# Logarithmic Finite-Size Corrections in the Three-Dimensional Mean Spherical Model

Jordan G. Brankov<sup>1</sup> and Daniel M. Danchev<sup>1</sup>

Received May 5, 1992

The finite-size scaling prediction about logarithmic corrections in the free energy arising from corners in the geometry of the system is tested on the threedimensional mean spherical model. The general case of boundary conditions which are periodic in  $d' \ge 0$  dimensions and free or fixed in the remaining 3 - d' dimensions is considered. Logarithmic and double-logarithmic size corrections stemming from corners, edges, and surfaces are obtained.

KEY WORDS: Finite-size scaling; logarithmic corrections; spherical model.

# **1. INTRODUCTION**

One of the fundamental predictions of finite-size scaling theory<sup>(1,2)</sup> for systems confined to a fully finite geometry with real boundaries is the appearance of a universal logarithmic term in the expansion for the free energy density f at the bulk critical point  $T = T_c$ :

$$(kT_c)^{-1}f(T_c;L) = L^{-d}Y(0) + uL^{-d}\ln L + \sum_{k=0}^d L^{-k}g^{(k)}(T_c) \quad (1.1)$$

Here k is the Boltzmann constant, and L is the linear size of the system, which for simplicity is assumed to occupy a hypercubic region of volume  $L^d$ , d being the space dimensionality. The first term in the right-hand side of Eq. (1.1) stems from the universal finite-size scaling function  $Y(tL^{1/\nu})$ , where  $t = (T - T_c)/T_c$  and v is the scaling exponent for the correlation length; the second term has a universal amplitute u which may depend on the boundary conditions; the terms  $L^{-k}g^{(k)}(T_c)$  originate from the regular

<sup>&</sup>lt;sup>1</sup> Institute of Mechanics and Biomechanics, Bulgarian Academy of Sciences, 1113 Sofia, Bulgaria.

part of the free energy density and describe contributions from the bulk (k=0), surfaces (k=1), edges (k=2,..., d-1), and corners (k=d).

The result (1.1) for d=2 has beed derived from conformal theory.<sup>(3)</sup> For general d, Privman<sup>(2)</sup> has argued that the term  $uL^{-d} \ln L$  is due to a resonance between the universal  $\mathcal{O}(L^{-d})$  contribution and the corner  $\mathcal{O}(L^{-d})$  nonuniversal contribution; see also ref. 4.

There are a few exactly solvable models at d > 2 which allow one to test the above prediction. Gelfand and Fisher<sup>(5,6)</sup> have obtained logarithmic finite-size corrections to the free energy  $\Delta F_d^{(\tau)}$  in the small-block limit of a *d*-dimensional Gaussian-type model under different boundary conditions  $(\tau)$ . However, the fact that such corrections were found to exist even under periodic boundary conditions has no explanation by conformal theory<sup>(3)</sup> or finite-size scaling arguments.<sup>(2)</sup> Similarly, the asymptotic number of a finite set of Hamiltonian walks on two-dimensional Manhatten lattices studied by Duplantier and David<sup>(7)</sup> exhibits size factors under both free and periodic boundary conditions. A related *d*-dimensional model is the constrained monomer-dimer model (CMD) (see ref. 8 and references therein), which is critical in the limit of infinite dimer activity. The logarithmic size contributions in the free energy  $F_{d,d'}$  of the CMD model have been obtained<sup>(8)</sup> under boundary conditions which are periodic in  $d' \ge 0$  dimensions and free in the remaining d - d' dimensions. The term  $2^{1-d} \ln L$  has been identified to stem from the  $2^d$  corners of the system with block geometry and fully free boundaries by considering the difference in the free energies  $F_{d,0} - F_{d,d'}$  with  $d' \ge 1$ .

In ref. 9 we have used a technique similar to the one used in ref. 8 to study the logarithmic finite-size corrections  $\Delta F_{d,d'}^{(0)}$  of the *d*-dimensional mean spherical model under free boundary conditions in d-d' dimensions and periodic boundaries in  $d' \ge 0$  dimensions. The critical behavior has been described in terms of the ratio  $L/\xi_L$ , where  $\xi_L$  is the correlation length of the finite system. The main results obtained in ref. 9 are as follows.

1. In the case of fully periodic boundary conditions, i.e., when d = d',

$$\Delta F_{d,d}^{(0)} = \begin{cases} \ln(L/\xi_L), & L/\xi_L \to 0\\ 0, & L/\xi_L = \mathcal{O}(1)\\ 0, & L/\xi_L \to \infty \end{cases}$$
(1.2)

Therefore, a logarithmic contribution appears only when  $L/\xi_L \rightarrow 0$  as  $L \rightarrow \infty$ . Standard finite-size analysis of the mean spherical constraint shows that this is the case of dimensions d equal to or higher than the upper critical one  $d_u = 4$ . Then,<sup>(10, 11)</sup>

$$\xi_L/L \propto \begin{cases} (\ln L)^{1/4}, & d=4\\ L^{(d-4)/4}, & d>4 \end{cases}$$
(1.3)

which implies

$$\Delta F_{d,d}^{(0)} = \begin{cases} -\frac{1}{4} \ln \ln L, & d=4\\ -\frac{d-4}{4} \ln L & d>4 \end{cases}$$
(1.4)

In the scaling regime, 2 < d < 4, one has  $L/\xi = \mathcal{O}(1)$  and therefore no terms proportional to  $\ln L$  appear in the free energy.

2. In the case of fully free boundary conditions, i.e., when d' = 0,

$$\Delta F_{d,0}^{(0)} = \begin{cases} -2^{-d} \ln L + \ln(L/\xi_L), & L/\xi_L \to 0\\ -2^{-d} \ln L, & L/\xi_L = \mathcal{O}(1)\\ -2^{-d} \ln \xi_L + d2^{-d}L/\xi_L, & L/\xi_L \to \infty \end{cases}$$
(1.5)

Therefore, a logarithmic contribution appears in all cases when  $\xi_L \rightarrow \infty$  as  $L \rightarrow \infty$ .

3. In the case of free boundaries in  $d-d' \ge 1$  dimensions and periodic boundaries in  $d' \ge 1$ ,

$$\Delta F_{d,d'}^{(0)} = \begin{cases} \ln(L/\xi_L), & L/\xi_L \to 0\\ 0, & L/\xi_L = \mathcal{O}(1)\\ 2^{-d}L/\xi_L, & L/\xi_L \to \infty, \quad d' = 1\\ 0, & L/\xi_L \to \infty, \quad d' \ge 2 \end{cases}$$
(1.6)

Therefore, a logarithmic contribution appears only in the case when  $L/\xi_L \rightarrow 0$  as  $L \rightarrow \infty$ , or in the special case when d' = 1 and  $L/\xi_L \propto \ln L$ , as  $L \rightarrow \infty$ .

Unfortunately, mathematical problems kept us from considering in the same way the case of fixed boundary conditions.

The aim of the present work is to complete the investigation of the logarithmic finite-size correction terms  $\Delta F_{d,d'}^{(\tau)}$  in the free energy of the mean spherical model by including the case of fixed boundary conditions ( $\tau = 1$ ). We use here an analytical approach similar to that of Shapiro and Rudnick,<sup>(12)</sup> but confine ourselves to d=3. One of our key findings is that under fully fixed boundary conditions ( $\tau = 1$ ) a new double-logarithmic term appears:

$$\Delta F_{3,0}^{(1)}(T_c; L) = 2^{-3}(1+9\pi)\ln L - 2^{-1}\ln\ln L \tag{1.7}$$

To clarify the origin of the last term in the right-hand side of (1.7), we consider also geometries without corners by imposing periodic boundary

conditions along d' = 1, 2, 3 dimensions. It turns out that besides the ln L term, which is due to the corners, there are ln L and ln ln L terms persisting in all cases with fixed surfaces:

$$\Delta F_{3,d'}^{(1)}(T_c;L) = \begin{cases} 2^{-1}\pi \ln L - 2^{-1} \ln \ln L, & d' = 1\\ 2^{-3}\pi \ln L - 2^{-1} \ln \ln L, & d' = 2\\ 0, & d' = 3 \end{cases}$$
(1.8)

The explanation of this fact can be sought in the fact that the critical finite-size correlation length behaves as  $\xi_L^{(1)} \propto L \ln^{1/2} L$  in the presence of free surfaces and as  $\xi_L^{(1)} \propto L$  in the absence of such.

The above results motivated a reexamination of the case of free boundary conditions by using the same techniques. Here we confirm and extend the results of our work in ref. 9.

