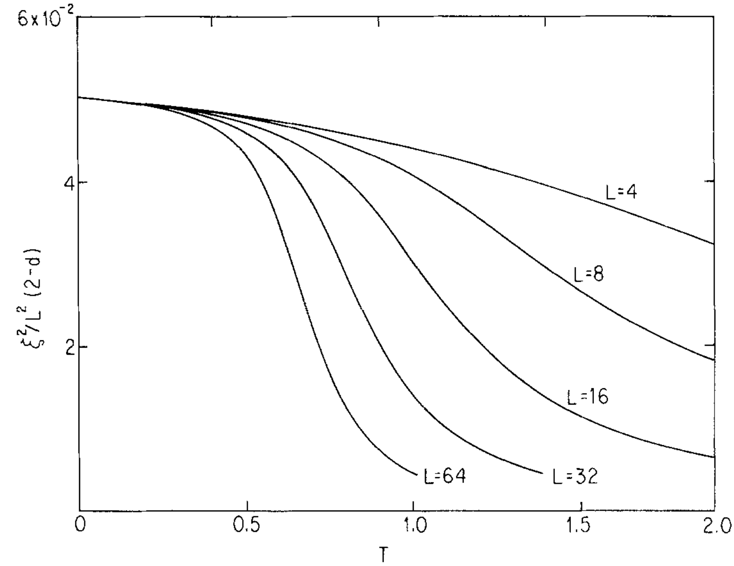


Fig. 4. Results of a PR experiment for $d = 2$ spherical model. Curves do not cross at the critical point; they collapse as the critical point is approached. Collapse is onto a linear function $(1 - aT)$.

Equations (80) and (81) fall precisely in this form (using $\xi_\infty^2 = \chi_\infty$ in Eq. (80)).

It is reasonable to ask whether this picture of the scaling of the two-dimensional spherical model is generic to critical transitions at the lower critical dimensionality. If it is, this is extremely relevant to PR studies of other systems at their lower critical dimensionality. (Examples are Ref. 19 where finite size scaling is applied to the determination of the lower critical dimension of the random field Ising model, and Monte Carlo studies of certain lattice gauge theories in four dimensions which are believed to behave like two-dimensional spin systems.[20] See also Ref. 25, which discusses the $O(2)$ Heisenberg model in $1+1$ dimension.) To address this question we consider the periodic one-dimensional Ising model, one being its lower critical dimensionality. A simple calculation on the one-dimensional Ising model yields (see Ref. 21, p. 138 for the correlation function of the finite model)

$$\chi_{L(\text{ising})} \simeq \frac{2L}{T}\left\{2 - \exp\left[-\left(\frac{2 - T\ln L}{T}\right)\right]\right\} \tag{86}$$

$$\xi^2_{L(\text{ising})} = L^2\left[(\ln\tanh\beta J)^2 + \left(\frac{2\pi}{L}\right)^2\right]^{-1} \tag{87}$$

(We have again used Eq. (35) as our definition of ξ_L.)

The following conclusions hold for both models:

1. Correlation lengths of both scale like

$$\xi_L/L = Y(\xi_\infty/L) \tag{88}$$

Thus, both exhibit apparent collapse of ξ_L/L for various L (shown in Fig. 5 for the Ising model). The asymptotic forms are
Ising

