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Critical Behavior of a Spherical Model with a Free Surface

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Critical phenomena in d-dimensional ferromagnetic spherical models on hypercubic lattices with free surfaces are studied. The surface specific heat and surface susceptibilities are obtained. The exponents characterizing the divergence of these surface quantities at the bulk critical temperature are found to satisfy recently proposed scaling relations. The variation of the susceptibility with distance from the surface is also discussed. The author's recent scaling theory for surface properties is investigated in detail, and found to give an exact representation for the free energy of a three-dimensional spherical model of finite thickness in finite bulk and surface magnetic fields. A scaling form for the surface free energy is derived.

KEY WORDS: Critical phenomena; spherical model; surface properties; scaling.

1. INTRODUCTION

The effect of a free surface on the critical behavior of magnetic systems has been discussed recently by several authors.[1–11] In the presence of a surface it is necessary to introduce[1–4] several new exponents to characterize the behavior of the surface thermodynamic properties in the critical region. Many of these "surface" exponents have been determined either analy-

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tically[5-7] or from exact series expansions[1,3,8,9] for several models and within mean-field theory.[3,10]

Attempts have also been made[1-4] to develop systematic scaling theories for surface critical phenomena based on general concepts. These arguments yield new scaling laws, which relate the various surface exponents to each other and/or the standard bulk exponents. These scaling relations are well satisfied[3,4] within mean-field theory and by the exponents of the two-dimensional Ising model, many of which are known exactly.[5,6] For the three-dimensional Ising model the exponents are only available through the numerical extrapolation of exact series expansions.[1,3,9] However, the available evidence appears to confirm the scaling predictions.[9,11] For more "realistic" magnetic models, such as the Heisenberg model, the available data[8] are so limited that no definite conclusions can yet be drawn. Since bulk scaling[12] appears to be valid for such models, one would also hope that surface scaling is also applicable to the Heisenberg model and ultimately to real magnetic systems, where the experimental investigation of surface effects is in its infancy.[13]

In this paper we extend an earlier analysis[7] of finite-size and surface effects on the critical behavior of the spherical model,[14] to discuss the response to a magnetic field applied locally to the surface. Aspects of this problem have been discussed for the Ising model in two dimensions by McCoy and Wu[5],[3] and, more recently, in three dimensions by Binder and Hohenberg[3] and Barber.[9] Our aim will be twofold; first, to calculate, for their own intrinsic interest, various surface properties of the spherical model, and second, to investigate the validity of scaling. We will show that for the spherical model it is in fact possible to analytically demonstrate the correctness of the scaling hypotheses and to calculate the appropriate scaling functions.

Our arguments are arranged as follows. In Section 2 we review the basic results of the earlier analysis[7] and extend the formulation to include a surface field. The surface specific heat is calculated in Section 3. In Section 4 we discuss the response of a spin in the surface layer to (a) the bulk magnetic field and (b) the surface field. Section 5 contains a similar discussion for an internal layer. In particular, we obtain the variation in the susceptibility as a function of distance from the surface. Sections 6–8 contain the discussion of scaling for the spherical model. A concluding summary is given in Section 9.

2. FORMULATION AND REVIEW OF BASIC RESULTS

As in the earlier work[7] (hereafter referred to as BF), we consider d-dimensional spherical models with nearest-neighbor ferromagnetic inter-

[3] Some of the results of this work were obtained independently in Ref. 6.

actions (of strength $J > 0$) on a hypercubic lattice. We suppose the lattice of spins is infinite in d' ($= d - 1$) dimensions ($d' \geqslant 2$) but finite with n "layers" in the dth dimension, the first and nth layers forming free surfaces, i.e., they each have only one neighboring layer. This geometry will be referred to as a *d'-dimensional, n-layer system*, with, in the terminology of BF, free edge boundary conditions. In the limit $n \to \infty$ we obtain a semi-infinite half-space as considered by Binder and Hohenberg[3] for the Ising model with $d = 3$. All spins are assumed to interact with a bulk magnetic field H, while spins in the first layer experience an additional surface field H_1.

Following the analysis of Sections 2 and 3 of BF, the free energy per spin of this system may be written as

$$F_d(T, h, h_1, n) = \tfrac{1}{2}k_B T \ln K + \frac{k_B T}{2n} \sum_{r=0}^{n-1} L_{d-1}(\phi + \Omega_r) - \frac{1}{4nJ} \sum_{r=0}^{n-1} \frac{[\epsilon_r(h, h_1)]^2}{\phi + \Omega_r} \quad (1)$$

where

$$L_d(z) = \int_0^{2\pi} \frac{d\theta_1}{2\pi} \cdots \int_0^{2\pi} \frac{d\theta_d}{2\pi} \ln\left[z + 2 \sum_{j=1}^{d} (1 - \cos \theta_j)\right] \quad (2)$$

$$\Omega_r = 4 \sin^2[\pi(r + 1)/(2n + 2)] - 4 \sin^2[\pi/(2n + 2)] \quad (3)$$

$$\epsilon_r(h, h_1) = [2/(n + 1)]^{1/2} \sum_{j=1}^{n} (h + h_1 \delta_{j,1}) \sin[\pi(r + 1)j/(n + 1)] \quad (4)$$

where $\delta_{j,k}$ is the Kronecker delta, and we have introduced the reduced variables

$$K = J/k_B T, \qquad h = mH, \qquad \text{and} \qquad h_1 = mH_1 \quad (5)$$

where T is the absolute temperature, k_B is Boltzmann's constant, and m is the magnetic moment per spin. Finally, the reduced spherical field ϕ is determined by the *spherical constraint*

$$(\partial F_d / \partial J\phi)_{T,h,h_1} = 1 \quad (6)$$

The sum in (4) is elementary and yields

$$\epsilon_r(h, h_1) = [2/(n + 1)]^{1/2}\{h_1 \sin[\pi(r + 1)/(n + 1)] + \alpha_r h \cot[\pi(r + 1)/(2n + 2)]\} \quad (7)$$

where

$$\begin{aligned} \alpha_r &= 0 \qquad r \ \text{odd} \\ &= 1 \qquad r \ \text{even} \end{aligned} \quad (8)$$

If we take the limit $n \to \infty$ in (1), we obtain the bulk free energy per spin,

$$F_d(T, h) = \tfrac{1}{2}k_B T \ln K + \tfrac{1}{2}k_B T L_d(\phi) - (h^2/4J\phi) \quad (9)$$

with ϕ determined by

$$W_d(\phi) = 2K[1 - (h^2/4J^2\phi^2)] \quad (10)$$

where

$$W_d(z) = L_d'(z) = \frac{d}{dz} L_d(z) = \frac{1}{(2\pi)^d} \int_0^{2\pi} \cdots \int_0^{2\pi} \frac{d\theta_1 \cdots d\theta_d}{z + 2 \sum_{j=1}^{d} (1 - \cos \theta_j)} \tag{11}$$

is the generalized Watson function of order d. The bulk thermodynamic properties now follow from (9) by the standard relations.[7,11,12] In particular, the bulk zero-field susceptibility per spin is given by

$$\chi_d(T) = \tfrac{1}{2}[J\phi_0(T)]^{-1} \tag{12}$$

with $\phi_0(T)$ determined by (10) with $h = 0$, namely

$$2K = W_d(\phi_0) \tag{13}$$

The bulk d-dimensional critical temperature $T_{c,d}$ is thus determined by

$$\phi_0(T_{c,d}) = 0 \tag{14}$$

or explicitly from (13) by

$$K_{c,d} = \frac{1}{2} W_d(0) = \frac{1}{4} \int_0^{2\pi} \frac{d\theta_1}{2\pi} \cdots \int_0^{2\pi} \frac{d\theta_d}{2\pi} \left[\sum_{j=1}^{d} (1 - \cos \theta_j) \right]^{-1} \tag{15}$$

where the integral is finite for $d \geqslant 3$.

We will also require the behavior of $\phi_0(T)$ as T approaches $T_{c,d}$ from above. The behavior of the functions $W_d(z)$ for small z was investigated in detail by BF (BF, Appendix A). The leading asymptotic behavior is summarized in Table I.

If we write

$$\Delta K = K_{c,d} - K \propto T - T_{c,d} \tag{16}$$

Table I. Expansions of Generalized Watson Functions $W_d(z)$

d	$W_d(z)$
1	$\frac{1}{2}z^{-1/2} - (z^{1/2}/16) + (3z^{3/2}/256) + O(z^{5/2})$
2	$[(\ln z^{-1})/4\pi] + [(5 \ln 2)/4\pi] + [(z \ln z^{-1})/32\pi]$ $+ [z(1 - 5 \ln 2)/32\pi] + O(z^2 \ln z)$
3	$W_3(0) - (z^{1/2}/4\pi) + O(z)$
4	$W_4(0) + [z(\ln z)/16\pi^2] + (C_4 z/16\pi^2) + O(z^2 \ln z)$
5	$W_5(0) + zW_5'(0) + (z^{3/2}/24\pi^2) + O(z^2)$
⋮	
$2k - 1$	$\sum_{r=0}^{k-2} [z^r W_{2k-1}^{(r)}(0)/r!] + [\Gamma(\frac{3}{2} - k) z^{k-(3/2)}/(4\pi)^{k-(1/2)}] + O(z^{k-1})$
$2k$	$\sum_{r=0}^{k-2} [z^r W_{2k}^{(r)}(0)/r!] + [(-)^k z^{k-1}(\ln z + C_{2k})/(4\pi)^k(k-1)!] + O(z^k \ln z)$

we find from Table I that as $\Delta K \to 0^+$,

$$\begin{aligned} \phi_0(T) &= 64\pi^2(\Delta K)^2 + O(\Delta K^3) && \text{for } d = 3 \\ &= 32\pi^2(\Delta K)/\ln(\Delta K^{-1}) + O[\Delta K/(\ln K)^{-2}] && \text{for } d = 4 \\ &= -2(\Delta K)/W_d'(0) + O[(\Delta K)^2] && \text{for } d \geqslant 5 \end{aligned} \tag{17}$$