The paper is organized as follows. In Section 2 we give a definition of the model and present convenient starting expressions for the further investigation. The method of analysis of the mean spherical constraint and the free energy for a large but finite system in two critical regimes is described in Section 3. The results for the asymptotic behavior of the solution of the mean spherical constraint are obtained in Section 4 separately for different boundary conditions: fully free; free along 3 - d' dimensions and periodic along d' = 1; 2 dimensions; fully fixed; and fixed along 3 - d'dimensions and periodic along d' = 1, 2 dimensions. The corresponding logarithmic corrections in the free energy are derived in Section 5. The paper closes with a discussion in Section 6.

# 2. THE MODEL

We consider the ferromagnetic mean spherical model (see, e.g., the review in ref. 13) on a finite *d*-dimensional hypercubic lattice  $\Lambda_d = L \times L \times \cdots \times L \in \mathbb{Z}^d$  of  $L^d$  sites. The Hamiltonian has the form

$$\beta \mathscr{H}_{\Lambda}^{(\tau)}(\{\sigma_i\}_{i \in \Lambda}) = -\frac{1}{2}K \sum_{\langle i,j \rangle} \sigma_i \sigma_j$$
(2.1)

Here  $\sigma_i \in \mathbb{R}^1$ ,  $i \in A$ , are the dynamical variables,  $\beta = 1/kT$  is the inverse temperature, and K is the dimensionless coupling. The summation in (2.1) is taken over all different pairs  $\langle i, j \rangle$  of nearest neighbors under the imposed boundary conditions. The dependence on the boundary conditions will be denoted by a superscript  $(\tau)$ ;  $\tau = 1$  for fixed and  $\tau = 0$  for free boundaries; the number of additional periodic boundaries is denoted by the

subscript d' = 0, 1, ..., d-1. In the mean spherical ensemble the partition function is given by

$$Z_{d,d'}^{(\tau)}(K,s;L) = \int_{\mathbb{R}} \cdots \int_{\mathbb{R}} \prod_{i \in A} dx \exp\left[-\beta \mathscr{H}_{A}^{(\tau)}(\{x_i\}_{i \in A}) - s \sum_{i \in A} x_i^2\right] \quad (2.2)$$

where s is the spherical field. The canonical free energy in units of  $(kT)^{-1}$ ,  $F_{d,d'}^{(\tau)}(K; L)$ , is defined by the Legendre transformation

$$F_{d,d'}^{(\tau)}(K;L) = \sup_{s} \{ -\ln Z_{d,d'}^{(\tau)}(K,s;L) - sL^{d} \}$$
(2.3)

The eigenvalues  $\varepsilon_{d,d'}^{(\tau)}$  of the quadratic form in the exponent of the integrand in the right-hand side of (2.2) are well known under the considered sets of boundary conditions (see, e.g., ref. 5). In the case of d' periodic and d-d' free boundaries we take

$$\varepsilon_{d,d'}^{(0)}(\mathbf{k};s,K) = s - K \sum_{\nu=1}^{d'} \cos \frac{2\pi k_{\nu}}{L_{\nu}} - K \sum_{\nu=d'+1}^{d} \cos \frac{\pi k_{\nu}}{L_{\nu}}$$
(2.4)

where  $\mathbf{k} = \{k_1, ..., k_d\}$ , with

$$k_v = 0, 1, ..., L - 1, \quad v = 1, ..., d$$
 (2.5)

In the case of d' periodic and d-d' fixed boundaries we take

$$\varepsilon_{d,d'}^{(1)}(\mathbf{k};s,K) = s - K \sum_{\nu=1}^{d} \cos \frac{2\pi k_{\nu}}{L_{\nu}} - K \sum_{\nu=d'+1}^{d} \cos \frac{\pi (k_{\nu}+1)}{L_{\nu}+1}$$
(2.6)

with the same set (2.5) of values for  $k_v$ , v = 1,..., d. Therefore, by performing the integration in (2.3), one obtains, apart from a normalization constant,

$$F_{d,d'}^{(\tau)}(K;L) = \sup_{s} \left\{ \frac{1}{2} \sum_{k_1=0}^{L-1} \cdots \sum_{k_d=0}^{L-1} \ln \varepsilon_{d,d'}^{(\tau)}(\mathbf{k};s,K) - sL^d \right\}$$
(2.7)

Now it is convenient to replace the spherical field s by another field  $\lambda$ , defined as

$$\lambda = 2s/K - 2d \qquad (\tau = 0)) \lambda = 2s/K - 2d' - 2(d - d') \cos \frac{\pi}{L + 1} \qquad (\tau = 1)$$
(2.8)

Then we can write

$$\ln \varepsilon_{d,d'}^{(\tau)}(\mathbf{k}; s, K) = \ln(K/2) + \ln[\lambda + \omega_{d,d'}^{(\tau)}(\mathbf{k})]$$
(2.9)

#### **Brankov and Danchev**

where

$$\omega_{d,d'}^{(0)}(\mathbf{k}) = 2\sum_{\nu=1}^{d'} \left(1 - \cos\frac{2\pi k_{\nu}}{L_{\nu}}\right) + 2\sum_{\nu=d'+1}^{d} \left(1 - \cos\frac{\pi k_{\nu}}{L_{\nu}}\right)$$
(2.10)

$$\omega_{d,d'}^{(1)}(\mathbf{k}) = 2\sum_{\nu=1}^{d} \left(1 - \cos\frac{2\pi k_{\nu}}{L_{\nu}}\right) + 2\sum_{\nu=d'+1}^{d} \left(1 - \cos\frac{\pi (k_{\nu}+1)}{L_{\nu}+1}\right) \quad (2.11)$$

Next, by using the identity

$$\ln[\lambda + \omega_{d,d'}^{(\tau)}(\mathbf{k})] = \ln \lambda + \int_0^\infty \frac{dx}{x} e^{-\lambda x} \{1 - \exp[-x\omega_{d,d'}^{(\tau)}(\mathbf{k})]\} \quad (2.12)$$

we obtain from (2.7)-(2.12) the following representation for the singular part of the free energy:

$$F_{d,d'}^{(\tau)}(K;L) = L^d \sup_{\lambda} g_{d,d'}^{(\tau)}(K;\lambda,L)$$
(2.13)

where

$$g_{d,d'}^{(\epsilon)}(K;\lambda,L) = \frac{1}{2} \left( \ln \lambda + \int_0^\infty \frac{dx}{x} e^{-\lambda x} \{ 1 - L^{-d} [S_L^{(p)}(x)]^{d'} [S_L^{(\epsilon)}(x)]^{d-d'} \} - \lambda K \right)$$
(2.14)

Here we have used the notation

$$S_{L}^{(p)}(x) = \sum_{k=0}^{L-1} \exp\left[-2x\left(1 - \cos\frac{2\pi k}{L}\right)\right]$$
(2.15)

$$S_{L}^{(0)}(x) = \sum_{k=0}^{L-1} \exp\left[-2x\left(1 - \cos\frac{\pi k}{L}\right)\right]$$
(2.16)

$$S_{L}^{(1)}(x) = \sum_{k=0}^{L-1} \exp\left[-2x\left(\cos\frac{\pi}{L+1} - \cos\frac{\pi(k+1)}{L+1}\right)\right]$$
(2.17)

Obviously, the supremum in the right-hand side of (2.13) is attained at a value  $\lambda = \lambda_L(K)$ , which obeys the equation

$$L^{-d} \int_0^\infty dx \, e^{-\lambda x} [S_L^{(p)}(x)]^{d'} [S_L^{(\tau)}(x)]^{d-d'} = K$$
(2.18)

Expressions (2.13)-(2.18) provide the basis of our further analysis.

780

# 3. THE METHOD

We take into account that in the bulk limit  $L \rightarrow \infty$ ,  $\lambda$  fixed, the left-hand side of (2.18) becomes<sup>(12,14)</sup>

$$\int_{0}^{\infty} dx \, e^{-\lambda x} [e^{-2x} I_0(2x)]^d = W_d(\lambda) \tag{3.1}$$

where  $W_d(\lambda)$  is the *d*-dimensional Watson integral, and rewrite Eq. (2.18) in the form

$$L^{-d} \int_{0}^{\infty} dx \, e^{-\lambda x} [S_{L}^{(p)}(x)]^{d'} [S_{L}^{(\tau)}(x)]^{d-d'} -\int_{0}^{\infty} dx \, e^{-\lambda x} [e^{-2x} I_{0}(2x)]^{d} = K - W_{d}(\lambda)$$
(3.2)

By applying the Poisson summation formula (see, e.g., ref. 14) to (2.15) and (2.16), we obtain

$$S_L^{(p)}(x) = \sum_{q = -\infty}^{\infty} L \int_0^1 d\alpha \exp(2i\pi q L\alpha) A^{(p)}(\alpha, x)$$
(3.3a)

$$S_{L}^{(0)}(x) = \sum_{q = -\infty}^{\infty} L \int_{0}^{1} d\alpha \exp(2i\pi q L\alpha) A^{(0)}(\alpha, x) + [A^{(0)}(0, x) - A^{(0)}(1, x)]/2$$
(3.3b)

where

$$A^{(p)}(\alpha, x) = \exp[-2x(1 - \cos 2\pi\alpha)]$$
 (3.4a)

$$A^{(0)}(\alpha, x) = \exp[-2x(1 - \cos \pi \alpha)]$$
 (3.4b)

Then, following the method of Shapiro and Rudnick,<sup>(12)</sup> we divide the first integral over x in (3.2) into two parts,

$$L^{-d} \int_{0}^{\varepsilon L^{2}} dx \, e^{-\lambda x} [S_{L}^{(p)}(x)]^{d'} [S_{L}^{(\tau)}(x)]^{d-d'} \equiv P_{d,d'}^{(\tau)}(\lambda;\varepsilon,L) \qquad (3.5a)$$

$$L^{-d} \int_{\varepsilon L^2}^{\infty} dx \, e^{-\lambda x} [S_L^{(p)}(x)]^{d'} [S_L^{(\tau)}(x)]^{d-d'} \equiv Q_{d,d'}^{(\tau)}(\lambda;\varepsilon,L) \quad (3.5b)$$

where  $\varepsilon > 0$  is to be determined.