$$\xi_L^2/L^2 \cong 1 - L^2/\xi_\infty^2 \tag{89}$$

Spherical

$$\xi_L^2/L^2 \cong 1 - \frac{1}{\ln(\xi_\infty/L)} \tag{90}$$

2. The susceptibilities of both scale like

$$\chi_L = \chi_\infty(T)\, Z(\xi_\infty/L) \tag{91}$$

The asymptotic forms are
Ising

$$\chi_L \cong \frac{L}{T}[1 - L/\xi_\infty] \tag{92}$$

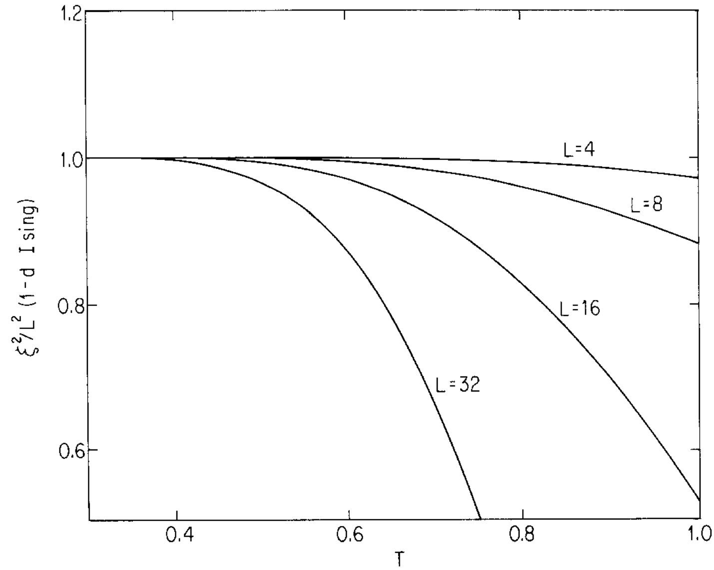


Fig. 5. Same as Fig. 4 for one-dimensional Ising model. Curves again show collapse, in this case onto a constant function.

Spherical

$$\chi_L \cong L^2 \ln(\xi_\infty / L^2) \tag{93}$$

The way in which Eqs. (92) and (93) satisfy Eq. (81) involves the various relationships between ξ_∞ and χ_∞

$$\chi_{\infty\ \text{spherical}} = \xi^2_{\infty\ \text{spherical}} \tag{94}$$

$$\chi_{\infty\ \text{ising}} = \frac{1}{T} \xi_{\infty\ \text{ising}} \tag{95}$$

Analyzing data using Eq. (91) will not in general be easy since χ_∞ is generally unknown. It would therefore be useful to be able to predict a simpler form, like (92) or (93). To do this requires knowledge of the precise relation between χ_∞ and ξ_∞. If, for example

$$\chi_\infty = T^p \xi_\infty^g \tag{96}$$

then scaling can be simplified to the useful form

$$\chi_L = L^g T^p W(\xi_\infty / L)$$

(c) $d \geqslant 4$

We shall first consider $d > 4$. For $4 < d < 6$, the infinite system satisfies

$$\beta_\infty(\alpha) = \beta_c - a\alpha + b\alpha^{(d-2)/2} + \cdots \tag{97}$$

The constraint equation is

$$\frac{-L^{d-2}}{T}[t - \varepsilon(L)] = f(\alpha L^2) + h(\alpha L^2) - L^{\alpha-2}\alpha a + \frac{g(\alpha L^2)}{L^2} + L^{d-2}O(\alpha^2) \tag{98}$$

Here

$$\varepsilon(L) = \frac{qT}{L^{d-2}}$$

$$h(\alpha L^2) = \left\{ \frac{2}{d-2} q[e^{-\alpha q L^2} - 1] - \frac{4q^{(d+2)/2}}{(d-2)(d-4)} e^{-\alpha L^2 q} \alpha L^2 - \frac{4}{(d-2)(d-4)} \sum_{n=0}^{\infty} \frac{(-1)^n (\alpha L^2 q)^{n+2}}{n!(n+3-d/2)} \right\} \tag{99}$$

It would appear that this violates scaling, as argued by Brezin[2]. For example

$$\chi_L(\tilde{t}=0) \sim aL^{d/2} \tag{100}$$

rather than like L^2 as expected. However, this also falls in the scaling form

$$\frac{-L^2}{T}\tilde{t} = -a\alpha L^2 + \frac{f(\alpha L^2) + h(\alpha L^2)}{L^{d-4}} \tag{101}$$

This is exactly the expected form

$$L^2\tilde{t} = W(\alpha L^2) + \frac{Z(\alpha L^2)}{L^{d-4}} \tag{102}$$

with

$$W(\alpha L^2) = a\alpha L^2 \tag{103}$$

and the correction term

$$Z(\alpha L^2) = -f(\alpha L^2) - h(\alpha L^2) \tag{104}$$

The shift is

$$\varepsilon(L) = \frac{T_c q}{L^{d-2}} \tag{105}$$

which now vanishes faster than the width of the finite size region, which vanishes like $1/L^2$.