On the other hand, for finite n, ϕ is determined in zero-field by

$$2K = (1/n) \sum_{r=0}^{n-1} W_{d-1}(\phi + \Omega_r) \tag{18}$$

For $d > 3$ this result with $\phi = 0$ determines the critical temperature $T_{c,d}(n)$ of the finite-layer system. However, when we consider the solution of (18) for $\phi \neq 0$ and $n \gg 1$ two limits must be distinguished[7]: (i) $n \to \infty$ with T above $T_{c,d}$ and fixed; and (ii) $n \to \infty$ with T in the critical region. In the first limit, corresponding to $n \to \infty$ with ϕ_0 a positive constant, we find [BF, Eq. (8.26)]

$$\phi(n, T) = \phi_0(T) - [W_d{}^\times(\phi_0)/W_d'(\phi_0)n] + O(n^{-2}) \tag{19}$$

with

$$W_d{}^\times(z) = W_d(z) - \tfrac{1}{2}W_{d-1}(z) - \tfrac{1}{2}W_{d-1}(z + 4) \tag{20}$$

In the other limit of interest we find[7]

$$\phi(n, T) = x/n^2 \tag{21}$$

with $x = x(n, T)$ determined by (see BF, Section 7.2)

$$8\pi n \, \Delta\dot{K} = \ln[\sinh(x - \pi^2)^{1/2}/(x - \pi^2)^{1/2}] + O(n^{-1}) \qquad \text{for } d = 3 \tag{22}$$

$$16\pi^2 n^2 \, \Delta\dot{K} = x \ln n + H_4{}^1(x) + O(n^{-1}) \qquad \text{for } d = 4 \tag{23}$$

and for $d \geqslant 5$

$$2n^2 \, \Delta\dot{K} = -W_d'(0)x + O(n^{-1}) \tag{24}$$

In these formulas the shifted temperature derivations are defined for all d by

$$\Delta\dot{K} = \Delta K + K_{c,d}\epsilon_d(n) \tag{25}$$

where $\epsilon_d(n)$ is the fractional shift. In three dimensions (see BF, Section 7.2)

$$\epsilon_3(n) = -[(\ln n)/8\pi K_{c,3}n] + \tfrac{1}{2}[W_3(0) - \tfrac{1}{2}W_2(4) - 7(\ln 2/8\pi)]/nK_{c,3} \tag{26a}$$

while for $d \geqslant 4$, $\epsilon_d(n)$ varies for large n as

$$\epsilon_d(n) \approx -|W_d{}^\times(0)/W_d(0)|n^{-1} + O(n^{-2}) \tag{26b}$$

that is, the shift exponent[1] λ is unity. The function $H_4{}^1(x)$ appearing in (23) is rather complex and is given in Table V of BF. For our present purposes it will be sufficient to note that

$$H_4^1(x) \approx -\tfrac{1}{2}x \ln x \qquad \text{as} \quad x \to \infty \tag{27}$$

$$H_4^1(x) \approx 2\pi x^{1/2} \qquad \text{as} \quad x \to 0 \tag{28}$$

For $d = 3$ and $d \geqslant 5$ we may invert (22) and (24) and express the scaled field x as a function of a single scaled temperature variable $n^{1/\nu}\,\Delta\dot{K}$, namely

$$x = \Phi(n^{1/\nu}\,\Delta\dot{K}) \tag{29}$$

where ν is the bulk correlation length exponent, which has the values[14]

$$\nu = 1 \quad (d = 3), \qquad \nu = \tfrac{1}{2}(\log)^{1/2} \quad (d = 4), \qquad \nu = \tfrac{1}{2} \quad (d \geqslant 5) \tag{30}$$

On the other hand, for $d = 4$ such a scaled representation is only valid if we drop the term $H_4^1(x)$ in (23). However, in view of (27) and (28) this term actually dominates in the limits $x \to \infty$ and $x \to 0$, both of which are of physical importance.

This completes our review of the results obtained by Barber and Fisher for spherical model layer systems. These results together with (1) for the free energy in the presence of a surface field form the basis of our present discussion of surface properties. We consider first the surface specific heat.

3. SURFACE SPECIFIC HEAT

From (1) the specific heat of an n-layer spherical model is given in zero field by

$$C_d(n, T) = -T\,\partial^2 F_d(T, 0, 0, n)/\partial T^2 = \tfrac{1}{2}k_B - J\,d\phi(n, T)/dT \tag{31}$$

In the limit $n \to \infty$ we recover the bulk specific heat [see BF, Eq. (2.16)],

$$C_d(T)/k_B = \tfrac{1}{2} + K^2\,d\phi_0/dK \tag{32}$$

where $\phi_0 = \phi_0(T)$ is, as usual, the solution of (18). In the critical region we find from (17) that as $\Delta K \to 0^+$

$$\begin{aligned} C_d(T) - \tfrac{1}{2} &= -128\pi^2 K_{c,3}^2\,\Delta K + O(\Delta K^2) && \text{for} \quad d = 3 \\ &= -32\pi^2 K_{c,4}^2/\ln(\Delta K^{-1}) + O[(\ln \Delta K)^{-2}] && \text{for} \quad d = 4 \\ &\to 2K_{c,d}^2/W_d'(0) && \text{for} \quad d \geqslant 5 \end{aligned} \tag{33}$$

where in the last expression the leading correction is $O(\Delta K^{1/2})$ for $d = 5$ and $O(\Delta K)$ for $d > 5$. On the other hand, for $T < T_{c,d}$

$$\phi_0 \equiv 0 \tag{34}$$

and hence

$$C_d(T)/k_B = \tfrac{1}{2} \qquad \text{all} \quad d, \quad T < T_{c,d} \tag{35}$$

From these results we observe that at $T_{c,d}$ (i) $C_3(T)$ is continuous, but dC_3/dT has a finite jump discontinuity; (ii) $C_4(T)$ is continuous, but dC_4/dT

diverges as

$$dC_4(T)/dT \sim \Delta K^{-1}/(\ln \Delta K)^2 \tag{36}$$

as $\Delta K \to 0^+$, and is zero beneath $T_{c,d}$; and (iii) $C_d(T)$ for $d \geqslant 5$ is discontinuous. This behavior may be characterized by the standard[12] critical exponent α with the values[14]

$$\alpha = -1 \quad (d = 3), \qquad \alpha = 0(\text{disc.}) \quad (d \geqslant 4) \tag{37}$$

with an additional logarithmic factor in four dimensions.[4]

The surface specific heat $C_d^{\times}(T)$ is defined by[1]

$$C_d^{\times}(T) = \tfrac{1}{2} \lim_{n \to \infty} n[C_d(n, T) - C_d(T)] \tag{38}$$

Thus, on substituting (19) in (31), we find

$$C_d^{\times}(T)/k_B = -\tfrac{1}{2}K^2(d\phi_0/dK)\{W_d^{\times\prime}(\phi_0)W_d'(\phi_0) - W_d^{\times}(\phi_0)W_d''(\phi_0)/[W_d'(\phi_0)]^2\} \tag{39}$$

where $W_d^{\times}(\phi_0)$ is defined in (20). For ϕ_0 small, that is, near $T_{c,d}$, the functions appearing in this expression for $C_d^{\times}(T)$ can be expanded (see Table I). Hence, on substituting (17) we obtain, for $\Delta K \to 0^+$,

$$C_d^{\times}(T)/k_B K_{c,d}^2 = 8\pi \ln(\Delta K^{-1}) + O(1) \qquad \text{for} \quad d = 3 \tag{40}$$

$$= \frac{8\pi^2 W_4(0)}{\Delta K[\ln(\Delta K)^{-1}]^2} + O[\Delta K^{-1/2}(\ln \Delta K^{-1})^{-3/2}] \qquad \text{for} \quad d = 4 \tag{41}$$

$$= \frac{-W_5^{\times}(0)}{32\sqrt{2}\pi^2[-W_5'(0)]^{5/2}}(\Delta K)^{-1/2} + O(\ln \Delta K) \qquad \text{for} \quad d = 5 \tag{42}$$

$$= \frac{-W_6^{\times}(0)}{[W_6'(0)]^3(4\pi)^3} \ln \Delta K + O(1) \qquad \text{for} \quad d = 6 \tag{43}$$

and for $d \geqslant 7$

$$C_d^{\times}(T)/k_B \to -\tfrac{1}{2}K_{c,d}^2[W_d^{\times\prime}(0)W_d'(0) - W_d^{\times}(0)W_d''(0)]/[W_d'(0)]^3 \tag{44}$$

as $T \to T_{c,d^+}$, where the corrections are $O(\Delta K^{1/2})$ for $d = 7$ and $O(\Delta K)$ for $d > 7$. On the other hand, for $T < T_{c,d}$, since $\phi \equiv 0$, $C_d^{\times}(T)$ vanishes identically for all d. From these results we find for the exponent $\alpha^{\times}$ the values

$$\alpha^{\times} = 0(\log) \quad (d = 3), \qquad \alpha^{\times} = 1 \quad (d = 4), \qquad \alpha^{\times} = \tfrac{1}{2} \quad (d = 5)$$
$$\alpha^{\times} = 0(\log) \quad (d = 6), \qquad \alpha^{\times} = 0(\text{disc.}) \quad (d \geqslant 7) \tag{45}$$

with, again, additional logarithmic factors in four dimensions.

[4] As is customary (see Ref. 12) we denote a discontinuity by $\alpha = 0(\text{disc})$ and a logarithmic divergence by $\alpha = 0(\log)$.

At first sight these exponent values appear to be in disagreement with the scaling theory of finite-size effects,[1] which predicts

$$\alpha^{\times} = \alpha + 1 \tag{46}$$

for the spherical model, since the shift exponent is unity. This conclusion is only verified for $d = 3$ and $d = 4$. However, this theory applies only to the singular part of the specific heat. A closer inspection of the expansions of (32) and (39) for $d \geqslant 5$ indicates that the singular part of the bulk specific varies as (for $k \geqslant 3$)

$$\begin{aligned} C_{d,s}(T) &\sim (\Delta K)^{k-(5/2)} \qquad \text{for} \quad d = 2k - 1 \\ &\sim (\Delta K)^{k-2} \ln \Delta K \qquad \text{for} \quad d = 2k \end{aligned} \tag{47}$$

while the singular part of the surface specific heat varies as

$$\begin{aligned} C^{\times}_{d,s}(T) &\sim (\Delta K)^{k-(7/2)} \qquad \text{for} \quad d = 2k - 1 \\ &\sim (\Delta K)^{k-3} \ln \Delta K \qquad \text{for} \quad d = 2k \end{aligned} \tag{48}$$

in accord with the scaling predication (46).