Let us consider first the term (3.5b). For  $\varepsilon$  fixed and L sufficiently large, due to the rapid convergence of the sums (2.15)–(2.17) we can use

$$S_L^{(p)}(x) \cong 1 + 2R_1(4\pi^2 x/L^2) + u_1(x;L) - Lv(x;L)$$
(3.6a)

$$S_L^{(0)}(x) \cong 1 + R_1(\pi^2 x/L^2) - u_2(x;L) - Lv(x;L) - e^{-4x}/2$$
 (3.6b)

where

$$R_{1}(z) = \sum_{q=1}^{\infty} e^{-zq^{2}}$$

$$u_{1}(x; L) = e^{-\pi^{2}x} [L/2\pi^{2}x - \operatorname{cosech}(2\pi^{2}x/L)]$$

$$u_{2}(x; L) = \frac{1}{2}e^{-\pi^{2}x} [\operatorname{cotanh}(\pi^{2}x/L) - L/\pi^{2}x]$$

$$v(x; L) = (4\pi x)^{-1/2} [1 - \operatorname{erf}(\pi x^{1/2})]$$
(3.7)

The expression for  $S_L^{(1)}(x)$  follows from (3.6b) and the exact relationship

$$S_{L}^{(1)}(x) = \exp\left[2x\left(1 - \cos\frac{\pi}{L+1}\right)\right] \left[S_{L+1}^{(0)}(x) - 1\right]$$
(3.8)

Hence,

$$S_{L}^{(1)}(x) \cong 1 + R_{2}(\pi^{2}x/(L+1)^{2}) - \exp[\pi^{2}x/(L+1)^{2}][u_{2}(x;L+1) + (L+1)v(x;L+1) + e^{-4x}/2] (3.9)$$

where

$$R_2(z) = \sum_{q=2}^{\infty} \exp[-z(q^2 - 1)]$$
(3.10)

By changing the integration variable in (3.5b), we obtain

$$Q_{d,d'}^{(\tau)}(\lambda;\varepsilon,L) = \varepsilon L^{2-d} \int_{1}^{\infty} dx \exp(-\lambda L^{2}\varepsilon x) \left[ S_{L}^{(p)}(\varepsilon L^{2}x) \right]^{d'} \left[ S_{L}^{(\tau)}(\varepsilon L^{2}x) \right]^{d-d'}$$
(3.11)

From (3.6)–(3.10) we have the estimates  $(x \ge 1)$ 

$$S^{(p)}(\varepsilon L^2 x) = 1 + \mathcal{O}[\exp(-4\pi^2 \varepsilon x)]$$
(3.12a)

$$S^{(0)}(\varepsilon L^2 x) = 1 + \mathcal{O}[\exp(-\pi^2 \varepsilon x)]$$
(3.12b)

$$S^{(1)}(\varepsilon L^2 x) = 1 + \mathcal{O}\{\exp[-3\pi^2 \varepsilon x L^2/(L+1)^2]\}$$
(3.12c)

782

 $(x \ge \varepsilon L^2)$ 

Therefore, from (3.11) and (3.12) it follows that:

Next we consider the term (3.5a). From (3.3) and (3.4) it is clear that if  $q \neq 0$  and  $L \rightarrow \infty$ , the main contribution in the integrals over  $\alpha$  comes from the neighborhood of  $\alpha = 0$ . Therefore, in this case we can use again the quadratic approximation of  $\cos z$  in (3.4). The remaining term with q = 0 can be integrated exactly. Thus, with the use of the Jacobi identity we obtain  $(0 \le x \le \varepsilon L^2)$ 

$$S_L^{(p)}(x) \cong Le^{-2x}I_0(2x) + L(\pi x)^{-1/2}R_1(L^2/4x) + u_1(x;L) \quad (3.15a)$$
  
$$S_L^{(0)}(x) \cong Le^{-2x}I_0(2x) + (1 - e^{-4x})/2$$

$$\begin{array}{l} (x) \cong Le \quad -\Gamma_0(2x) + (1 - e^{-x})/2 \\ + L(\pi x)^{-1/2} R_1(L^2/x) - u_2(x;L) \end{array}$$
(3.15b)

Note that due to relationship (3.8) the term (3.5a) for fixed boundary conditions,  $\tau = 1$ , can be written as

$$P_{d,d'}^{(1)}(\lambda;\varepsilon,L) = L^{-d} \int_0^{\varepsilon L^2} dx \ e^{-\tilde{\lambda}x} \left[ S_L^{(p)}(x) \right]^{d'} \left[ S_{L+1}^{(\tau)}(x) - 1 \right]^{d-d'} (3.16)$$

where

$$\tilde{\lambda} = \lambda - 2(d - d') \left(1 - \cos\frac{\pi}{L + 1}\right)$$
(3.17)

Now we evaluate the contributions in the integral (3.5a) from different products of the terms which enter into the right-hand sides of (3.15a) and (3.15b).

1. First, we note that

$$0 \le u_i(x; L) \le \mathcal{O}(1)e^{-\pi^2 x} \qquad (i = 1, 2)$$
(3.18)

Therefore, the contribution from integrands containing the factors  $u_i(x; L)$  may be estimated as (p = 1, ..., d)

$$L^{-p} \int_{0}^{eL^{2}} dx \ e^{-\lambda x} [e^{-2x} I_{0}(2x)]^{d-p} [u_{i}(x;L)]^{p}$$
$$= \mathcal{O}(L^{-p}) \times \text{analytical in } \lambda \text{ function}$$
(3.19)

#### **Brankov and Danchev**

and similarly in the case of products containing as cofactors other combinations of the terms  $e^{-2x}I_0(2x)$ ,  $(1-e^{-4x})/2$ , and  $u_i(x; L)$  with i=1, 2.

2. Second, we consider products containing the factors  $(\pi x)^{-1/2} R_1(L^2/ax)$  with a = 1 or 4. Let us divide the integration interval into two parts. The integrals over [0, M] are readily estimated,

$$\int_{0}^{M} dx \, e^{-\lambda x} [e^{-2x} I_{0}(2x)]^{d-p} [(\pi x)^{-1/2} R_{1}(L^{2}/ax)]^{p}$$
$$= \mathcal{O}(1) \int_{0}^{M} dx \, x^{-p/2} \exp(-pL^{2}/ax)$$
$$= \mathcal{O}[L^{-2} \exp(-pL^{2}/aM)]$$
(3.20)

To estimate the contribution from the remaining part of the interval, we choose M sufficiently large, so that

$$\int_{M}^{\varepsilon L^{2}} dx \ e^{-\lambda x} \left[ e^{-2x} I_{0}(2x) \right]^{d-p} \left[ (\pi x)^{-1/2} R_{1}(L^{2}/ax) \right]^{p}$$

$$\propto \int_{M}^{\varepsilon L^{2}} dx \ x^{-d/2} e^{-\lambda x} \exp(-pL^{2}/ax)$$
(3.21)

Now we have to specify the regime of  $\lambda L^2$  as  $\lambda \to 0$  and  $L \to \infty$ .