The origin of the discrepancy between the two results (Eq. (102) and (98)) is that the correction term has a pole at $\alpha = 0$. Thus, although it becomes asymptotically small as $L \to \infty$ for fixed α, it diverges as $\alpha \to 0$

$$Z(\alpha L^2) \sim -\frac{1}{\alpha L^2} \qquad \text{as} \quad \alpha L^2 \to 0 \tag{106}$$

We see that the correction can only be ignored if $\alpha > 1/L^{d-2}$. The conclusion is that the predicted scaling form holds only for $t > \varepsilon(L)$. In a small region above Tc finite size scaling fails in the manner discovered by Brezin. This is illustrated in Fig. 6 and 7.

The nonanalyticity of the correction function provides the clue to the explanation of this behavior—the scaling is controlled by the presence of a dangerous irrelevant variable. A variable u is called a dangerous irrelevant variable if it is irrelevant in the RG sense (i.e., u flows to a fixed point of

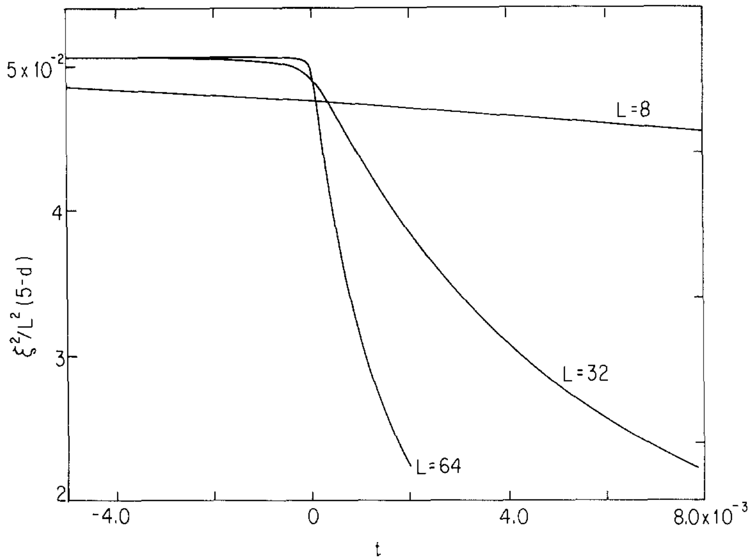


Fig. 6. PR experiment for $d=5$ spherical model. Curves cross at $t=\varepsilon(L)$.

zero under action of RG), but the scaling functions are not analytic functions of u near the fixed point of u. For example, consider the scaling equation of the susceptibility

$$\chi_\infty(t, u) = b^{\gamma/\nu} X(tb^{1/\nu}, ub^{y}) \tag{107}$$

and assume that the fixed point is

$$t = u = 0 \tag{108}$$

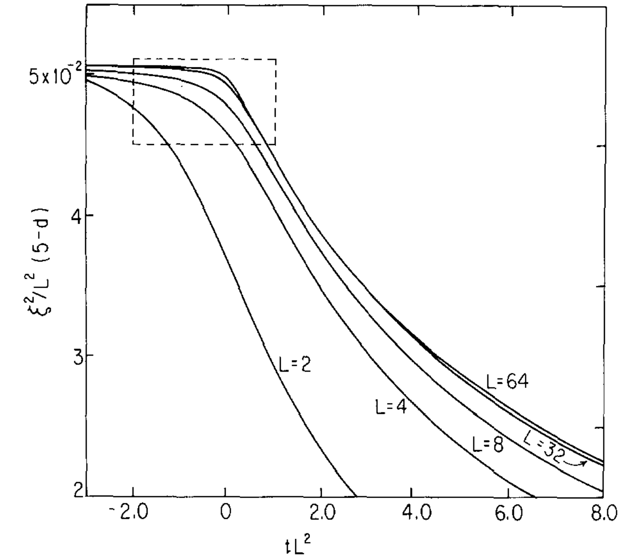
u is irrelevant so $y<0$. If the scaling function has the property that near the fixed point it is not analytic in u, say

$$X(x, y) \to \frac{W(x)}{\sqrt{y}} \quad \text{as} \quad \begin{matrix} x\to 0 \\ y \to 0 \end{matrix} \tag{109}$$