The temperature dependence (40) of $C_3{}^{\times}(T)$ could have been anticipated from an earlier calculation[15] of the surface specific heat of an ideal boson film, since the critical behavior of the spherical model and ideal Bose gases are essentially equivalent.[16] As for the boson film, we observe that the amplitude of the divergence of $C_3{}^{\times}(T)$ is positive, and hence the total specific heat for finite n is *enhanced* above the bulk value. Since $W_d{}^{\times}(0)$ and $W_d{}'(0)$ are, in general, negative, a similar conclusion applies in all dimensions. This anomalous behavior is related to the enhancement of the critical temperature, which occurs for finite n and $d > 3$ with free edge boundary conditions.[7] Both these effects are a consequence of the effect of the boundary conditions on the constraint field. A detailed discussion of these phenomena has been given elsewhere (see Refs. 1, 7, and 15), and we will not consider them further here.

4. SUSCEPTIBILITIES AT THE SURFACE

In the presence of a surface field, as well as a bulk magnetic field, three susceptibilities should be distinguished.[3] In zero field ($h = h_1 = 0$) they may be defined for an n-layer system by

$$\chi(n, T) = -[\partial^2 F/\partial h^2]_{h=h_1=0} \tag{49}$$

$$\chi_1(n, T) = -[\partial^2 F/\partial h_1 \, \partial h]_{h=h_1=0} \tag{50}$$

$$\chi_{1,1}(n, T) = -[\partial^2 F/\partial h_1{}^2]_{h=h_1=0} \tag{51}$$

The first, $\chi(n, T)$, measures the response of the system as a whole to a bulk magnetic field. In the limit $n \to \infty$, at fixed T away from T_c, $\chi(n, T)$ approaches the zero-field bulk susceptibility $\chi(T)$ as[1,2]

$$\chi(n, T) \approx \chi(T) + (2/n)\chi^{\times}(T) + \cdots \tag{52}$$

where the surface susceptibility $\chi^{\times}(T)$ diverges at the bulk critical temperature T_c with an exponent $\gamma^{\times}$. For the spherical model $\chi^{\times}(T)$ and thus its exponent $\gamma^{\times}$ were obtained by Barber and Fisher[7] (BF, Section 8.3).

On the other hand, $\chi_1(n, T)$ and $\chi_{1,1}(n, T)$ are local susceptibilities measuring the response of a surface spin to, respectively, a bulk magnetic field and a surface field. Since both are intrinsically surface quantities, we expect that

$$\chi_1(n, T) \approx \chi_1(T)/n + \cdots \tag{53}$$

$$\chi_{1,1}(n, T) \approx \chi_{1,1}(T)/n + \cdots \tag{54}$$

as $n \to \infty$ with T fixed and not equal to T_c. These relations define the *surface layer susceptibility* $\chi_1(T)$ and the *local surface susceptibility* $\chi_{1,1}(T)$, where we have adopted the terminology of Binder and Hohenberg.[3] At T_c both, in general, can be expected[3] to diverge with exponents γ_1 and $\gamma_{1,1}$, respectively. In this section we calculate $\chi_1(T)$ and $\chi_{1,1}(T)$ for the spherical model.

Substituting (7) in (1) and differentiating gives

$$J\chi_1(n, T) = \frac{2}{n(n+1)} \sum_{s=0}^{[1/2n-1/2]} \frac{\cos^2[\pi(2s+1)/(2n+2)]}{\phi + \Omega_{2s}} \tag{55}$$

and

$$J\chi_{1,1}(n, T) = \frac{1}{n(n+1)} \sum_{r=0}^{n-1} \frac{\sin^2[\pi(r+1)/(n+1)]}{\phi + \Omega_r} \tag{56}$$

where $[x]$ denotes the integer part of x, and ϕ is determined by (18). Both the summations appearing in these expressions are of order n. Hence, on converting the sums to integrals and recalling (19), we find

$$J\chi_1(T) = \frac{2}{\pi} \int_0^{\pi/2} \frac{\cos^2\theta \, d\theta}{\phi_0 + 4\sin^2\theta} \tag{57}$$

and

$$J\chi_{1,1}(T) = \frac{2}{\pi} \int_0^{\pi/2} \frac{\sin^2 2\theta \, d\theta}{\phi_0 + 4\sin^2\theta} \tag{58}$$

where ϕ_0 is the solution of the bulk spherical constraint (14). Both integrals may easily be transformed to standard integrals,[17] to give

$$J\chi_1(T) = -\tfrac{1}{4} + \tfrac{1}{4}\phi_0^{-1/2}(\phi_0 + 4)^{1/2} \tag{59}$$

$$= \tfrac{1}{2}\phi_0^{-1/2} + O(1) \qquad \text{as} \quad \phi_0 \to 0 \tag{60}$$

and

$$J\chi_{1,1}(T) = \tfrac{1}{2} + \tfrac{1}{4}\phi_0 - \tfrac{1}{4}\phi_0^{1/2}(\phi_0 + 4)^{1/2} \tag{61}$$

$$= \tfrac{1}{2}(1 - \phi_0^{1/2}) + O(\phi_0), \qquad \phi_0 \to 0 \tag{62}$$

The expressions (59) and (61) for $\chi_1(T)$ and $\chi_{1,1}(T)$ are illustrated graphically for $d = 3$ as a function of T/T_c in Fig. 1. For comparison we also plot the bulk susceptibility (13) and the surface susceptibility $\chi^\times(T)$ given by [BF, Eq. (8.27)]

$$J\chi^\times(T) = \phi_0^{-2}[W_d^\times(\phi_0)/4W_d'(\phi_0)] + \tfrac{1}{4}\phi_0^{-1} - \tfrac{1}{4}\phi_0^{-1}(\phi_0 + 4)^{-3/2} \tag{63}$$

where $W_d^\times(z)$ is defined in (20). In plotting these curves we have used the tabular data of Mannari and Kawabata[18] to evaluate $W_3(\phi_0)$ and $W_3'(\phi_0)$.

The layer susceptibility $\chi_1(T)$ is clearly divergent at T_c; substituting (17) in (42) we find, as $\Delta K \to 0$,

$$\begin{aligned} J\chi_1(T) &\approx (\Delta K)^{-1}/16\pi && \text{for } d = 3 \\ &\approx (\Delta K)^{-1/2}(\ln \Delta K^{-1})^{1/2}/8\pi\sqrt{2} && \text{for } d = 4 \\ &\approx \tfrac{1}{2}[-\tfrac{1}{2}W_d'(0)]^{1/2}(\Delta K)^{-1/2} && \text{for } d \geqslant 5 \end{aligned} \tag{64}$$

from which we can identify the exponent γ_1.

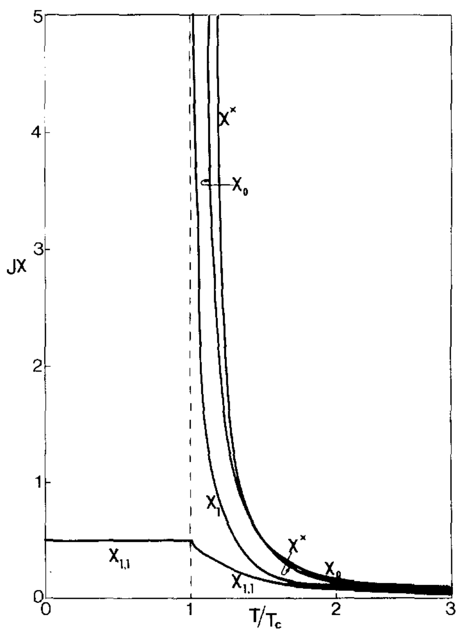

Fig. 1. Plot of bulk susceptibility χ_0, surface susceptibility $\chi^\times$, surface layer susceptibility χ_1, and local surface susceptibility $\chi_{1,1}$ versus T/T_c for $d = 3$ spherical model. Note that $\chi_{1,1}$ remains finite, but has an infinite slope at T_c.

Table II. Susceptibility Exponents for the Spherical Model with a Free Surface

Dimension, d	Bulk susceptibility, γ	Surface susceptibility, $\gamma^{\times}$	Layer susceptibility, γ_1	Local susceptibility, $\gamma_{1,1}$
3	2	3(log)	1	-1
4	1(log)	2(log)	$\frac{1}{2}(\log)^{1/2}$	$-\frac{1}{2}(\log)^{-1/2}$
≥ 5	1	2	$\frac{1}{2}$	$-\frac{1}{2}$

On the other hand, $\chi_{1,1}(T)$ is finite at T_c; substitution of (17) yielding,

$$\begin{aligned} J\chi_{1,1}(T) - \tfrac{1}{2} &\approx -8\pi(\Delta K) && \text{for} \quad d = 3 \\ &\approx -4\pi\sqrt{2}(\Delta K/\ln \Delta K^{-1})^{1/2} && \text{for} \quad d = 4 \\ &\approx [-\tfrac{1}{2}W_d'(0)]^{-1/2}(\Delta K)^{1/2} && \text{for} \quad d \geqslant 5 \end{aligned} \tag{65}$$

as $\Delta K \to 0^+$. However, beneath T_c we have $\phi_0 = 0$, and hence

$$d\chi_{1,1}/dT = 0 \qquad T < T_c, \quad \text{all} \quad d \tag{66}$$

Thus in three dimensions $d\chi_{1,1}/dT$ is discontinuous at T_c, while in four or more dimensions $d\chi_{1,1}/dT$ diverges as T approaches T_c from above. By definition the critical behavior of $d\chi_{1,1}/dT$ is characterized by an exponent $1 + \gamma_{1,1}$, and hence we may determine $\gamma_{1,1}$, which characterizes the singular part of $\chi_{1,1}(T)$.

The exponents γ_1 and $\gamma_{1,1}$ are summarized in Table II, where, for completeness, we also give $\gamma^{\times}$ and γ. Elsewhere[4] we have argued, on the basis of a scaling ansatz for $F(n, h, h_1, T)$ [see also Section 7], that γ_1 and $\gamma_{1,1}$ should satisfy

$$2\gamma_1 - \gamma_{1,1} = \gamma + \nu \tag{67}$$

where ν is the bulk correlation length exponent, given in (30). For the exponent values listed in Table II this relation may be easily checked and is found to be quite exact, including the case $d = 4$, where factors of $\ln(\Delta T)$ also occur.