(a) If  $\lambda L^2 \to \infty$  as  $\lambda \to 0$  and  $L \to \infty$ , the integral in (3.21) can be approximated by

$$\lambda^{d/2 - 1} \int_{0}^{\infty} dx \, x^{-d/2} e^{-x} \exp(-p\lambda L^{2}/ax)$$
  

$$\propto \lambda^{d/4 - 1} L^{-d/2} \exp[-2(p\lambda L^{2}/a)^{1/2}]$$
(3.22)

(b) If  $\lambda L^2 = \mathcal{O}(1)$  or  $\lambda L^2 \to 0$  as  $\lambda \to 0$  and  $L \to \infty$ , after changing the integration variable  $x \to L^2/t$  in the right-hand side of (3.21), we obtain

$$L^{2-d} \int_{1/\varepsilon}^{L^2/M} dt \ t^{-d/2-2} \exp(-\lambda L^2/t - pt/a) = \mathcal{O}(L^{2-d})$$
(3.23)

3. Finally, notice that (p = 1, ..., d)

$$L^{-p} \int_{0}^{\epsilon L^{2}} dx \ e^{-\lambda x} [e^{-2x} I_{0}(2x)]^{d-p} [(1-e^{-4x})/2]^{p}$$
  
=  $(2L)^{-p} \int_{0}^{\epsilon L^{2}} dx \ e^{-\lambda x} [e^{-2x} I_{0}(2x)]^{d-p}$   
+  $\mathcal{O}(L^{-p}) \times \text{analytical in } \lambda \text{ function}$  (3.24)

Collecting the above results, for the integral (3.5a) with  $\tau = 0$  we obtain

$$P_{d,d'}^{(0)}(\lambda;\varepsilon,L) = \sum_{p=0}^{d-d'} {d-d' \choose p} (2L)^{-p} \int_0^{\varepsilon L^2} dx \ e^{-\lambda x} [e^{-2x} I_0(2x)]^{d-p} + \mathcal{O}(L^{2-d}) + O(L^{-1})$$
(3.25)

Turning to the case of fixed boundary conditions [see (3.16)], we note that  $\lambda L^2 \to \infty$  as  $\lambda \to 0$  and  $L \to \infty$  implies  $\tilde{\lambda} L^2 \to \infty$  and  $\tilde{\lambda} \to 0^+$ , while  $\lambda L^2 = \mathcal{O}(1)$  or  $\lambda L^2 \to 0$  as  $\lambda \to 0$  and  $L \to \infty$  implies  $\tilde{\lambda} L^2 = \mathcal{O}(1)$ . Therefore, essentially repeating the steps given by (3.18)–(3.24), we obtain

$$P_{d,d'}^{(1)}(\lambda;\varepsilon,L) = (1+L^{-1})^{d-d'} \sum_{p=0}^{d-d'} {d-d' \choose p} [-2(L+1)]^{-p} \times \int_0^{\varepsilon L^2} dx \ e^{-\bar{\lambda}x} [e^{-2x} I_0(2x)]^{d-p} + \mathcal{O}(L^{2-d}) + \mathcal{O}(L^{-1})$$
(3.26)

We are ready now to study the mean spherical constraint (3.2) in the three-dimensional case, d=3, under the boundary conditions specified by  $\tau = 0, 1$  and d' = 0, 1, 2.

# 4. THE MEAN SPHERICAL CONSTRAINT

We make use of the asymptotic expansion<sup>(13)</sup>

$$W_3(\lambda) = K_c - \lambda^{1/2} / 4\pi + \mathcal{O}(\lambda) \tag{4.1}$$

and rewrite Eq. (3.2) at d = 3 in the form [see (3.5)]

$$P_{3,d'}^{(\tau)}(\lambda;\varepsilon,L) + Q_{3,d'}^{(\tau)}(\lambda;\varepsilon,L) - W_3(\lambda) = K - K_c + \lambda^{1/2}/4\pi + \mathcal{O}(\lambda)$$
(4.2)

(i) Let us consider first the case of fully free boundary conditions,  $\tau = 0$ , d' = 0. To proceed, we need to specify the behavior of  $\lambda L^2$  as  $\lambda \to 0$  and  $L \to \infty$ .

(a) Let  $\lambda L^2 \to \infty$  as  $\lambda \to 0$  and  $L \to \infty$ . Then we make use of (3.1) to obtain (p = 0, 1, ..., d)

$$\int_{0}^{\varepsilon L^{2}} dx \ e^{-\lambda x} \left[ e^{-2x} I_{0}(2x) \right]^{d-p} = W_{d-p}(\lambda) + \mathcal{O}(e^{-\varepsilon \lambda L^{2}}) \tag{4.3}$$

By inserting (4.3) in (3.25) and taking into account (3.13), we obtain that Eq. (4.2) at  $\tau = 0$  and d' = 0 becomes

$$3W_{2}(\lambda)/2L + 3W_{1}(\lambda)/4L^{2} + (8\lambda L^{3})^{-1} + \mathcal{O}(L^{-1})$$
  
=  $K - K_{c} + \lambda^{1/2}/4\pi + \mathcal{O}(\lambda)$  (4.4)

Since<sup>(13)</sup>

$$W_{2}(\lambda) = (1/4\pi) \ln \lambda^{-1} + \mathcal{O}(1)$$
  

$$W_{1}(\lambda) = (1/2)\lambda^{-1/2} + \mathcal{O}(\lambda^{1/2})$$
(4.5)

Eq. (4.4) can be written in the form

$$(3/8\pi) \ln \lambda^{-1} = (K - K_c) L + \lambda^{1/2} L / 4\pi + \mathcal{O}(\lambda L) + \mathcal{O}(1)$$
(4.6)

Therefore, if  $(K - K_c)L = \mathcal{O}(1)$ , the solution of (4.6) is  $\lambda_L^{1/2} \cong 3(\ln L)/L$ , in conformity with the assumption  $\lambda L^2 \to \infty$  as  $\lambda \to 0$  and  $L \to \infty$ .

An equivalent form of Eq. (4.6) is

$$-(3/4\pi)\ln(\lambda^{1/2}L) - \lambda^{1/2}L/4\pi = (K - K_{c,L}^{(0)})L + \mathcal{O}(\lambda L) + \mathcal{O}(1)$$
(4.7)

where we have introduced a shifted critical coupling

$$K_{c,L}^{(0)} = K_c + 3(\ln L)/4\pi L \qquad (d = 3, d' = 0)$$
(4.8)

Hence, if  $(K - K_{c,L}^{(0)})L = \mathcal{O}(1)$ , the mean spherical constraint has no solution  $\lambda = \lambda_L \to 0$  with the assumed property  $\lambda_L L^2 \to \infty$  as  $L \to \infty$ .

(b) Let  $\lambda L^2 = \mathcal{O}(1)$  or  $\lambda L^2 \to 0$  as  $\lambda \to 0$  and  $L \to \infty$ . Obviously, for the integral in (3.25) with p = d = 3 one has

$$(2L)^{-3} \int_0^{\varepsilon L^2} dx \ e^{-\lambda x} = (2L)^{-3} \lambda^{-1} (1 - e^{-\varepsilon \lambda L^2}) \tag{4.9}$$

To consider the integrals with p = 1 and p = 2, we divide the integration interval into two parts and notice that for any fixed M > 0,

$$(2L)^{-p} \int_0^M dx \ e^{-\lambda x} [e^{-2x} I_0(2x)]^{3-p} = \mathcal{O}(L^{-p})$$
(4.10)

To evaluate the integral over the remaining part of the interval, we choose M sufficiently large and make use of the asymptotic form of the modified Bessel function:

$$(2L)^{-p} \int_{M}^{eL^{2}} dx \ e^{-\lambda x} [e^{-2x} I_{0}(2x)]^{3-p}$$
  

$$\approx (4\pi)^{(p-3)/2} (2L)^{-p} \int_{M}^{eL^{2}} dx \ e^{-\lambda x} x^{(p-3)/2}$$
(4.11)

786

Now, by expanding the exponent in the right-hand side of (4.11) into power series, we obtain (p = 1)

$$(2L)^{-1} \int_{M}^{\varepsilon L^{2}} dx \ e^{-\lambda x} [e^{-2x} I_{0}(2x)]^{2} = (4\pi L)^{-1} \ln L + \mathcal{O}(L^{-1}) \quad (4.12)$$

and (p=2)

$$(2L)^{-2} \int_{M}^{\varepsilon L^{2}} dx \, e^{-\lambda x} e^{-2x} I_{0}(2x) = \mathcal{O}(L^{-1})$$
(4.13)

By inserting (4.9)–(4.13) in (3.25) and taking into account (3.14), we find that Eq. (4.2) at  $\tau = 0$  and d' = 0 becomes

$$(\lambda L^{2})^{-1} + (3/4\pi) \ln L + (8\lambda L^{2})^{-1} [1 - \exp(-\varepsilon\lambda L^{2})]$$
  
=  $(K - K_{c})L + \lambda^{1/2}L/4\pi + \mathcal{O}(1)$  (4.14)

Obviously, if  $(K-K_c)L = \mathcal{O}(1)$ , this equation has no solution  $\lambda = \lambda_L \to 0$ with the assumed property  $\lambda_L L^2 = \mathcal{O}(1)$  or  $\lambda_L L^2 \to 0$  as  $L \to \infty$ . A solution  $\lambda_L = \mathcal{O}(L^{-2})$  exists only if  $(K-K_{c,L}^{(0)})L = \mathcal{O}(1)$ , where  $K_{c,L}^{(0)}$  is given by (4.8).