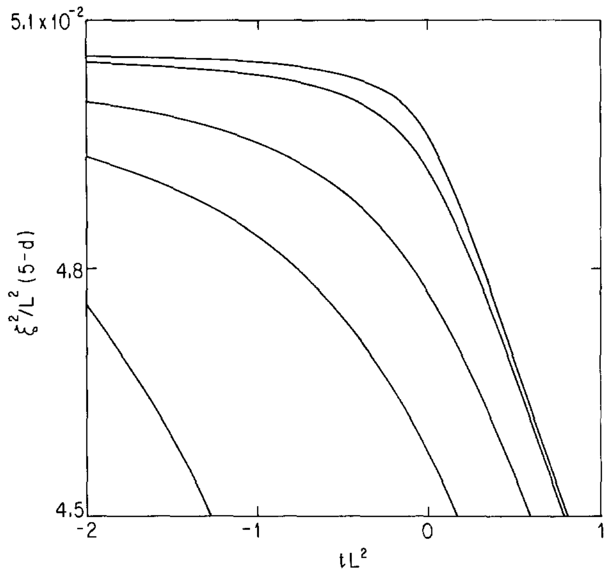
then u is called a dangerous variable. Note that away from the fixed point X can be analytic in u

$$X(1, y) = X(1, 0) + yX_y(1, 0) + \cdots \tag{110}$$

These variables provide the accepted mechanism of the failure of hyperscaling above the upper critical dimension of general critical systems (see Ref. 15 for an explanation of how that works). Since hyperscaling fails for



(a)



(b)

Fig. 7. (a) ξ^2/L^2 vs. $tL^{1/\nu}$ for $d=5$ spherical model. Shift is no longer $\propto L^{1/\nu}$, so the scaled curves appear shifted. Except for the shift, the curves scale in a region not too close to $t=0$, but fail to scale close to $t=0$ (dashed box). (b) Nonscaling region of Fig. 7a (dashed box) enlarged.

the spherical model in more than four dimensions, a dangerous irrelevant variable must be involved. To see how this would affect the finite size scaling, assume that the scaling ansatz equation (5) holds, but u is now dángerous. Then not too close to criticality, $\tilde{t}L^{1/\nu} \sim 1$, Eq. (7) holds and

$$\chi_L(t) = L^{\gamma/\nu} X(\tilde{t}L^{1/\nu}) + L^{(\gamma - p)/\nu} Y(\tilde{t}L^{1/\nu}) \tag{111}$$

However, as $L^{1/\nu}\tilde{t} = 0$ is approached, Eq. (109) holds and the scaling form is

$$\chi_L(t) = \frac{L^{\gamma/\nu} W(\tilde{t}L^{1/\nu})}{L^{y/2}\sqrt{u}} \tag{112}$$

This is precisely the behavior described above for the spherical model in more than four dimensions. In fact, if we introduce a u into the spherical model by rewriting the constraint equation

$$L^2\tilde{t} = a\alpha L^2 - \frac{uL^{4-d}}{\alpha L^2} \tag{113}$$

then u is a very reasonable choice for our irrelevant variable because: (1) corrections are proportional to u; (2) u scales as uL^{4-d}; (3) $u = 0$ reproduces the Gaussian model result of a classical phase transition even in a finite system.

(In appendix B we show how to introduce a u into the spherical model rigorously with the same result). The equation for the susceptibility

$$\chi_L = L^2 \left\{ \frac{1}{L^2\tilde{t}} \left[\frac{2}{1 + \left(1 + \dfrac{4uL^{4-d}}{(\tilde{t}L^2)^2}\right)^{1/2}} \right] \right\} \tag{114}$$

has precisely the properties described above. Thus, we claim that it is not finite size scaling that fails above the upper critical dimension, but hyperscaling.

An infinite system above the upper critical dimension is known to exhibit mean field critical behavior. We now address the question of whether that is true for the finite system as well. It has been argued by Brezin[2] that it is not true, because mean field theory shows no finite size effects. The Gaussian model shows no finite size effects, but the definition of mean field theory appropriate to this question is the theory which predicts the behavior of ϕ^4 theory, namely that defined by the free energy[22]

$$F(t, h, u) \equiv L^{-d} \ln \int_{-\infty}^{\infty} d\psi \exp\{-L^d[t\psi^2 - h\psi + u\psi^4]\} \tag{115}$$

For L infinite, this yields conventional mean field theory. For finite L, we dub this theory rounded mean field theory (RMF), because it exhibits finite rounding. RMF predicts both the scaling form of the spherical model, Eq. (102), and the dangerous irrelevant variable structure, Eq. (112). Near the critical point, the susceptibility of RMF is

$$\chi_L(t \sim 0) \sim \frac{L^{d/2}}{\sqrt{u}} - \frac{L^d t}{u} \tag{116}$$

identical to that of the spherical model obtained by expanding Eq. (114) for small $\tilde{t}$.