5. SUSCEPTIBILITY ON INTERIOR LAYERS

It is also of interest to calculate the susceptibility on the lth layer ($l = 1$ corresponding to the surface) of a semiinfinite simple cubic lattice half-space. Again we distinguish the layer susceptibility $\chi_l(T)$, measuring the response of a spin in the lth layer to a bulk field, and the local susceptibility $\chi_{l,l}(T)$

characterizing the response to a local field applied only to the lth layer. At T_c both $\chi_l(T)$ and $\chi_{l,l}(T)$ are expected[3] to diverge with exponents γ_l and $\gamma_{l,l}$, respectively.

For the spherical model $\chi_l(T)$ and $\chi_{l,l}(T)$ may be obtained by a straightforward generalization of our previous arguments. Consider, to begin with, an n-layer system with a field h_l coupling to spins in the lth layer ($l < n$). The resulting free energy is given by (1) with $\epsilon_r(h, h_1)$ replaced by

$$\begin{aligned}\epsilon_r(h, h_l) &= [2/(n+1)]^{1/2} \sum_{j=1}^{n} (h + h_l \delta_{j,l}) \sin[\pi(r+1)j/(n+1)] \\ &= [2/(n+1)]^{1/2} \{h_l \sin[\pi(r+1)l/(n+1)] \\ &\quad + \alpha_r h \cot[\pi(r+1)/2(n+1)]\}\end{aligned} \tag{68}$$

where $\alpha_r = 0$ (1) if r is odd (even). Hence we obtain

$$\begin{aligned}J\chi_l(n,T) &= -[\partial^2 F/\partial h\, \partial h_l]_{h=h_l=0} \\ &= \frac{1}{n(n+1)} \\ &\quad \times \sum_{s=0}^{[1/2n-1/2]} \frac{\sin[\pi(2s+1)l/(n+1)] \cot[\pi(2s+1)/2(n+1)]}{\phi + \Omega_{2s}}\end{aligned} \tag{69}$$

and

$$\begin{aligned}J\chi_{l,l}(n,T) &= -[\partial^2 F/\partial h_l^2]_{h=h_l=0} \\ &= \frac{1}{n(n+1)} \sum_{r=0}^{n-1} \frac{\sin^2[\pi(r+1)l/(n+1)]}{\phi + \Omega_r}\end{aligned} \tag{70}$$

with ϕ given by (18) and Ω_r by (3).

In the limit $n \to \infty$, corresponding to a semi-infinite half-space bounded by a free surface, we may replace the summations by integrations, to yield

$$J\chi_l(T) = \lim_{n\to\infty} nJ\chi_l(n,T) = \frac{1}{2\pi} \int_0^{\pi} \frac{\sin l\theta \cot \frac{1}{2}\theta \, d\theta}{\phi_0 + 4\sin^2 \frac{1}{2}\theta} \tag{71}$$

and

$$J\chi_{l,l}(T) = \lim_{n\to\infty} nJ\chi_{l,l}(n,T) = \frac{1}{\pi} \int_0^{\pi} \frac{\sin^2 l\theta}{\phi_0 + 4\sin^2 \frac{1}{2}\theta} \, d\theta \tag{72}$$

where ϕ_0 is again the solution of (13). The integrals appearing in these expressions are evaluated in Appendix A. Hence we obtain

$$J\chi_l(T) = \tfrac{1}{2}\phi_0^{-1}[1 - e^{-l\Gamma(\phi_0)}] \tag{73}$$

and

$$J\chi_{l,l}(T) = \tfrac{1}{2}\phi_0^{-1/2}(\phi_0 + 4)^{-1/2}[1 - e^{-2l\Gamma(\phi_0)}] \tag{74}$$

where

$$\Gamma(\phi_0) = \ln[1 + \tfrac{1}{2}\phi_0 + \tfrac{1}{2}\phi_0^{1/2}(\phi_0 + 4)^{1/2}] \tag{75}$$

As $\phi_0 \to 0$, corresponding to $T \to T_{c^+}$,

$$\Gamma(\phi_0) = \phi_0^{1/2} + O(\phi_0^{3/2}) \tag{76}$$

and hence for *fixed l*

$$J\chi_l(T) = \tfrac{1}{2}l\phi_0^{-1/2} + O(1), \qquad \phi_0 \to 0 \tag{77}$$

and

$$J\chi_{l,l}(T) = \tfrac{1}{2}l - \tfrac{1}{2}l^2\phi_0^{1/2} + O(\phi_0), \qquad \phi_0 \to 0 \tag{78}$$

Comparison of these expressions with (42) and (44) for χ_1 and $\chi_{1,1}$, respectively, shows that for all *finite l*,

$$\gamma_l = \gamma_1 \qquad \text{and} \qquad \gamma_{l,l} = \gamma_{1,1} \tag{79}$$

where the exponents γ_1 and $\gamma_{1,1}$ are given in Table II. On the other hand, the amplitude increases with l. The result (79) confirms, for the spherical model, a conjecture originally made by McCoy and Wu[(5)] for the layer magnetization of the two-dimensional Ising model, that the "layer" exponents γ_l, $\gamma_{l,l}$, etc., are independent of l for all finite l.

If we recall (12) relating ϕ_0 to the bulk susceptibility $\chi(T)$, we may write (73) as

$$\chi_l(T) = \chi(T)[1 - e^{-l\Gamma(\phi_0)}] \tag{80}$$

which clearly illustrates that as $l \to \infty$ at fixed T above T_c, $\chi_l(T)$ tends to the bulk susceptibility, as expected on physical grounds. On the other hand, we find from (74) that in the same limit $\chi_{l,l}(T)$ tends to

$$J\chi_{\infty,\infty}(T) = \tfrac{1}{2}\phi_0^{-1/2}(\phi_0 + 4)^{-1/2} \tag{81}$$

Physically, we may describe this quantity as the response of a spin in an infinite d-dimensional hypercubic lattice to a magnetic field applied only to the $(d - 1)$-dimensional layer containing the spin. Since

$$J\chi_{\infty,\infty}(T) \approx \tfrac{1}{4}\phi_0^{-1/2} + O(\phi_0^{1/2}) \qquad \text{as} \quad \phi_0 \to 0 \tag{82}$$

we find, on comparing this expression with (60), that $\chi_{\infty,\infty}(T)$ diverges at T_c with the same exponent (γ_1, given in Table I) as $\chi_1(T)$. Note, however, that $\chi_{\infty,\infty}(T)$ is *not* equal to $\chi_1(T)$. Moreover, there appear to be no convincing grounds for assuming that $\gamma_{\infty,\infty}$ and γ_1 are generally identical. Indeed, the direct estimation of $\gamma_{\infty,\infty}$ for a more realistic model, such as the Ising model, would be of some interest.

In view of (76) and the exponent relation (30), we may write (80) in the critical region in the physically illuminating form

$$\chi_l(T) \approx \chi(T)[1 - \exp(-alt^{\nu})] \tag{83}$$

where, as usual, $t = (T - T_c)/T_c$, ν is the bulk correlation length exponent [given by (30)], and a is a constant. This form for $\chi_l(T)$, which may be written as

$$\chi_l(T) \approx \chi(T)f(l/\xi(T)) \tag{84}$$

where $\xi(T)$ is the bulk correlation length, is a rather natural postulate for the variation of a thermodynamic near a free surface. In the context of the magnetization near a surface it has been discussed recently by Fisher[11] (see also Ref. 13).

If we assume that

$$f(x) \approx f_0 x^{\sigma} \qquad \text{as} \quad x \to 0 \tag{85}$$

corresponding to $T \to T_c$ at fixed l, we can conclude, with $l = 1$, that

$$\gamma_1 = \gamma - \sigma\nu \tag{86}$$

Unfortunately, it does not seem possible to fix a priori the value of σ. For the spherical model (83) gives

$$\sigma = 1 \qquad \text{all} \quad d \tag{87}$$

and hence

$$\gamma_1 = \gamma - \nu \tag{88}$$

which is, of course, confirmed by the exact values of γ_1 given in Table I.

The exponent relation (88) is, however, special to the spherical model, although it is tempting to conjecture that the scaling function $f(x)$ appearing in (84) would be more generally linear for small x. This assumption is, however, untenable; the values[3,5] $\gamma_1 = \frac{11}{8}$; $\gamma = \frac{7}{4}$, and $\nu = 1$ for the two-dimensional Ising model indicate, via (86), the value $\sigma = \frac{3}{8}$ for this model. The general applicability of an assumption of the form (84) appears therefore to be limited in the absence of any heuristic arguments to predict σ.

This completes our discussion of the response of a spherical model to a local surface or "layer" field. In the next section we being our investigation of the validity of scaling for this system.

6. SCALING REPRESENTATIONS FOR $\chi_1(n, T)$ AND $\chi_{1,1}(n, T)$

In Section 4 we calculated the surface layer susceptibility $\chi_1(T)$ and the local surface susceptibility $\chi_{1,1}(T)$ defined by (53) and (54), respectively. Both $\chi_1(T)$ and $\chi_{1,1}(T)$ were found to be nonanalytic at the bulk critical temperature $T_{c,d}$.

On the other hand, for finite n, inspection of (55) and (56) indicates that the divergence of $\chi_1(n, T)$ and $\chi_{1,1}(n, T)$ is determined by

$$\phi(n, T) = 0 \tag{89}$$

with ϕ determined by (18). Explicitly, we have, for sufficiently large n,

$$J\chi_1(n, T) \approx 2n^{-2}\phi^{-1} + O(1), \qquad \phi \to 0 \tag{90}$$

$$J\chi_{1,1}(n, T) \approx \pi n^{-4}\phi^{-1} + O(1), \qquad \phi \to 0 \tag{91}$$

Hence for $d > 3$, $\chi_1(n, T)$ and $\chi_{1,1}(n, T)$ diverge at the *shifted* layer critical temperature $T_{c,d}(n)$. If we compare (90) and (91) with the analogous expansion [see BF, Eq. (8.16)] for $\chi(n, T)$, defined in (49), namely

$$J\chi(n, T) \approx 2\pi^{-1}n^{-1}\phi^{-1} + O(1), \qquad \phi \to 0 \tag{92}$$

we see that for all *finite n*, and $d > 3$,

$$\chi_1(n, T) \sim \chi_{1,1}(n, T) \sim \chi(n, T) \approx \dot{t}^{-\dot{\gamma}} \qquad \text{as} \quad \dot{t} \to 0 \tag{93}$$

where $\dot{\gamma}$ is the exponent of the $(d-1)$-dimensional bulk susceptibility (see Table II) and

$$\dot{t} = [T - T_{c,d}(n)]/T_{c,d} \tag{94}$$

That is, all three susceptibilities, with n finite, diverge at $T_{c,d}(n)$ with the *same* exponent, although their respective amplitudes are different.