Summarizing the above results, we have that the solution  $\lambda = \lambda_L$  of the mean spherical constraint in the case of fully free boundary conditions is

$$\lambda_L \approx [3(\ln L)/L]^2 \quad \text{if} \quad (K - K_c)L = \mathcal{O}(1)$$
  

$$\lambda_L = \mathcal{O}(L^{-2}) \quad \text{if} \quad (K - K_{c,L}^{(0)})L = \mathcal{O}(1)$$
(4.15)

(ii) Consider now the case of 3-d' dimensions with free boundaries and d' = 1, 2 dimensions with periodic boundaries.

(a) If  $\lambda L^2 \to \infty$  as  $\lambda \to 0$  and  $L \to \infty$ , from (3.13), (3.25), (4.3), and (4.5) we obtain (4.2) in the form

$$[(3-d')/8\pi] \ln \lambda^{-1} = (K-K_c)L + \lambda^{1/2}L/4\pi + \mathcal{O}(\lambda L) + \mathcal{O}(1) \quad (4.16)$$

Therefore, if  $(K-K_c)L = \mathcal{O}(1)$ , the solution of (4.16) is  $\lambda_L^{1/2} \cong (3-d')(\ln L)/L$ .

Equation (4.16) has the equivalent form

$$- [(3 - d')/4\pi] \ln(\lambda^{1/2}L) - \lambda^{1/2}L/4\pi$$
  
=  $(K - K_{c,L}^{(0)})L + \mathcal{O}(\lambda L) + \mathcal{O}(1)$  (4.17)

where

$$K_{c,L}^{(0)} = K_c + (3 - d')(\ln L)/4\pi L$$
(4.18)

Hence, if  $(K - K_{c,L}^{(0)})L = \mathcal{O}(1)$ , Eq. (4.17) has no solution  $\lambda = \lambda_L \to 0$  with the above assumed property  $\lambda_L L^2 \to \infty$  as  $L \to \infty$ .

(b) If  $\lambda L^2 = \mathcal{O}(1)$  or  $\lambda L^2 \to 0$  as  $\lambda \to 0$  and  $L \to \infty$ , by inserting (4.10)–(4.13) in (3.25) and taking into account (3.14), we find that Eq. (4.2) becomes

$$(\lambda L^2)^{-1} + [(3-d')/4\pi] \ln L = (K-K_c)L + \lambda^{1/2}L/4\pi + \mathcal{O}(1)$$
(4.19)

Obviously, if  $(K-K_c)L = \mathcal{O}(1)$ , this equation has no solution  $\lambda = \lambda_L \to 0$ with the assumed property  $\lambda_L L^2 = \mathcal{O}(1)$  or  $\lambda_L L^2 \to 0$  as  $L \to \infty$ . A solution  $\lambda_L = \mathcal{O}(L^{-2})$  exists only if  $(K-K_{c,L}^{(0)})L = \mathcal{O}(1)$ , where  $K_{c,L}^{(0)}$  is given by (4.18).

Summarizing the above results, we find that the solution  $\lambda = \lambda_L$  of the mean spherical constraint in the case of 3 - d' free and d' = 1, 2 periodic boundaries is

$$\lambda_L \approx [(3-d') \ln L)/L]^2 \quad \text{if} \quad (K-K_c)L = \mathcal{O}(1)$$
  

$$\lambda_L = \mathcal{O}(L^{-2}) \quad \text{if} \quad (K-K_{c,L}^{(0)})L = \mathcal{O}(1) \quad (4.20)$$

Note that expressions (4.18) and (4.20) at d' = 0 reduce to expressions (4.8) and (4.15), respectively.

(iii) Next we consider the case of fully fixed boundary conditions,  $\tau = 1, d' = 0.$ 

(a) If  $\lambda L^2 \to \infty$  as  $\lambda \to 0$  and  $L \to \infty$ , then  $\tilde{\lambda} L^2 \to \infty$  and  $\tilde{\lambda} \to 0^+$  as  $L \to \infty$  [see (3.17)]. Therefore, we can make use of (3.1) to obtain (p=0, 1, ..., d)

$$\int_{0}^{\varepsilon L^{2}} dx \, e^{-\tilde{\lambda}x} [e^{-2x} I_{0}(2x)]^{d-p} = W_{d-p}(\tilde{\lambda}) + \mathcal{O}(e^{-\varepsilon \tilde{\lambda}L^{2}}) \tag{4.21}$$

Now it is convenient to use in Eq. (4.2) the expansion (4.1) in terms of  $\overline{\lambda}$  instead of  $\lambda$ . Then, by inserting (4.21) in (3.26) and taking into account (3.13), we find that Eq. (4.2) becomes

$$[1 + \mathcal{O}(L^{-1})][3W_{3}(\tilde{\lambda})/L - 3W_{2}(\tilde{\lambda})/2L + 3W_{1}(\tilde{\lambda})/4L^{2}] - (8\tilde{\lambda}L^{3})^{-1} + \mathcal{O}(L^{-1}) = K - K_{c} + \tilde{\lambda}^{1/2}/4\pi + \mathcal{O}(\tilde{\lambda})$$
(4.22)

With the aid of expansions (4.1) and (4.5), we can write Eq. (4.22) in the form

$$-(3/8\pi)[1+\mathcal{O}(L^{-1})]\ln\tilde{\lambda}^{-1}$$
  
=  $(K-K_c)L+\tilde{\lambda}^{1/2}L/4\pi+\mathcal{O}(\tilde{\lambda}L)+\mathcal{O}(1)$  (4.23)

788

Therefore, due to the opposite sign (in comparison with the case of free boundaries) of the surface contribution  $3W_2(\tilde{\lambda})/2L$ , if  $(K-K_c)L = \mathcal{O}(1)$ , the mean spherical constraint (4.23) has no solution  $\lambda = \lambda_L \to 0$  with the property  $\lambda_L L^2 \to \infty$  as  $L \to \infty$ .

(b) If  $\lambda L^2 = \mathcal{O}(1)$  or  $\lambda L^2 \to 0$  as  $\lambda \to 0$  and  $L \to \infty$ , then  $\tilde{\lambda} L^2 = \mathcal{O}(1)$  and  $\tilde{\lambda} \to 0$ . Since now  $\tilde{\lambda}$  may be negative [see (3.17)], the asymptotic expansion (4.1) will be used for  $\lambda$  rather than for  $\tilde{\lambda}$ . Thus, by inserting in (3.26) the counterparts of (4.9)–(4.13) and taking into account (3.14), we can write Eq. (4.2) as

$$-(3/4\pi L)[1 + \mathcal{O}(L^{-1})] \ln L + \mathcal{O}(L^{-1}) + \int_{0}^{\varepsilon L^{2}} dx \ e^{-\tilde{\lambda}x} [e^{-2x} I_{0}(2x)]^{3} - W_{3}(\lambda) - (1 - e^{-\varepsilon \tilde{\lambda}L^{2}})/8\tilde{\lambda}L^{3} + 1/\lambda L^{3} = K - K_{c} + \lambda^{1/2}/4\pi + \mathcal{O}(\lambda)$$
(4.24)

Now we write

$$\int_{0}^{\varepsilon L^{2}} dx \ e^{-\tilde{\lambda}x} [e^{-2x}I_{0}(2x)]^{3} = \int_{0}^{\varepsilon L^{2}} dx \ e^{-\lambda x} [e^{-2x}I_{0}(2x)]^{3} + \int_{0}^{\varepsilon L^{2}} dx \ (e^{-\tilde{\lambda}x} - e^{-\lambda x}) [e^{-2x}I_{0}(2x)]^{3}$$
(4.25)

The first integral in the right-hand side of (4.25) can be evaluated as

$$W_{3}(\lambda) - \int_{eL^{2}}^{\infty} dx \ e^{-\tilde{\lambda}x} [e^{-2x}I_{0}(2x)]^{3} = W_{3}(\lambda) + \mathcal{O}(L^{-1})$$
(4.26)

and for the second integral we have the estimate

$$\mathcal{O}(L^{-2}) + \int_{M}^{\delta L^{2}} dx \ e^{-\lambda x} \{ \exp[3\pi^{2} x/(L+1)^{2}] - 1 \} (4\pi x)^{-3/2} = \mathcal{O}(L^{-1})$$
(4.27)

Thus Eq. (4.24) reduces to

$$-(3/4\pi)\ln L + \lambda^{-1}L^{-2} = (K - K_c)L + \lambda^{1/2}L/4\pi + \mathcal{O}(1)$$
(4.28)

If  $(K-K_c)L = \mathcal{O}(1)$ , the solution of the above equation is  $\lambda = \lambda_L \approx 4\pi/3L^2 \ln L$ ; it has the property  $\lambda_L L^2 \to 0$  as  $L \to \infty$ , hence  $\tilde{\lambda}_L \to 0^-$ . Finally we notice that if a shifted critical coupling is introduced,

$$K_{c,L}^{(1)} = K_c - 3(\ln L)/4\pi L \tag{4.29}$$

then Eq. (4.28) has a solution  $\lambda = \lambda_L = \mathcal{O}(L^{-2})$  when  $(K - K_{c,L}^{(1)})L = \mathcal{O}(1)$ .