For $d = 4$, mean field theory must be renormalized to produce the correct results of Ginzburg–Landau–Wilson theory, as is well known from RG theory.[23] Renormalizing RMF theory yields

$$\begin{aligned} F &= L^{-4} \ln \int d\psi \exp\{-L^4[(t\psi^2 + u\psi^4)\,\omega^{-1}(L) - h\psi]\} \\ &= L^{-4} E(tL^2\omega(L)^{-1/2}, hL^3\omega(L)^{1/4}) \end{aligned} \tag{117}$$

where

$$\omega(L) = \frac{1}{1 + A \ln L} \tag{118}$$

This form follows from a standard development of the free energy of a four-dimensional system.[23] It holds only in the finite size regime. Taking two derivatives with respect to h we obtain when $h = 0$,

$$\chi_L = -\frac{1}{L^4} \frac{\partial^2 E}{\partial h^2}\bigg|_{h=0} = L^2\omega^{1/2}E(0, 0) + L^4 t E_1(0, 0) + \cdots \tag{119}$$

The constraint equation of the finite spherical model is

$$L^2\left[-t/T + \frac{\varepsilon(L)}{T}\right] = -\alpha L^2 \ln L^2 + f(\alpha L^2) + h(\alpha L^2) + \cdots \tag{120}$$

$$\begin{aligned} \varepsilon(L) &= Tcg/L^2 \\ h(\alpha L^2) &= q^2 \left\{ \gamma\alpha L^2 - b\alpha L^2 + \alpha L^2 \ln q^2 \right. \\ &\quad \left. + \frac{1}{q}\,[e^{-\alpha L^2 q} - 1] - \sum_{n=0}^{\infty} \frac{(-1)^n(\alpha L^2 q)^{n+1}}{n \cdot n!} \right\} \\ \gamma &= \text{constant} \end{aligned} \tag{121}$$

Expanding for the susceptibility as before,

$$\chi_L = L^2(\ln L^2)^{1/2} - L^4\tilde{t} \tag{122}$$

This is identical to the RMF result. Thus, mean field theory does predict the finite size behavior of the spherical model. (We also note that the generalized scaling forms for the $d=2$ system hold for the $d=4$ system as well.)

In Brezin's study of the finite spherical model,[2] he concludes the model indicates that it is not possible to compute the universal scaling functions from an epsilon expansion. His reasons are that mean field theory does not represent the limiting theory as it exhibits no finite size effects, and that the scaling functions are singular as epsilon approaches zero. However, we have shown that RMF theory does represent the correct theory in the limit d goes to d_u. The question remains, does the singularity of the scaling function present any difficulty in performing an epsilon expansion. It is clear that it does not. Note that although the scaling function for the susceptibility $d<4$

$$\chi_L(t) = L^2 X(L^{1/\nu}\tilde{t}\, 0) = \frac{L^2 qd}{\varepsilon}\left[L^{1/\nu}\tilde{t} + \left((L^{1/\nu}\tilde{t})^2 + \frac{4qd}{2\varepsilon}\right)^{1/2}\right]^{-1} \tag{123}$$

is singular in epsilon, $X(L^{1/\nu}\tilde{t}, u)$ is not, as we have seen (see Eq. (69)). This is because the expansion about $u=0$ becomes ill behaved at $d=4$, because u is becoming a dangerous irrelevant variable. It is no different in the infinite system. Here the susceptibility is

$$\chi_\infty(t) = \left[\frac{2}{d-2}\Gamma\left(\frac{4-d}{2}\right)\right]^{2/(d-2)} t^{-2/(d-2)} \tag{124}$$

This is also singular in epsilon. No one would assert that an epsilon expansion cannot be used to evaluate the scaling functions in the infinite spherical model, because it can. In fact, in ϕ^4 theory u also becomes a dangerous irrelevant variable as epsilon goes to zero, so the same picture is reproduced there, as is well known. Therefore, there is nothing in the results of the finite spherical model which suggests that an epsilon expansion cannot be used to investigate a finite system.