For a two-dimensional n-layer system (89) is only satisfied at $T = 0$, where [see BF, Eq. (F.16)]

$$\phi(n, T) \approx 2\pi^2 n^{-2} \exp(8\pi n\, \Delta\dot{K}) \sim \exp(-c/T) \tag{95}$$

with $\Delta\dot{K}$ defined in (26). Hence, for $d = 3$ and n finite, $\chi_1(n, T)$ and $\chi_{1,1}(n, T)$ are finite and analytic functions of T except at $T = 0$, where they diverge exponentially as $\exp(c/T)$ with c a positive constant. The behavior of $\chi(n, T)$ is similar [see BF, Appendix F].

Clearly the critical behavior of $\chi_1(n, T)$ and $\chi_{1,1}(n, T)$ for finite n is qualitatively different in all dimensions from that exhibited in the limit $n \to \infty$. Yet on physical grounds we would expect[1,2] that the expansions (53) and (54) are valid for sufficiently large n and T away from T_c. In the critical region they must, however, break down.

In this regime the scaling theory of finite-size effects developed by Fisher[1,2] predicts that the singular parts of the thermodynamic properties of an n-layer system may be represented in the form

$$Y(n, T) \approx n^{\omega} X(n^{1/\nu}\dot{t}) \qquad n \to \infty, \quad \dot{t} \to 0 \tag{96}$$

where $\dot{t}$ is defined in (94) and ν is the bulk correlation length exponent. The exponent ω is determined by the requirement that (96) reproduce the correct critical behavior in the limit $n \to \infty$ at fixed T. Hence for $Y = \chi_1$ or $\chi_{1,1}$ we require

$$X(z) = X_0 z^{-\psi} \qquad \text{as} \quad z \to \infty \tag{97}$$

with $\psi = \gamma_1$ and $\gamma_{1,1}$, respectively, to give the correct t dependence (54), and

$$\omega = -1 + (\psi/\nu) \tag{98}$$

to give the correct n dependence (53). For the spherical model the exponent values given in Table II give for all d

$$\omega_1 = -1 + (\gamma_1/\nu) = 0 \tag{99}$$

$$\omega_{1,1} = -1 + (\gamma_{1,1}/\nu) = -2 \tag{100}$$

In the earlier work [BF, Section 9] the scaled form (96) was confirmed for the susceptibility $\chi(n, T)$. We will now show that $\chi_1(n, T)$ and $\chi_{1,1}(n, T)$ may also be written in this form and explicitly obtain the appropriate scaling functions.

To do so, we recall that in the critical region the spherical field ϕ has the form (21). Hence we must analyze (55) and (56) in the limit $n \to \infty$ with $x = \phi n^2$ fixed.

We consider $\chi_1(n, T)$ first. On substituting (21) in (55) and approximating $\sin[\pi/(2n + 2)]$ by $\pi/(2n + 2)$, we obtain

$$J\chi_1(n, T) = 2 \sum_{s=0}^{[1/2n-1/2]} \frac{\cos^2[\pi(2s + 1)/(2n + 2)]}{x - \pi^2 + 4n^2 \sin^2[\pi(2s + 1)/(2n + 2)]} + O(n^{-1}) \tag{101}$$

The asymptotic evaluation for large n of sums of this type has been discussed in detail by Barber and Fisher [BF, Section 4.1]. Following their analysis, we replace the sine in (101) by its argument, the cosine by unity, and extend the sum to infinity. The error incurred in this process can be bounded, as in the earlier work, and is $O(n^{-1})$. Hence we find

$$\begin{aligned} J\chi_1(n, T) &= 2 \sum_{s=0}^{\infty} [x - \pi^2 + 4\pi^2(s - \tfrac{1}{2})^2]^{-1} + O(n^{-1}) \\ &= R_{00}^{1/2}[\tfrac{1}{4}(x - \pi^2)]/2\pi^2 + O(n^{-1}) \end{aligned} \tag{102}$$

where we have introduced the modified remnant function[7,19]

$$R_{00}^{1/2}(z) = \sum_{s=1}^{\infty} [z + (r - \tfrac{1}{2})^2]^{-1} = \tfrac{1}{2}\pi z^{-1/2} \tanh(\pi z^{1/2}) \tag{103}$$

Hence we finally obtain for $n \gg 1$ with $x = \phi n^2$ fixed

$$J\chi_1(n, T) = \tfrac{1}{2}(x - \pi^2)^{-1/2} \tanh[\tfrac{1}{2}(x - \pi^2)^{1/2}] + O(n^{-1}) \tag{104}$$

To obtain the corresponding expression for $\chi_{1,1}(n, T)$, we first make use of the identity

$$(\sin^2 2\theta)/(4u + 4\sin^2\theta) = \tfrac{1}{2} + u + \cos 2\theta - u(1+u)(u + \sin^2\theta)^{-1} \quad (105)$$

with

$$\theta = \pi(r+1)/(2n+2) \quad (106)$$

and

$$u = (x/4n^2) - \sin^2[\pi/(2n+2)] = (x - \pi^2)/4n^2 + O(n^{-3}) \quad (107)$$

to write (56) as

$$J\chi_{1,1}(n, T) = (n+1)^{-1}(\tfrac{1}{2} + u) + \frac{1}{n(n+1)}\sum_{r=0}^{n-1}\cos[\pi(r+1)/(n+1)] - u(1+u)s_1 \quad (108)$$

where

$$s_1 = \frac{1}{n(n+1)}\sum_{r=0}^{n-1}\{u + \sin^2[\pi(r+1)/(2n+2)]\}^{-1} \quad (109)$$

may be reduced to a simple remnant function as follows. Substituting (107) for u gives

$$s_1 = 4\sum_{r=0}^{n-1}\{x - \pi^2 + 4n^2\sin^2[\pi(r+1)/(2n+2)]\}^{-1} + O(n^{-1}) \quad (110)$$

Proceeding as before, we replace the sine by its argument and extend the sum to infinity. The resulting error is again of order n^{-1}, and hence we obtain

$$\begin{aligned} s_1 &= 4\sum_{r=1}^{\infty}(x - \pi^2 + \pi^2 r^2)^{-1} + O(n^{-1}) = 4R_{00}(x/\pi^2 - 1)/\pi^2 + O(n^{-1}) \\ &= 2(x-\pi^2)^{-1}[(x-\pi^2)^{1/2}\coth(x-\pi^2)^{1/2} - 1] + O(n^{-1}) \end{aligned} \quad (111)$$

Substituting this result together with (107) in (108) and noting that the remaining sum over cosines in (108) vanishes[20] identically, we obtain the required expression

$$J\chi_{1,1}(n, T) = \tfrac{1}{2}n^{-1} - \tfrac{1}{2}n^{-2}(x-\pi^2)^{1/2}\coth(x-\pi^2)^{1/2} + O(n^{-3}) \quad (112)$$

In this expression the second term represents the singular part to which the scaling form should apply.[1,2]

We now recall [see (29)] that in the critical region for $d = 3$ and $d \geqslant 5$ the scaled field x is a function of the single scaled variable $n^{1/\nu}\Delta\dot{K} \sim n^{1/\nu}\Delta\dot{t}$. Hence for $d = 3$ and $d \geqslant 5$ we may write (104) and (112) as

$$J\chi_1(n, T) = X_1(n^{1/\nu}\Delta\dot{K}) + O(n^{-1}) \quad (113)$$

$$J\chi_{1,1}(n, T) = \tfrac{1}{2}n^{-1} + n^{-2}X_{1,1}(n^{1/\nu}\Delta\dot{K}) + O(n^{-3}) \quad (114)$$

which, in view of (99) and (100), confirm the scaling hypothesis (96) in these dimensions. In four dimensions, however, since x is not a function of a single scaled variable over the whole range $0 < x < \infty$, such a scaled form does not exist. A similar failure was found for $\chi(n, T)$ [see BF, Section 9.3], and is not surprising in view of similar difficulties with thermodynamic scaling[16] for $d = 4$.

The scaling functions $X_1(z)$ and $X_{1,1}(z)$ may be easily determined. For $d \geqslant 5$ they are given explicitly, from (22) and (24), by

$$X_1(z) = \tfrac{1}{2}(w_d z - \pi^2)^{-1/2} \tanh[\tfrac{1}{2}(w_d z - \pi^2)^{1/2}] \tag{115}$$

$$X_{1,1}(z) = -\tfrac{1}{2}(w_d z - \pi^2)^{1/2} \coth(w_d z - \pi^2)^{1/2} \tag{116}$$

where

$$w_d = -2/W_d'(0) > 0 \tag{117}$$

In three dimensions a closed form does not seem to exist, but the scaling functions may be specified parametrically by

$$X_1(z) = \tfrac{1}{2}y^{-1} \tanh \tfrac{1}{2}y \tag{118}$$

$$X_{1,1}(z) = \tfrac{1}{2}y \coth y \tag{119}$$

$$8\pi z = \ln[(\sinh y)/y] \tag{120}$$

It is straightforward now to show that as $z \to \infty$ we have

$$X_1(z) = (z^{-1}/16\pi) - [\ln(16\pi z)/2(8\pi z)^2] + O[(\ln z)/z^3] \quad \text{for } d = 3 \tag{121}$$

$$= \tfrac{1}{2}w_d^{-1/2}z^{-1/2} + O(z^{-3/2}) \quad \text{for } d \geqslant 5 \tag{122}$$

and

$$X_{1,1}(z) = 4\pi z + \tfrac{1}{2}\ln(16\pi z) + O[(\ln z)/z] \quad \text{for } d = 3 \tag{123}$$

$$= -\tfrac{1}{2}w_d^{1/2}z^{1/2} + O(z^{-1/2}) \quad \text{for } d \geqslant 5 \tag{124}$$

The leading terms in these expressions are in precise accord with (101), with $\psi = \gamma_1$ or $\gamma_{1,1}$ as given in Table II. If we replace z by $n^{1/\nu}\,\Delta K$, we recover, as required, the limiting critical behavior (64) and (65).