Summarizing the above results, we find that the solution  $\lambda = \lambda_L$  of the mean spherical constraint in the case of fully fixed boundary conditions is given by

$$\lambda_L \approx (4\pi/3 \ln L) L^{-2} \quad \text{if} \quad (K - K_c) L = \mathcal{O}(1)$$
  

$$\lambda_L = \mathcal{O}(L^{-2}) \quad \text{if} \quad (K - K_c^{(1)}) L = \mathcal{O}(1)$$
(4.30)

(iv) Finally, we consider the case of 3-d' dimensions with fixed boundaries and d' = 1, 2 dimensions with periodic boundaries.

(a) If  $\lambda L^2 \to \infty$  as  $\lambda \to 0$  and  $L \to \infty$ , we cast (4.2) in the form [compare with (4.23)]

$$- [(3-d')/8\pi] [1 + \mathcal{O}(L^{-1})] \ln \tilde{\lambda}^{-1}$$
$$= (K - K_c)L + \tilde{\lambda}^{1/2}L/4\pi + \mathcal{O}(\tilde{\lambda}L) + \mathcal{O}(1)$$
(4.31)

Therefore, if  $(K - K_c)L = \mathcal{O}(1)$ , the mean spherical constraint (4.31) has no solution  $\lambda = \lambda_L \to 0$  with the property  $\lambda_L L^2 \to \infty$  as  $L \to \infty$ .

(b) If  $\lambda L^2 = \mathcal{O}(1)$  or  $\lambda L^2 \to 0$  as  $\lambda \to 0$  and  $L \to \infty$ , Eq. (4.2) can be written as [compare with (4.28)]

$$-[(3-d')/4\pi] \ln L + \lambda^{-1}L^{-2} = (K-K_c)L + \lambda^{1/2}L/4\pi + \mathcal{O}(1)$$
(4.32)

If  $(K-K_c)L = \mathcal{O}(1)$ , the solution of the above equation is  $\lambda = \lambda_L \approx 4\pi/(3-d')L^2 \ln L$ ; it has the property  $\lambda_L L^2 \to 0$  as  $L \to \infty$ , hence  $\tilde{\lambda}_L \to 0^-$ . If  $(K-K_{c,L}^{(1)})L = \mathcal{O}(1)$ , where

$$K_{c,L}^{(1)} = K_c - (3 - d')(\ln L)/4\pi L$$
(4.33)

then Eq. (4.32) has a solution  $\lambda = \lambda_L = \mathcal{O}(L^{-2})$ .

Summarizing the above results, we find that the solution  $\lambda = \lambda_L$  of the mean spherical constraint in the case of 3 - d' fixed and d' = 1, 2 periodic boundaries is given by

$$\lambda_L \approx [4\pi/(3-d')\ln L]L^{-2} \quad \text{if} \quad (K-K_c)L = \mathcal{O}(1)$$
  

$$\lambda_L = \mathcal{O}(L^{-2}) \quad \text{if} \quad (K-K_{c,L}^{(1)})L = \mathcal{O}(1) \quad (4.34)$$

Note that expressions (4.33) and (4.34) at d' = 0 reduce to expressions (4.29) and (4.30), respectively.

Now we are ready to study the logarithmic finite-size constributions to the free energy in the critical regimes  $(K-K_c)L = \mathcal{O}(1)$  and  $(K-K_{c,L}^{(\tau)})L = \mathcal{O}(1)$ .

# 5. LOGARITHMIC FINITE-SIZE CORRECTIONS IN THE FREE ENERGY

We confine ourselves to deriving corrections in the free energy (2.13), (2.14) which are proportional to  $\ln L$  and  $\ln \ln L$ ; these logarithmic corrections will be denoted by  $\Delta F_{d,d'}^{(\tau)}(K;L)$ . Note that besides the terms which are obtainable directly in the desired form, in the bulk critical regime  $(K-K_c)L = \mathcal{O}(1)$ , due to the logarithmic dependence of  $\lambda = \lambda_L(K)$  on L, we have to take into account some special  $\lambda$ -dependent terms in the asymptotic from of  $g_{d,d'}^{(\tau)}(K;\lambda,L)$  as  $\lambda \to 0$  and  $L \to \infty$ .

1. In the case of free boundary conditions at d=3 [see (4.15) and (4.20)], logarithmic corrections of the proper form may arise from  $\lambda$ -dependent terms proportional to

$$L^{-3}(\lambda_L^{1/2}L) = (3-d')L^{-3}\ln L$$
  

$$L^{-3}\ln\lambda_L = 2L^{-3}(\ln\ln L - \ln L) + \mathcal{O}(L^{-3})$$
(5.1)

2. In the case of fixed boundary conditions at d=3 [see (4.30) and (4.34)], logarithmic corrections of the proper form may arise from  $\lambda$ -dependent terms proportional to

$$L^{-3}(\lambda_L L^2)^{-1} = [(3-d')/4\pi] L^{-3} \ln L$$
  

$$L^{-3} \ln \lambda_L = -L^{-3}(2 \ln L + \ln \ln L) + \mathcal{O}(L^{-3})$$
(5.2)

The following observation greatly simplifies our task. Note that the integral

$$\int_{0}^{\infty} dx \, x^{-1} e^{-(1+\lambda)x} \{ 1 - L^{-d} [S_{L}^{(p)}(x)]^{d'} [S_{L}^{(\tau)}(x)]^{d-d'} \}$$
(5.3)

is an analytical at  $\lambda = 0$  function of  $\lambda$  both for finite L and in the limit  $L \to \infty$ . Therefore, by denoting

s.p. 
$$\Phi(\lambda_L, L) = \text{singular part of } \Phi(\lambda_L, L) \text{ at } \lambda_L = 0$$
  
as  $L \to \infty$  and  $\lambda_L \to 0$  (5.4)

we can write [see (3.5)]

s.p. 
$$g_{d,d'}^{(\tau)}(K; \lambda_L, L)$$
  
= s.p.  $\frac{1}{2} \left( \ln \lambda_L + \int_0^\infty \frac{dx}{x} e^{-\lambda_L x} (1 - e^{-x}) \{ 1 - L^{-d} [S_L^{(p)}(x)]^{d'} [S_L^{(\tau)}(x)]^{d-d'} \} \right)$   
- s.p.  $\frac{1}{2} L^{-d} \int_0^\infty \frac{dx}{x} e^{-\lambda_L x} (1 - e^{-x}) [S_L^{(p)}(x)]^{d'} [S_L^{(\tau)}(x)]^{d-d'}$   
= -s.p.  $\frac{1}{2} \int_{\lambda_L}^1 d\mu \left[ P_{d,d'}^{(\tau)}(\mu; \varepsilon, L) + Q_{d,d'}^{(\tau)}(\mu; \varepsilon, L) \right]$ 
(5.5)

Now we note that the  $\lambda_L$ -dependent terms of the form (5.1) and (5.2), being proportional to  $\lambda_L^{1/2}$ ,  $\ln \lambda_L$ , and  $\lambda_L^{-1}$ , are singular at  $\lambda_L = 0$ . Such contributions can arise only from terms divergent at  $\mu = 0$ , to be denoted by d.t., in the integrand of the integral over  $\mu$  in the right-hand side of (5.5).

From (3.11), by direct integration and using estimates (3.12), we obtain

$$\int_{\lambda_{L}}^{1} d\mu \, Q_{d,d'}^{(\tau)}(\mu;\varepsilon,L)$$

$$= L^{-d} \int_{1}^{\infty} \frac{dx}{x} \exp(-\varepsilon \lambda_{L} L^{2} x) \left[ S_{L}^{(p)}(\varepsilon L^{2} x) \right]^{d'} \left[ S_{L}^{(\tau)}(\varepsilon L^{2} x) \right]^{d-d'}$$

$$+ \mathcal{O}(L^{-d} e^{-\varepsilon L^{2}})$$

$$= \begin{cases} \mathcal{O}(L^{-d} e^{-\varepsilon \lambda_{L} L^{2}}) & \text{if } \lambda_{L} L^{2} \to \infty \\ \mathcal{O}(L^{-d}) & \text{if } \lambda_{L} L^{2} = \mathcal{O}(1) \\ -L^{-d} \ln(\lambda_{L} L^{2}) + \mathcal{O}(L^{-d}) & \text{if } \lambda_{L} L^{2} \to 0 \end{cases}$$
(5.6)

To proceed, we have to specify the boundary conditions.