5. SUMMARY

We have shown that the Ewald sum technique provides a method of studying the fully finite spherical model which facilitates both numerical and analytic study. Numerically, there are no restrictions on the values of

L, T, or H that can be reached. Analytically, expansions can be generated both away from criticality and in the finite size scaling region. The numerical results were applied to produce graphs of the correlation length in all dimensions less than six. The analytic results were used to study the form of finite size scaling. We have shown that finite size scaling holds in all dimensions except two and four. In two dimensions a universal form for the modified scaling form was proposed. In four dimensions the scaling was that predicted by renormalized mean field theory. In more than four dimensions, the scaling is dictated by the presence of a dangerous irrelevant variable, and is precisely that predicted by mean field theory. Thus, the possibility of performing an epsilon expansion cannot be ruled out.

ACKNOWLEDGMENTS

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APPENDIX A

In this section we describe how to perform the sum

$$\xi^2/L^2 = \frac{1}{2\pi^2}\left[d - \frac{\sum_l \sum_{i=1}^{d} \cos\left(\frac{2\pi}{L} l_i\right) G(l)}{\sum_l G(l)}\right] \tag{A.1}$$

The methods involved are elementary, but it is a somewhat tedious computation.

First consider the sum

$$\sum_l \sum_{i=1}^{d} \cos\left(\frac{2\pi}{L} l_i\right) G(l)$$

$$= \sum_l \sum_{i=1}^{d} \cos\left(\frac{2\pi}{L} l_i\right) \sum_{n_1,\ldots,n_d} \frac{\cos\left[\frac{2\pi}{L}(n_1 l_1 + \cdots + n_d l_d)\right]}{\beta L^d\left[\alpha + J\sum_{j=1}^{d}\left(1 - \cos\frac{2\pi n_j}{L}\right)\right]} \tag{A.2}$$

Expanding $\cos((2\pi/L)\sum_1^d n_i l_i)$ via trigonometric identities results in the identity

$$\cos\left(\frac{2\pi}{L}\sum_{i=1}^{d} n_i l_i\right)=\prod_{i=1}^{d} c_i-\sum_{\substack{i,j=1\\ i<j}}^{d} s_i s_j \prod_{k\neq i,j}^{d} c_k + \sum_{\substack{i,j,k,l\\ i<j<k<l}}^{d} s_i s_j s_k s_l \prod_{m\neq i,j,k,l}^{d} c_m+\cdots \tag{A.3}$$

where we have defined

$$c_i\equiv\cos\left(\frac{2\pi}{L}l_i n_i\right)$$
$$s_i\equiv\sin\left(\frac{2\pi}{L}l_i n_i\right) \tag{A.4}$$

The series in (A.3) terminates at $\prod_{i=1}^{d} s_i$ for d even and $(-1)^{(d-1)/2}\sum_{i_1,\dots,i_{d-1},i_1<i_2\cdots<i_{d-1}} s_{i_1}\cdots s_{i_{d-1}}c_{i_d}$ for d odd.

The sum on l of all the terms with sines will be zero by the identity

$$\sum_{l=1}^{L}\sin\left(\frac{2\pi}{L}ln\right)=0 \tag{A.5}$$

The remaining term,

$$\sum_{l_1,\dots,l_d=1}^{L}\sum_{i=1}^{d}\cos\left(\frac{2\pi}{L}l_i\right)\sum_{n,\dots,n_d}\frac{\cos\left(\frac{2\pi}{L}n_1 l_i\right)\cdots\cos\left(\frac{2\pi}{L}n_d l_d\right)}{\beta L^d\left[\alpha+J\sum_1^d\left(1-\cos\frac{2\pi}{L}n_i\right)\right]} \tag{A.6}$$

can be summed on l via the identities:

$$\sum_{l=1}^{L}\cos\left(\frac{2\pi ln}{L}\right)=L\delta_{n,0}$$
$$\sum_{l=1}^{L}\cos\left(\frac{2\pi ln}{L}\right)\cos\left(\frac{2\pi l}{L}\right)=\frac{L}{2}(\delta_{n,1}+\delta_{n,L-1}) \tag{A.7}$$

Thus, (A.6) reduces to

$$\frac{1}{\beta L^d}\sum_{n_1,\dots,n_j}\sum_{j=1}^{d}\frac{L}{2}(\delta_{n_j,1}+\delta_{n_j,L-1})\prod_{i\neq j}^{d}L\delta_{n_i,0}\left[\alpha+J\sum_{k=1}^{d}\left(1-\cos\frac{2\pi n_k}{L}\right)\right]^{-1}$$
$$=\frac{d}{\beta\left[\alpha+J\left(1-\cos\frac{2\pi}{L}\right)\right]} \tag{A.8}$$