In the limit $z \to 0$, corresponding to $\Delta K \to 0$ at fixed n, we obtain

$$X_1(z) = \tfrac{1}{4} - \pi z + O(z^2) \quad \text{for } d = 3 \tag{125}$$

$$= (4/w_d)z^{-1} + O(1) \quad \text{for } d \geqslant 5 \tag{126}$$

and

$$X_{1,1}(z) = \tfrac{1}{2} - 8\pi z + O(z^2) \quad \text{for } d = 3 \tag{127}$$

$$= (\pi^2/2w_d)z^{-1} + O(1) \quad \text{for } d \geqslant 5 \tag{128}$$

For $d \geqslant 5$ the leading terms of these expansions reproduce the divergence (93) at $T_{c,d}(n)$.

For $d = 3$, $X_1(z)$ and $X_{1,1}(z)$ tend to finite limits as $z \to 0$, reflecting the absence of a nonzero critical temperature for a two-dimensional layer system with n finite. On the other hand, if we consider the limit $z \to -\infty$, corresponding to $T \to 0$ at fixed n, the scaling representations should[7] reproduce the exponential divergence of $\chi_1(n, T)$ and $\chi_{1,1}(n, T)$ at $T = 0$. To obtain the behavior of $X_1(z)$ and $X_{1,1}(z)$ in this limit, we notice first that for $z < 0$, y is pure imaginary, i.e., $y = i\theta$. The limit $z \to -\infty$ then corresponds to $\theta \to \pi$. Hence we find as $z \to -\infty$

$$X_1(z) = \pi^{-2} e^{8\pi|z|} + \pi^{-2} - \pi^{-3} + O(e^{-|z|}) \tag{129}$$

and

$$X_{1,1}(z) = -\tfrac{1}{2} e^{8\pi|z|} + \tfrac{1}{2}\pi^{-1} + \tfrac{1}{2} + O(e^{-|z|}) \tag{130}$$

Substituting these expansions in (113) and (114) gives for $T \to 0$ at fixed n

$$J\chi_1(n, T) \approx \pi^{-2} \exp(8\pi n|\Delta \dot{K}|) \tag{131}$$

and

$$J\chi_{1,1}(n, T) \approx \tfrac{1}{2}n^{-2} \exp(8\pi n|\Delta \dot{K}|) \tag{132}$$

Comparison of these predictions with the results of the direct analysis, obtained by substituting (95) in (90) and (91), confirms the validity of the scaling representations for large fixed n in the limit $T \to 0$.

Thus we have seen for $d = 3$ and $d \geqslant 5$ that the scaling theory of finite-size effects, which has previously been confirmed[7,15] for bulk properties, also describes the behavior of intrinsically surface properties for spherical models of finite thickness. In four dimensions a single scaling form does not exist. However, (104), together with (23), remains a valid representation in the critical region. In particular, the limit $x \to \infty$ reproduces the bulk critical behavior (64) and (65), while in the limit $x \to 0$ we recover (93).

7. SCALING REPRESENTATION FOR FREE ENERGY IN FINITE FIELD

The analysis of the previous section, together with the earlier work,[7] has shown that in zero field the thermodynamic properties of a finite n-layer spherical model are in accord with the scaling theory of finite-size effects.[1,2] Elsewhere[4] we have extended this theory to nonzero bulk and surface fields. This generalized scaling theory suggests that the singular part of the free energy of an n-layer system should have the form

$$F_{d,s}(T, h, h_1, n) \approx n^{(\alpha-2)/\nu} Q(n^{1/\nu}\dot{t}, n^{\Delta/\nu}h, n^{\Delta_1/\nu}h_1) \tag{133}$$

as $n \to \infty$ and $h, h_1, t \to 0$, where $\Delta = \beta + \delta$ is the bulk gap exponent[12] and the new surface field exponent Δ_1 is given by[4]

$$\Delta_1 = \Delta - \gamma_1 + \gamma_{1,1} \tag{134}$$

In this section we will confirm that the free energy of an n-layer spherical model has this form and explicitly obtain the scaling function Q. For simplicity, we will only discuss the case $d = 3$.

The appropriate free energy to consider[7] is, however, not $F_3(T, h, h_1, n; \phi)$, which is an explicit function of the spherical field ϕ, but rather the free energy per spin $A_3(T, h, h_1, n)$ at constant spherical constraint,

$$\mathscr{S}^2 = \sum_i \langle s_i^2 \rangle = N \tag{135}$$

This free energy is related to $F_3(T, h, h_1, n; \phi)$ by a Legendre transformation. Thus we find (see BF, Section 10.2)

$$A_d(T, h, h_1, n) = F_d(T, h, h_1, n; \phi) - J\phi - 2J\cos[\pi/(n+1)] \tag{136}$$

where ϕ is the solution of

$$\partial F_d/\partial\phi = J \tag{137}$$

Since for a three-dimensional spherical model[14]

$$\Delta = \tfrac{5}{2}, \qquad \alpha = -1, \qquad \nu = 1 \tag{138}$$

we find from Table II

$$\Delta_1 = \tfrac{1}{2} \tag{139}$$

Thus for a two-dimensional n-layer spherical model (133) predicts that

$$2\beta A_{3,s}(T, h, h_1, n) \approx n^{-3} Q(nt, n^{5/2}h, n^{1/2}h_1) \tag{140}$$

as $n \to \infty$ and $t, h, h_1 \to 0$.

In the critical region we still have $\phi = x/n^2$, with x now a function of h, h_1, and T. Hence from (136)

$$A_{3,s}(T, h, h_1, n) = F_{3,s}(T, h, h_1; n; x/n^2) - Jx/n^2 \tag{141}$$

Now from (1) and (7) we see that F_3 consists of five terms. The first $(\frac{1}{2}k_B T \ln K)$ is clearly nonsingular in the critical region and can be ignored. The two terms explicitly dependent on h_1 were analyzed in the previous section, while the term proportional to h^2 was analyzed by Barber and Fisher.[7] Hence from (104), (112), and BF, Eq. (9.11), we find, as $n \to \infty$ with x a positive constant, that

$$\begin{aligned} 2\beta F_{3,s}(T, h, h_1, n) = {} & L_s(x) - n^{-3}y^2 Q_1(x) - 2n^{-3} y y_1 Q_2(x) \\ & + y_1^2 n^{-3} Q_3(x) + O(n^{-4}) \end{aligned} \tag{142}$$

where $L_s(x)$ is the singular part of

$$L(x) = (1/n) \sum_{r=0}^{n-1} L_2(x/n^2 + \Omega_r) \tag{143}$$

$$Q_1(x) = \tfrac{1}{2}(x - \pi^2)^{-1}\{1 - 2(x - \pi^2)^{-1/2} \tanh[\tfrac{1}{2}(x - \pi^2)^{1/2}]\} \tag{144}$$

$$Q_2(x) = (x - \pi^2)^{-1/2} \tanh[\tfrac{1}{2}(x - \pi^2)^{1/2}] \tag{145}$$

$$Q_3(x) = (x - \pi^2)^{1/2} \coth(x - \pi^2)^{1/2} \tag{146}$$

and we have introduced the scaled field variables

$$y = (Jk_BT)^{-1/2}hn^{5/2}, \qquad y_1 = (Jk_BT)^{-1/2}h_1n^{1/2} \tag{147}$$

It remains to analyze $L(x)$. This is done in Appendix B, where we show that, as $n \to \infty$ with x a positive constant,

$$L(x) = L(0) + 2x(K + \Delta\dot{K})/n^2 + Q_0(x)/n^3 + O[(\ln n)/n^4] \tag{148}$$

where $\Delta\dot{K}$ is defined in (28) and

$$Q_0(x) = (\pi/4)[R_{2,0}(-1) - R_{2,0}(x/\pi^2 - 1)] \tag{149}$$

The remnant function[19] $R_{2,0}(z)$ is defined by

$$R_{2,0}(z) = \sum_{r=1}^{\infty} (r^2 + z)[\ln(1 + z/r^2) - z] = \int_0^z \ln[(\sinh \pi w^{1/2})/\pi w^{1/2}]\, dw \tag{150}$$

The constant term $L(0)$ in (148) is nonsingular and may be neglected. Hence if we introduced the scaled temperature variable

$$\dot{z} = n\,\Delta\dot{K} \tag{151}$$

we may write (142) as

$$2\beta F_{3,s}(x) = 2xK/n^2 + n^{-3}[2\dot{z}x + Q_0(x) - y^2Q_1(x) - 2yy_1Q_2(x) + y_1{}^2Q_3(x)] + O[(\ln n)/n^4] \tag{152}$$

From (137) the scaled field x is given in leading order by

$$2\dot{z} + Q_0{}'(x) - \tfrac{1}{2}y^2Q_1{}'(x) - 2yy_1Q_2{}'(x) + y_1{}^2Q_3{}'(x) = 0 \tag{153}$$

In zero field (i.e., $y = y_1 = 0$) this reduces to (22). In principle, at least, we can solve (153) to give as $n \to \infty$

$$x \simeq \Phi(\dot{z}, y, y_1) \tag{154}$$

Finally, if we substitute (152) in (141), we obtain the required expression,

$$2\beta A_{3,s}(T, h, h_1, n) = n^{-3}[2\dot{z}x + Q_0(x) - y^2Q_1(x) - 2yy_1Q_1(x) + y_1{}^2Q_3(x)] + O[(\ln n)/n^4] \tag{155}$$

which, in view of (154), is precisely of the form (140). The scaling function $Q(z, y, y_1)$ may be specified parametrically by, on combining (144)–(146) and (153),

$$Q(\dot{z}, y, y_1) = 2\dot{z}(\rho^2 + \pi^2) + \tfrac{1}{4}\pi[R_{2,0}(-1) - R_{2,0}(\rho^2/\pi^2)] - \tfrac{1}{2}y^2\rho^{-2} + [y^2\rho^{-3} - 2yy_1\rho^{-1}]\tanh\tfrac{1}{2}\rho + y_1{}^2\rho\coth\rho \qquad (156)$$

$$4\dot{z} = (1/2\pi)\ln[(\sinh\rho)/\rho] - y^2\rho^{-4} + \rho^{-3}(3y^2\rho^{-2} - 2yy_1) \times \tanh\tfrac{1}{2}\rho - \tfrac{1}{2}\rho^{-2}(y^2\rho^{-2} - 2yy_1)\,\mathrm{sech}^2\,\tfrac{1}{2}\rho - \rho^{-1}y_1{}^2\coth\rho + y_1{}^2\,\mathrm{cosech}^2\,\rho \qquad (157)$$

8. SCALING REPRESENTATION FOR SURFACE FREE ENERGY

An alternative[4,11] approach to a scaling theory for surface properties is to scale not with n but with the reduced shifted temperature $\dot{t}$. That is, in place of (133) we postulate[4,11] the form

$$F_{d,s}(T, h, h_1, n) \approx \dot{t}^{2-\alpha}\bar{Q}(n\dot{t}^{\nu}, h/\dot{t}^{\Delta}, h_1/\dot{t}^{\Delta_1}) \qquad (158)$$

to be valid as $n \to \infty$ and $\dot{t}, h, h_1 \to 0$. While these alternative scaling assumptions are equivalent and lead to the same exponent relations, there appear[11] to be some advantages to t-scaling. In particular, we can deduce[4,11] a scaling form for the surface free energy which is analogous to the standard scaling assumption for the bulk free energy.