1. In the case of free boundary conditions it suffices to consider  $\mu \to 0$ and  $\mu L^2 \ge \lambda_L L^2 \to \infty$ . Then from (3.25) and (4.3) we obtain

d.t. 
$$P_{d,d'}^{(0)}(\mu;\varepsilon,L) = \sum_{p=0}^{d-d'} {d-d' \choose p} (2L)^{-p} \, d.t. \, W_{d-p}(\mu)$$
 (5.7)

Thus, by inserting (5.7) in (5.5), performing the integration over  $\mu$  with the aid of expansions (4.5), and taking into account (5.6), we obtain for the logarithmic corrections of the proper form in the free energy density at  $(K-K_c)L = O(1)$ 

$$\Delta F_{d,d'}^{(0)}(K;L) = \begin{cases} 2^{-d-1} \ln \lambda_L + d2^{-d} L \lambda_L^{1/2} & d' = 0\\ 2^{-d} L \lambda_L^{1/2} & d' = 1\\ 0 & d' \ge 2 \end{cases}$$
(5.8)

Finally, setting d=3 in (5.8) and making use of (5.1), we get

$$\Delta F_{3,d'}^{(0)}(K;L) = \begin{cases} \ln L + 2^{-3} \ln \ln L & d' = 0\\ 2^{-2} \ln L & d' = 1\\ 0 & d' \ge 2 \end{cases}$$
(5.9)

2. In the case of fixed boundary conditions from (3.26) we have

d.p. 
$$P_{d,d'}^{(1)}(\mu; \varepsilon, L)$$
  
=  $(1 + L^{-1})^{d-d'} \sum_{p=0}^{d-d'} {d-d' \choose p} [-2(L+1)]^{-p}$   
 $\times$  d.p.  $\int_{0}^{\varepsilon L^{2}} dx \ e^{-\tilde{\mu}x} [e^{-2x} I_{0}(2x)]^{d-p}$  (5.10)

Since the right-hand side of (5.10) depends on  $\mu$  through [see (3.17)]

$$\tilde{\mu} = \mu - \delta_L$$

$$\delta_L \equiv \delta_L(d, d') = 2(d - d') \left(1 - \cos\frac{\pi}{L+1}\right) = \pi^2 (d - d') L^{-2} + \mathcal{O}(L^{-3})$$
(5.11)

we have, for p = 0, 1, ..., d,

s.p. 
$$\int_{\lambda_L}^{1} d\mu \int_{0}^{eL^2} dx \ e^{-\tilde{\mu}x} [e^{-2x} I_0(2x)]^{d-p}$$
  
= s.p.  $\int_{0}^{eL^2} dx \ x^{-1} \{ \exp[x(\delta_L - \lambda_L)] - 1 \} [e^{-2x} I_0(2x)]^{d-p} = 0$  (5.12)

because the right-hand side is regular at  $\lambda_L = 0$  when  $\lambda_L L^2 \rightarrow 0$ . Therefore, logarithmic corrections (to be denoted by l.c.) may arise only from the  $\lambda_L$ -independent part of the integral in the left-hand side of (5.12). Indeed, for p = d we have

l.c. 
$$\int_{\lambda_L}^{1} d\mu \int_{0}^{\varepsilon L^2} dx \ e^{-\tilde{\mu}x} = 1.c. \int_{0}^{1} d\mu \ \tilde{\mu}^{-1} [1 - \exp(-\varepsilon \tilde{\mu} L^2)] = 2 \ln L$$
 (5.13)

Further, for p = d - 1,

$$\begin{aligned} &\text{l.c. } \int_{\lambda_{L}}^{1} d\mu \int_{0}^{\varepsilon L^{2}} dx \ e^{-\tilde{\mu}x} e^{-2x} I_{0}(2x) \\ &= \text{l.c. } (4\pi)^{-1/2} \int_{0}^{1} d\mu \int_{M}^{\varepsilon L^{2}} dx \ x^{-1/2} e^{-\tilde{\mu}x} \\ &= \mathcal{O}(1) \text{ l.c. } \int_{0}^{1} d\mu \ |\tilde{\mu}|^{-1/2} = 0 \end{aligned}$$
(5.14)

for p = d - 2,

$$\begin{aligned} \text{l.c.} & \int_{\lambda_{L}}^{1} d\mu \int_{0}^{\epsilon L^{2}} dx \ e^{-\tilde{\mu}u} [e^{-2x} I_{0}(2x)]^{2} \\ &= \text{l.c.} \ (4\pi)^{-1} \int_{0}^{1} d\mu \int_{M}^{\epsilon L^{2}} dx \ x^{-1} e^{-\tilde{\mu}x} \\ &= \text{l.c.} \ (4\pi)^{-1} \int_{0}^{1} d\mu \ln |\tilde{\mu}|^{-1} \\ &= 2\pi (d-d') (2L)^{-2} \ln L \end{aligned}$$
(5.15)

and for  $p \ge d-3$ ,

l.c. 
$$\int_{\lambda_L}^{1} d\mu \int_{0}^{eL^2} dx \ e^{-\tilde{\mu}x} [e^{-2x} I_0(2x)]^{d-p}$$
  
=  $\mathcal{O}(1)$  l.c.  $\int_{0}^{1} d\mu \ |\tilde{\mu}|^{(d-p-2)/2} = 0$  (5.16)

Thus, collecting the results (5.5), (5.6), and (5.10)–(5.16), for the logarithmic corrections of the proper form in the free energy at  $(K-K_c)L = \mathcal{O}(1)$  we obtain

$$\Delta F_{d,0}^{(1)}(K;L) = -[1 + \pi d^2 (d-1)/2](-2)^{-d} \ln L + 2^{-1} \ln(\lambda_L L^2)$$
(5.17a)

$$\Delta F_{d,1}^{(1)}(K;L) = -\pi (d-1)^2 (-2)^{-d} \ln L + 2^{-1} \ln(\lambda_L L^2)$$
(5.17b)

$$\Delta F_{d,2}^{(1)}(K;L) = -\pi (d-2)(-2)^{-d} \ln L + 2^{-1} \ln(\lambda_L L^2)$$
(5.17c)

and

$$\Delta F_{d,d'}^{(1)}(K;L) = 2^{-1} \ln(\lambda_L L^2), \qquad d' \ge 3$$
(5.17d)

Finally, setting d=3 in (5.17) and making use of (5.2), we get at  $(K-K_c)L=\mathcal{O}(1)$ 

$$\Delta F_{3,d'}^{(1)}(K;L) = \begin{cases} 2^{-3}(1+9\pi)\ln L - 2^{-1}\ln\ln L & d'=0\\ 2^{-1}\pi\ln L - 2^{-1}\ln\ln L & d'=1\\ 2^{-3}\pi\ln L - 2^{-1}\ln\ln L & d'=2 \end{cases}$$
(5.18)

3. Next we consider the case of free boundary conditions in the shifted critical regime  $(K - K_{c,L}^{(0)})L = \mathcal{O}(1)$  when  $\lambda_L = \mathcal{O}(L^{-2})$ . Now logarithmic corrections of the proper form may arise from  $\lambda_L$ -dependent terms in the right-hand side of (5.5) proportional to

$$L^{-d} \ln \lambda_L = -2L^{-d} \ln L + \mathcal{O}(L^{-d})$$
 (5.19a)

$$L^{-d+2}\lambda_L \ln \lambda_L = -L^{-d}(\lambda_L L^2) \ln L + \mathcal{O}(L^{-d})$$
(5.19b)

794

The term (5.19a) arises after the integration over  $\mu$  of  $W_0(\mu) = \mu^{-1}$  [see (5.7)], and already has been taken into account in (5.8); the term (5.19b) is due to the weak singularity of  $W_2(\mu)$  [see (4.5)],

l.c. 
$$\int_{\lambda_L}^{1} d\mu W_2(\mu) = (4\pi)^{-1}$$
 l.c.  $\int_{\lambda_L}^{1} d\mu \ln \mu^{-1} = (4\pi)^{-1} \lambda_L \ln \lambda_L$  (5.20)

Thus, from (5.5)–(5.8) and (5.20) we obtain

$$\Delta F_{d,d'}^{(0)}(K;L) = \begin{cases} -\left[1 - d(d-1)(2\pi)^{-1}\lambda_L L^2\right]2^{-d}\ln L & d' = 0\\ (d-1)2^{-d}\pi^{-1}\lambda_L L^2\ln L & d' = 1\\ 2^{-d}\pi^{-1}\lambda_L L^2\ln L & d' = 2\\ 0 & d' \ge 3 \end{cases}$$
(5.21)