The final sum can be shown to be

$$\sum_{l=1}^{L} G(l) = \frac{1}{\beta\alpha} \tag{A.9}$$

by methods above. Together, this yields the desired result

$$\xi^2 = \frac{dL^2}{2\pi^2}\left[1 - \frac{\alpha}{\alpha + J\left(1 - \cos\frac{2\pi}{L}\right)}\right] \tag{A.10}$$

APPENDIX B

In this Appendix we show how the spherical model can be modified to accommodate an adjustable variable u. This variable will play the same role as u in ϕ^4 theory: in more than four dimensions u will be a dangerous irrelevant variable, and in less than four dimensions $u - u^*$ will be the leading irrelevant variable, with u^* nonzero. In RG theory, this variable governs the size of the critical region. Since the size of the critical region of the spherical model is finite, such a variable must exist. Our modified model will be identical to the spherical model for some value of u, but will allow u to vary.

The modification is threefold. First, we introduce a Gaussian damping term into the partition function. In the absence of a spherical constraint the new partition function is

$$\int \exp\left[\beta J {\sum}' \sigma_i \sigma_j - \omega \sum_i \sigma_i^2\right] \prod_i d\sigma_i \tag{B.1}$$

where the sum $\sum'$ is over nearest neighbor pairs. This Gaussian model partition function is singular when the temperature T is such that

$$\beta_c J d = \omega \tag{B.2}$$

where $\beta_c = 1/kT_c$, and d equals the spatial dimensionality of the system. When $T < T_c$ the partition function (B.1) is undefined. The purpose of this first modification is to keep the transition temperature finite, even in the absence of spherical constraint.

Our next step is to introduce the *soft* spherical constraint

$$\left(\frac{u}{\pi N}\right)^{1/2} e^{-(u/N)(\sum_i \sigma_i^2 - N)^2} \tag{B.3}$$

In the limit $u=\infty$ this factor becomes a delta function and the strict spherical model constraint is recovered. As the variable u goes to zero the constraint disappears and our model is once again a pure Gaussian model. It seems clear now, and we will establish shortly, that this latter limit is singular. Our softening of the spherical constraint parallels closely Wilson's softening of the spin-by-spin constraint in fixed-length spin models to derive the Ginsburg–Landau–Wilson effective Hamiltonian as a description of the Ising system.[23]

The partition function of our soft-constraint spherical model is

$$
\begin{aligned}
Z_u &= \left(\frac{u}{\pi N}\right)^{1/2} \int \exp\left[\beta J \sum{}' \sigma_i \sigma_j - \omega \sum \sigma_i^2 - \frac{u}{N}(\sigma_i^2 - N)^2\right] \prod_i d\sigma_i \\
&= \int_{-i\infty}^{i\infty} d\lambda \int \prod_i dJ_i \exp\left[\beta J \sum{}' \sigma_i \sigma_j - \omega \sum \sigma_i^2 - \lambda\left(\sum \sigma_i^2 - N\right) + \frac{\lambda^2 N}{4u}\right]
\end{aligned} \tag{B.4}
$$

The new variable λ, introduced by means of an identity on Gaussian integrals, will play a key role in the analysis to follow.

For fixed λ the integration over the spin variables, σ_i, is carried out by going over to their spatial fourier transforms, $s(q)$. Carrying out this transformation and integrating over the values of $s(q)$, we are left with the following single integral for the partition function

$$
Z_u = \int_{-i\infty}^{i\infty} \exp\left[-\frac{1}{2}\sum_g \ln\left(\lambda + \omega - \beta J \sum_i \cos g_i\right) + \lambda N + \frac{\lambda^2 N}{4u}\right] d\lambda \tag{B.5}
$$

The integral over λ can be carried out by the method of steepest descents. We replace the integral by the integrand with λ taking on the value at which it satisfied the extremum equation

$$
\frac{d}{d\lambda}\left[\frac{1}{2}\sum_g \ln\left(\lambda + \omega - \beta J \sum_i \cos g_i\right) + \lambda N - \frac{N\lambda^2}{4u}\right] = 0
$$

or

$$
\lambda = u\left[\frac{1}{N}\sum_g \frac{1}{\lambda + \omega - \beta J d + \beta J \sum (1 - \cos g_i)} - 2\right] \tag{B.6}
$$

Our final modification of the spherical model is to take this steepest descents result as yielding the exact partition function, even when N, the number of degrees of freedom, is finite. Thus, we are looking at a mean, softened constraint, spherical model.