For a three-dimensional n-layer spherical model (158) takes the explicit form, recalling the exponent values (138) and (139),

$$2\beta A_{3,s}(T, h, h_1, n) \approx \Delta\dot{K}^3\bar{Q}(n\,\Delta\dot{K}, h/\Delta\dot{K}^{5/2}, h_1/\Delta\dot{K}^{1/2}) \qquad (159)$$

where we have scaled, for convenience, with $\Delta\dot{K} \sim \dot{t}$. If we introduce the scaled field variables

$$\dot{v} = (Jk_BT)^{-1/2}h/\Delta\dot{K}^{5/2} = \dot{z}^{-5/2}y_1, \quad \dot{v}_1 = (Jk_BT)^{-1/2}h_1/(\Delta K)^{1/2} = \dot{z}^{-1/2}y_1 \quad (160)$$

where y and y_1 are defined in (147) and $\dot{z}$ in (151), we find on comparing (159) and (140) that

$$\bar{Q}(\dot{z}, \dot{v}, \dot{v}_1) = \dot{z}^{-3}Q(\dot{z}, \dot{z}^{5/2}\dot{v}, \dot{z}^{1/2}\dot{v}_1) \qquad (161)$$

Hence the t-scaling function $\bar{Q}$ follows immediately from (156) and (157).

Now if we consider the limit $n \to \infty$ at fixed T not equal to T_c, we may define[1] the surface free energy $A^{\times}(T, h, h_1)$ by the expansion[5]

$$A(T, h, h_1, n) \approx A_{\infty}(T, h) + (2/n)A^{\times}(T, h, h_1) + \cdots \qquad (162)$$

[5] In this definition we assume for symmetry that h_1 couples to spins in the "top" and "bottom" surfaces, i.e., the first and nth layers. This, however, creates no difficulties and we simply double all terms dependent on h_1 in our previous results for the free energy. This assumption will be made for the remainder of our discussion. In particular all terms in (156) and (157) containing v_1 will be doubled.

where $A_\infty(T, h)$ is the bulk free energy. If we assume that bulk scaling[12] holds, we may write in the critical region

$$A_\infty(T, h) \approx \Delta K^3 \bar{Q}_\infty(h/\Delta K^{5/2}) \tag{163}$$

and hence we can expect that

$$\lim_{z\to\infty} \bar{Q}(z, v, v_1) = \bar{Q}_\infty(v) \tag{164}$$

To investigate the surface free energy on the basis of (159) we require the leading corrections to (164) for large z.

From (161) and the parametric equations (156) and (157) for Q we observe that for large $\dot{z}$ the parameter $\rho \propto \dot{z}$. A more detailed analysis gives as $\dot{z} \to \infty$

$$\rho = \dot{z}A(\dot{v})\{1 + B(\dot{v})\ln[2zA(\dot{v})]/\dot{z} + C(\dot{v}, \dot{v}_1)/\dot{z} + O[(\ln \dot{z}/\dot{z})^2]\} \tag{165}$$

where

$$B(\dot{v}) = [5A(\dot{v}) - 32\pi]^{-1} \tag{166}$$

$$C(\dot{v}, \dot{v}_1) = 2\pi B(\dot{v})[2\dot{v}_1{}^2 A^{-1} + 4\dot{v}\dot{v}_1 A^{-3} - 3\dot{v}^2 A^{-5}] \tag{167}$$

with $A(\dot{v})$ the solution of

$$A^5 - 8\pi A^4 = 2\pi \dot{v}^2 \tag{168}$$

The required expansion of $\bar{Q}$ now follows if we substitute (165) in (156). Hence we obtain as $\dot{z} \to \infty$ at fixed $\dot{v}$ and $\dot{v}_1$

$$\bar{Q}(\dot{z}, \dot{v}, \dot{v}_1) = \bar{Q}_\infty(\dot{v}) + \bar{Q}_1(\dot{v})\ln[2\dot{z}A(\dot{v})]/\dot{z} + \bar{Q}^\times(\dot{v}, \dot{v}_1)/\dot{z} + O[(\ln \dot{z}/\dot{z})^2] \tag{169}$$

where

$$\bar{Q}_\infty(\dot{v}) = [2A^2(\dot{v})/3] - [5\dot{v}^2/6A^2(\dot{v})] \tag{170}$$

$$\bar{Q}_1(\dot{v}) = A^2(\dot{v})/4\pi \tag{171}$$

$$\bar{Q}^\times(\dot{v}, \dot{v}_1) = 2(\dot{v}_1{}^2 - 2)A(\dot{v}) + [A^2(\dot{v})/4\pi] - [4\dot{v}\dot{v}_1/A(\dot{v})] \tag{172}$$

Clearly (169) is consistent with (164) and yields in the limit $n \to \infty$ the bulk free energy in the form (163) with the bulk scaling function $\bar{Q}_\infty(v)$ determined by (170) and (168). To obtain the surface free energy defined by (162), we must recall from (25) and (26b) that

$$\Delta\dot{K} = \Delta K - [(\ln n)/8\pi n] + (a/n) \tag{173}$$

where the amplitude a is given in (26a). Hence on substituting this expression for $\Delta\dot{K}$ and (169) in (159), we find that all terms proportional to $(\ln n)/n$ cancel, and we are left with a correction term of order n^{-1}, as expected. Comparison with (162) yields immediately the surface free energy in the form

$$\beta A_s^\times(T, h, h_1) \approx \{[A(v)\,\Delta K]^2 \ln[2A(v)\,\Delta K]/16\pi\} + \tfrac{1}{4}(\Delta K)^2[3a\bar{Q}_\infty(v) + Q^\times(v, v_1) - 5av\bar{Q}_\infty'(v)/2] \tag{174}$$

where v and v_1 are given by (160) but with $\Delta\dot{K}$ replaced by ΔK. One may easily check that this expression gives the correct critical behavior for the surface properties of a three-dimensional spherical model.

In the absence of a bulk magnetic field, i.e., $v = 0$, we have from (168)

$$A(0) = 8\pi \tag{175}$$

and hence the surface free energy takes the simple form

$$\beta A_s^\times(T, 0, h_1) \approx 4\pi(\Delta K^2)\ln(16\pi\,\Delta K) + 4\pi(\Delta K^2)(8\pi a - 1 + v_1^2) \tag{176}$$

The second term in this expression is of the form postulated by Binder and Hohenberg[3] for the surface free energy of a spin system in the presence of a surface field. However, this term alone would not yield the correct behavior for the surface specific heat [see (40)]. This failure for the spherical model of the Binder–Hohenberg postulate is a direct consequence of the "anomalous" shift in the critical temperature.[7] For more realistic models, where the shift exponent appears to exceed unity, such a form should correctly reproduce all of the surface thermodynamics in the absence of a bulk field.[4] This completes our discussion of scaling for a spherical model with a free surface.

9. CONCLUSION

We conclude by summarizing the main results of this paper.

(i) Critical phenomena in d-dimensional ferromagnetic spherical models with free surfaces were studied. In particular, the surface specific heat $C^\times(T)$ and the various surface susceptibilities were discussed (Sections 3 and 4).

(ii) The critical exponents $\alpha^\times$, γ_1, and $\gamma_{1,1}$ describing the divergence at the bulk critical temperature of $C^\times(T)$, the surface layer susceptibility $\chi_1(T)$, and local surface susceptibility $\chi_{1,1}(T)$ were obtained. The values of these exponents are summarized in Eq. (45) and Table II.

(iii) These exponents satisfy in all dimensions the various scaling relations for surface exponents which have recently been proposed.[1–4]

(iv) The generalized scaling theory[4] for systems of finite thickness in finite fields was investigated in detail (see Section 7) and shown to be an exact representation of the free energy for $d = 3$. The appropriate scaling function was explicitly determined.

(v) This scaling theory can be recast[4,11] in terms of t-scaled rather than n-scaled variables. This was done in Section 8, where a scaled form for the surface free energy was obtained. In zero bulk field this result is almost of the form proposed by Binder and Hohenberg[3]; the difference can be attributed to the "anomalous" shift in the critical temperature, which occurs for the spherical model.[7]

(vi) In the t-scaling formulation the surface field h_1 is scaled by t^{Δ_1}, which introduces[4,11] a new surface gap exponent. Quite generally[4,11]

$$\Delta_1 = \Delta - \gamma_1 + \gamma_{1,1} \tag{177}$$

where $\Delta = \beta + \gamma$ is the bulk gap exponent. Hence from the values of Table II we find that $\Delta_1 = \frac{1}{2}$ for the spherical model in all dimensions. Since this value is also found[4,11] within mean-field theory and for the two-dimensional Ising model, there appear to be reasonable grounds for conjecturing[11] that Δ_1 has a universal value of $\frac{1}{2}$. The existing estimates[3,9] for the surface exponents of the three-dimensional Ising model are not inconsistent with this assumption.[9,11] (See the section, Note Added in Proof.)

(vii) Finally, the variation of the susceptibility near a free surface was also discussed (see Section 5). On any layer a finite distance from the free surface the layer susceptibility $\chi_l(T)$ and the local layer susceptibility $\chi_{l,l}(T)$ are found to diverge with the same exponents as $\chi_1(T)$ and $\chi_{1,1}(T)$, respectively. In the critical region both $\chi_l(T)$ and $\chi_{l,l}(T)$ may be written in the form discussed recently by Fisher,[11] with a temperature-independent extrapolation length. However, this approach seems of limited application[11] to other systems.