4. Finally, we consider the case of fixed boundary conditions in the shifted critical regime  $(K - K_{c,L}^{(1)})L = \mathcal{O}(1)$ . Now  $\lambda_L$  and  $\delta_L$  [see (5.11)] are of the same order of magnitude,  $O(L^{-2})$ . One readily verifies that (5.13), (5.14), and (5.16) still hold, while (5.15) changes to

$$\begin{aligned} &\text{l.c.} \int_{\lambda_{L}}^{1} d\mu \int_{0}^{eL^{2}} dx \ e^{-\tilde{\mu}x} [e^{-2x} I_{0}(2x)]^{2} \\ &= 1.\text{c.} (4\pi)^{-1} \int_{\lambda_{L}}^{1} d\mu \ln |\tilde{\mu}|^{-1} \\ &= 1.\text{c.} (4\pi)^{-1} \tilde{\lambda}_{L} \ln |\tilde{\lambda}_{L}| = -(2\pi)^{-1} \tilde{\lambda}_{L} \ln L \end{aligned}$$
(5.22)

where  $\tilde{\lambda}_L = \lambda_L - \delta_L$  [see (3.17) and (5.11)]. Therefore, in this regime we obtain

$$\Delta F_{d,d'}^{(1)}(K;L) = \begin{cases} -\left[1 - d(d-1)(2\pi)^{-1}\tilde{\lambda}_L L^2\right](-2)^{-d}\ln L & d' = 0\\ (d-1)(-2)^{-d}\pi^{-1}\tilde{\lambda}_L L^2\ln L & d' = 1\\ (-2)^{-d}\pi^{-1}\tilde{\lambda}_L L^2\ln L & d' = 2\\ 0 & d' \ge 3 \end{cases}$$
(5.23)

The structure of the logarithmic corrections now parallels that for free boundary conditions in the corresponding shifted critical regime [compare (5.21) and (5.23)].

# 6. **DISCUSSION**

We have shown that the logarithmic finite-size corrections in the free energy of the three-dimensional mean spherical model depend on the type of the critical regime: there is a bulk critical regime when

$$x_1 \equiv (K - K_c) L = \mathcal{O}(1) \tag{6.1}$$

and a shifted critical regime when

$$\dot{x}_1 \equiv (K - K_{c,L}^{(\tau)})L = \mathcal{O}(1) \tag{6.2}$$

where the shifted critical coupling  $K_{c,L}^{(\tau)}$  [see (4.18) and (4.33)] depends on the boundary conditions. To compare with our previous results<sup>(9)</sup> concerning the case of free boundaries, we note that the finite-size correlation length  $\xi_L(K)$  is related to the solution  $\lambda = \lambda_L(K)$  of the mean spherical constraint (2.18) by

$$\xi_L(K) = [\lambda_L(K)]^{-1/2}$$
(6.3)

Hence Eq. (5.8) coincides with (1.5) and (1.6) in the bulk critical regime, when  $L/\xi_L \rightarrow \infty$  [see (4.20)]. This is the result corresponding to the short-block limit considered by Gelfand and Fisher<sup>(5,6)</sup> for the Gaussian model. The total logarithmic contribution (5.9) has been divided<sup>(9)</sup> into a contribution from the corners, proportional to  $\ln \lambda_L$ ,

$$\Delta F_{3,0}^{(0,c)}(K;L) = -2^{-3} \ln L + 2^{-3} \ln \ln L$$
(6.4)

and a contribution from the edges, proportional to  $L\lambda_L^{1/2}$ ,

$$\Delta F_{3,d'}^{(0,e)}(K;L) = \begin{cases} (9/8) \ln L & d' = 0\\ (1/4) \ln L & d' = 1 \end{cases}$$
(6.5)

Note that the contribution per edge depends on d' = 0, 1 since  $\lambda_L$  does [see (4.15), (4.20)].

Unexpectedly, in the shifted critical regime (6.2) there are logarithmic finite-size contributions which arise from two-dimensional surfaces [see (5.20)]. However, now there are no logarithmic edge contributions of the considered form, since  $L\lambda_L^{1/2} = \mathcal{O}(1)$ . Thus we can distinguish between contributions from the corners, proportional to  $\ln \lambda_L$ ,

$$\Delta F_{3,0}^{(0,c)}(K;L) = -2^{-3} \ln L \tag{6.6}$$

and from the surfaces, proportional to  $\lambda_L \ln \lambda_L$ ,

$$\Delta F_{3,d'}^{(0,s)}(K;L) = \begin{cases} (3/8\pi)\lambda_L L^2 \ln L & d'=0\\ (1/4\pi)\lambda_L L^2 \ln L & d'=1\\ (1/8\pi)\lambda_L L^2 \ln L & d'=2 \end{cases}$$
(6.7)

A characteristic feature of the surface contributions (6.7) is that the amplitude of the ln L term depends on the scaled temperature variable (6.2) through the factor  $\lambda_L L^2$ .

The bulk critical regime of the model with fixed boundaries corresponds to the long-block limit,  $L/\xi_L \rightarrow \infty$  [see (4.34) and (6.3)]. In this case there is a double logarithmic term proportional to  $\ln(L/\xi_L)$  [see (5.6) and (5.18)] which has no transparent geometrical origin; it persists with constant amplitude in all geometries with fixed surfaces ( $d' \leq 2$ ):

$$\Delta F_{3,d'}^{(1,*)}(K;L) = -2^{-1} \ln \ln L \tag{6.8}$$

Apart from the term (6.8), one may classify the logarithmic finite-size contributions as due to corners [see (5.10) and (5.13)],

$$\Delta F_{3,0}^{(1,c)}(K;L) = 2^{-3} \ln L \tag{6.9}$$

and two-dimensional surfaces [see (5.10) and (5.15)],

$$\Delta F_{3,d'}^{(1,s)}(K;L) = \begin{cases} (9\pi/8) \ln L & d' = 0\\ (\pi/2) \ln L & d' = 1\\ (\pi/8) \ln L & d' = 2 \end{cases}$$
(6.10)

Logarithmic edge contributions are absent [see (5.10) and (5.14)].

In the shifted critical regime there is no double logarithmic term of the type (6.8) [see (5.6)]. The logarithmic contribution from the corners is the same as (6.9), and the one due to surfaces [see (5.10) and (5.22)] is

$$\Delta F_{3,d'}^{(1,s)}(K;L) = \begin{cases} -(3/8\pi)\tilde{\lambda}_L L^2 \ln L & d' = 0\\ -(1/4\pi)\tilde{\lambda}_L L^2 \ln L & d' = 1\\ -(1/8\pi)\tilde{\lambda}_L L^2 \ln L & d' = 2 \end{cases}$$
(6.11)

The amplitudes of the ln L terms depend on the scaled temperature variable (6.2) through the factor  $\tilde{\lambda}_L L^2$ .

In conclusion, we point out that the results (6.4), (6.6), and (6.9) confirm the hypothesis for universal amplitudes of the logarithmic size corrections due to corners. These amplitudes are independent of the choice of the critical regime, but depend on the boundary conditions. Not predicted by finite-size scaling arguments is the appearance of double logarithmic terms [see (6.4) and (6.8)] in the bulk critical regime. The generality of our results about the universal amplitudes of the logarithmic contributions stemming from edges [see (6.5)] or surfaces [see (6.10)] in the bulk critical regime needs further investigation.

# ACKNOWLEDGMENT

This work was supported by the Bulgarian National Foundation for Scientific Research, grant MM-74/91.

# REFERENCES

- 1. V. Privman, ed., Finite Size Scaling and Numerical Simulation of Statistical Systems (World Scientific, Singapore, 1990).
- 2. V. Privman, Phys. Rev. B 38:9261 (1988).
- 3. J. L. Cardy and I. Peschel, Nucl. Phys. B 300[FS22]:377 (1988).
- 4. V. Privman, Physica A 177:241 (1991).
- 5. M. P. Gelfand and M. E. Fisher, Physica A 166:713 (1990).
- 6. M. P. Gelfand and M. E. Fisher, Int. J. Thermophys. 9:713 (1988).
- 7. B. Duplantier and F. David, J. Stat. Phys. 51:327 (1988).
- 8. J. G. Brankov and V. B. Priezzhev, J. Phys. A 25:4297 (1992).
- 9. J. G. Brankov and D. M. Danchev, J. Phys. A, submitted.
- 10. E. Brezin, J. Phys. (Paris) 43:15 (1982).
- 11. M. Luck, Phys. Rev. B 31:3069 (1985).
- 12. J. Shapiro and J. Rudnick, J. Stat. Phys. 43:51 (1986).
- 13. G. S. Joyce, in *Phase Transitions and Critical Phenomena*, Vol. 2, C. Domb and M. S. Green, eds. (Academic Press, New York, 1972), pp. 375-492.
- 14. S. Singh and R. K. Pathria, Phys. Rev. B 31:4483 (1985).
- 15. M. N. Barber and M. E. Fisher, Ann. Phys. 77:1 (1973).