From this point on the analysis proceeds straightforwardly. In more than four dimensions we can neglect all contributions to the sum in (B.6) except the $\mathbf{q}=0$ one. The extremum equation is,

$$\lambda=\frac{u}{N[\lambda+\omega-\beta Jd]} \tag{B.7}$$

where the subtraction in the square brackets has also been neglected. Writing $\lambda+w-\beta Jd\equiv\alpha$ we have

$$\alpha-\omega+\beta Jd=\frac{u}{\alpha}L^{-d} \tag{B.8}$$

Defining ΔT via

$$\beta=\frac{1}{K(T_c+\Delta T)} \tag{B.9}$$

We have, neglecting terms of order ΔT^2,

$$\alpha-\frac{Jd}{KT^2}\Delta T-\frac{uL^{-d}}{\alpha}=0$$

which when multiplied by L^2 yields

$$\alpha L^2-\frac{Jd}{KT_c^2}(\Delta TL^2)-\frac{uL^{4-d}}{\alpha L^2}=0 \tag{B.10}$$

which, except for scale factors and some modification of notation, is identical to constraint equation (113) in the text.

REFERENCES

1. M. E. Fisher, in *Critical Phenomena*, Proc. 51st Enrico Fermi Summer School, Varena, M. S. Green, ed. (Academic Press, New York, 1972).
2. E. Brezin, *J. Physique* **43**:15 (1982).
3. V. Privman and M. E. Fisher, *J. Phys. A* **16**:L295 (1983).
4. M. P. Nightingale, *Physica* **83A**:561 (1976).
5. M. P. Nightingale, *J. Appl. Phys.* **53**:7927 (1982).
6. V. Privman, *Physica* **123A**:428 (1984).
7. M. N. Barber and M. E. Fisher, *Ann. Phys.* **77**:1 (1973).
8. E. Brezin, *Ann. N.Y. Acad. Phys.* **410**:339 (1983).
9. S. Singh and R. K. Pathria, *Phys. Rev.* **B31**:4483 (1985).
10. J. Rudnick, H. Guo, and D. Jasnow, *J. Stat. Phys.* **41**:353 (1985).
11. M. N. Barber, in *Phase Transitions and Critical Phenomena*, Vol. 8, C. Domb and J. L. Lebowitz, eds. (Academic Press, New York, 1983).

12. J. M. Luck, *Phys. Rev.* **B31**:3069 (1985).
13. M. E. Fisher and V. Privman, *Phys. Rev.* **B37**:447 (1985).
14. G. S. Joyce, in *Phase Transitions and Critical Phenomena*, Vol. 2, C. Domb and M. S. Green, eds. (Academic Press, New York, 1972).
15. M. E. Fisher, in *Critical Phenomena*, Proc. of Summer School at University of Stellenbosch, South Africa, F. J. W. Hayne, ed. (Springer-Verlag, Berlin, 1983).
16. M. Abramowitz and I. Stegun, *Handbook of Mathematical Functions* (National Bureau of Standards, 1964), P. 378 Eqs. (9.8.1) and (9.8.2).
17. P. P. Ewald, *Ann. Phys. (4)* **64**:253 (1921).
18. M. P. Tosi, in *Solid State Physics*, Vol. 16, F. Seitz and D. Turnbull, eds. (Academic Press, New York) 1964.
19. L. Jacobs and M. Nauenberg, *Physica A* **128A**:529 (1984).
20. M. Creutz, *Quarks, Gluons and Lattices* (Cambridge University Press, London, 1983), Chap. 17.
21. C. J. Thompson, *Mathematical Statistical Mechanics* (Princeton University Press, Princeton, 1972).
22. K. Binder, M. Nauenberg, V. Privman, and A. P. Young, *Phys. Rev.* **B31**:1498 (1985).
23. K. Wilson and J. Kogut, *Phys. Rep.* **12**:75 (1974).
24. H. W. J. Blote and M. P. Nightingale, *Physica* **112A**:405 (1981).
25. C. J. Hamer and M. N. Barber, *J. Phys. A* **14**:259 (1981).