APPENDIX A. EVALUATION OF $\chi_l(T)$ AND $\chi_{l,l}(T)$

In this appendix we evaluate

$$J\chi_l(T) = \frac{1}{2\pi}\int_0^{\pi} \frac{\sin l\theta \cot \frac{1}{2}\theta}{\phi_0 + 4\sin^2\frac{1}{2}\theta}\, d\theta \tag{A.1}$$

and

$$J\chi_{l,l}(T) = \frac{1}{\pi}\int_0^{\pi} \frac{\sin^2 l\theta}{\phi_0 + 4\sin^2\frac{1}{2}\theta}\, d\theta \tag{A.2}$$

We consider $\chi_l(T)$ first. Introducing the identities

$$\cot\tfrac{1}{2}\theta = (1 + \cos\theta)/\sin\theta \tag{A.3}$$

$$2\sin^2\tfrac{1}{2}\theta = 1 - \cos\theta \tag{A.4}$$

we obtain, since the integrand is periodic of period 2π,

$$J\chi_l(T) = \frac{1}{4\pi}\int_0^{2\pi} \frac{\sin l\theta}{\sin\theta}\, \frac{1 + \cos\theta}{\phi_0 + 2 - 2\cos\theta}\, d\theta \tag{A.5}$$

If we now change integration variable to $z = e^{i\theta}$, we may rewrite this integral as

$$J\chi_l(T) = -\frac{1}{4\pi i}\oint \frac{dz}{z^l}\frac{z^{2l}-1}{z-1}\frac{z+1}{z^2-(\phi_0+2)z-1} \tag{A.6}$$

where the contour of integration is the unit circle, $|z| = 1$. It is convenient to write

$$z^2-(\phi_0+2)z-1 = (z-z_+)(z-z_-) \tag{A.7}$$

where

$$z_\pm = 1+\tfrac{1}{2}\phi_0 \pm \tfrac{1}{2}[\phi_0(\phi_0+4)]^{1/2} \tag{A.8}$$

Since $\phi_0 > 0$, only the pole at $z = z_-$ lies within the contour of integration. Hence by Cauchy's theorem (A.6) may be written

$$J\chi_l(T) = -\tfrac{1}{2}[R_0+R_1] \tag{A.9}$$

where

$$R_0 = \frac{1}{(l-1)!}\left\{\frac{d^{l-1}}{dz^{l-1}}\left[\frac{z^{2l}-1}{z-1}\frac{z+1}{(z-z_+)(z-z_-)}\right]\right\}_{z=0} \tag{A.10}$$

and

$$R_1 = \frac{z_-^{2l}-1}{z_-^{l}(z_--1)}\frac{z_-+1}{z_--z_+} = \frac{z_-^{l}-z_-^{-l}}{z_--1}\frac{z_-+1}{z_--z_+} \tag{A.11}$$

To evaluate R_0, we note that

$$\frac{d^n}{dx^n}(uv) = \sum_{k=0}^{n}\frac{n!}{(n-k)!\,k!}\frac{d^kv}{dx^k}\frac{d^{n-k}u}{dx^{n-k}} \tag{A.12}$$

Hence

$$R_0 = \sum_{k=0}^{n}\alpha_k\beta_k \tag{A.13}$$

where

$$\alpha_k = \frac{1}{k!}\left\{\frac{d^k}{dz^k}\left[\frac{z+1}{(z-z_+)(z-z_-)}\right]\right\}_{z=0} \tag{A.14}$$

and

$$\beta_k = \frac{1}{(l-1-k)!}\left\{\frac{d^{l-1-k}}{dz^{l-1-k}}\left[\frac{z^{2l}-1}{z-1}\right]\right\}_{z=0} \tag{A.15}$$

Since

$$\frac{z^{2l}-1}{z-1} = \frac{(z^l-1)(z^l+1)}{z-1} = 1+z+z^2+\cdots+z^{2l-1} \tag{A.16}$$

we find

$$\beta_k = 1 \tag{A.17}$$

while decomposing $(z + 1)/(z - z_+)(z - z_-)$ into partial fractions yields

$$\alpha_k = (z_+ - z_-)^{-1}[(z_- + 1)z_-^{-1-k} - (z_+ + 1)z_+^{-1-k}] \tag{A.18}$$

Recalling that

$$z_+ z_- = 1 \tag{A.19}$$

we find on substituting (A.18) in (A.13)

$$R_0 = (z_+ - z_-)^{-1}\left[(1 + z_+) \sum_{k=0}^{l-1} z_+^{k} - (1 + z_-) \sum_{k=0}^{l-1} z_-^{k}\right] \tag{A.20}$$

The remaining sums are geometric series, and hence finally, after some elementary algebra,

$$R_0 = \frac{1}{z_- - z_+} \frac{z_- + 1}{z_- - 1} (z_+^{l} + z_-^{l} - 2) \tag{A.21}$$

Substituting (A.21) and (A.11) in (A.9) gives

$$2J\chi_l(T) = (z_+ + 1)(1 - z_+^{-l})/(z_+ - 1)(z_+ - z_-) \tag{A.22}$$

Finally, substituting (A.8) for $z_\pm$ and simplifying, we obtain (79) of the text, namely

$$J\chi_l(T) = \tfrac{1}{2}\phi_0^{-1}[1 - e^{-l\Gamma(\phi)}] \tag{A.23}$$

with

$$\Gamma(\phi) = \ln z_+ \tag{A.24}$$

To evaluate $J\chi_{l,l}(T)$, we first rewrite (A.2), using (A.3), in the form

$$J\chi_{l,l}(T) = \tfrac{1}{2}[I_0(\phi_0) - I_{2l}(\phi_0)] \tag{A.25}$$

where

$$I_m(\phi_0) = \frac{1}{\pi} \int_0^{\pi} \frac{\cos m\theta}{\phi + 2 - 2\cos\theta} \, d\theta \tag{A.26}$$

This final integral again may be transformed to a contour integral around the unit circle and evaluated as before. We find

$$I_m(\phi_0) = (z_+^{m} + z_+^{-m})/(z_+ - z_-) \tag{A.27}$$

where $z_\pm$ are given in (A.5). Substituting this result in (A.25) yields, on simplification, Eq. (74) of the text, namely

$$J\chi_{l,l}(T) = \tfrac{1}{2}\phi_0^{-1/2}(\phi_0 + 4)^{-1/2}[1 - e^{-2l\Gamma(\phi_0)}] \tag{A.28}$$

with $\Gamma(\phi_0)$ defined in (A.24).

APPENDIX B. ASYMPTOTIC EVALUATION OF $L(x)$

In this appendix we analyze $L(x)$, defined in (139), in the limit $n \to \infty$ with x a positive constant. To do so, we make use of the relation [see (11)]

$$L_2(z) = L_2(0) + \int_0^z W_2(z')\,dz' \tag{B.1}$$

to write (139) as

$$L(x) = L(0) + \int_0^{x/n^2} W^1_{3,n}(\phi')\,d\phi' \tag{B.2}$$

where

$$W^1_{3,n}(\theta) = (1/n) \sum_{r=0}^{n-1} W_2(\phi + \Omega_r) \tag{B.3}$$

This sum has been analyzed by Barber and Fisher,[7] who showed that as $n \to \infty$ with $\phi = x/n^2$ [see BF, Eq. (4.66)]

$$W^1_{3,n}(x/n^2) = W_3(x/n^2) + [W_3{}^\times(x/n^2)/n] + [D_3{}^1(x)/n] + O[(\ln n)/n^2] \tag{B.4}$$

where $W_3{}^\times(z)$ is defined in (20) and

$$D_3{}^1(x) = [2x^{1/2} - \ln 4x - 2R_{1,0}(x/\pi^2 - 1)]/8\pi \tag{B.5}$$

with $R_{1,0}(z)$ a remnant function.[19] Substituting (B.4) in (B.2), and noting the recursion relation[19]

$$R_{\sigma+1,\tau}(z) = \int_0^z dw\, R_{\sigma,\tau}(w) \tag{B.6}$$

for remnant functions, we obtain

$$\begin{aligned} L(x) = L(0) &+ L_3(x/n^2) - L_3(0) + \{[L_3{}^\times(x/n^2) - L_3{}^\times(0)]/n\} \\ &+ \{(4x^{3/2}/3) - x\ln 4x + x - 2\pi^2[R_{2,0}(x/\pi^2 - 1) - R_{2,0}(-1)]\}/8\pi n^3 \\ &+ O[(\ln n)/n^4] \end{aligned} \tag{B.7}$$

where

$$L_3{}^\times(z) = L_3(z) - \tfrac{1}{2}L_2(z) - \tfrac{1}{2}L_2(z+4) \tag{B.8}$$

From (B.1) and Table I we find for small z that

$$\begin{aligned} L_3(z) &= L_3(0) + W_3(0)z - z^{3/2}/6\pi + O(z^2) \\ L_2(z) &= L_2(0) - [z(\ln z)/4\pi] + [(5\ln 2 + 1)z/4\pi] + O(z^2 \ln z) \end{aligned} \tag{B.9}$$

so that (B.7) gives

$$L(x) = L(0) + [xW_3(0)/n^2] - [x(\ln n)]4\pi n^3] + \{[W_3(0) - 7(\ln 2)/8\pi - \tfrac{1}{2}W_2(4)]x - (\pi/4)[R_{2,0}(x/\pi^2 - 1) - R_{2,0}(-1)]\}/n^3 + O[(\ln n)/n^4] \tag{B.10}$$

Finally, if we recall (26a), we obtain Eq. (148) of the text.

NOTE ADDED IN PROOF

It should be pointed out that recent Monte Carlo calculations by Binder and Hohenberg (to be published) on the surface layer magnetization of the $d = 3$ Ising model indicate that the exponent Δ_1 has the value $\Delta_1 \simeq 5/8$, contradicting the assumption discussed above. The general scaling relations[3,4,11] for surface exponents, however, appear to be valid. In addition, the recent calculations by Lubensky and Rubin (to be published) using the renormalization group and ϵ-expansion techniques [K. G. Wilson, *Phys. Rev.* **B4**:3174, 3184 (1971); K. G. Wilson and M. E. Fisher, *Phys. Rev. Letts.* **28**: 240 (1972)] also predict that Δ_1 does not possess a universal value.

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