Finite-size scaling in the presence of an inhomogeneous external field: An analytical-model treatment

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(Received 4 March 1994)

The validity of finite-size scaling in the presence of an inhomogeneous external field vanishing in the thermodynamic-limit is studied using a fully finite three-dimensional mean spherical model. The external field is chosen to change sign stepwise in one space dimension and to be translationally invariant in the other two dimensions, in which the lattice is assumed periodic. The boundary conditions in the direction of broken translational invariance are (i) periodic, and (ii) free, and (iii) fixed. Exact expressions for the magnetization profile are derived and studied. An extended, coordinate-dependent finite-size scaling is found to hold near the shifted critical temperature. Different scaling forms hold near the bulk critical temperature: in case (ii) the distance from the boundary scales with the finite-size correlation length, and in case (iii) with the linear size of the system.

I. INTRODUCTION

Vanishing external fields are usually used to break the symmetry of the Hamiltonian and to single out pure Gibbs phases in the low-temperature region. For that purpose the amplitude H of the field is set to zero after the thermodynamic limit is taken. This approach, applied to classical and quantum systems with various symmetry-breaking sources, constitutes the basis of Bogoliubov's definition of quasiaverages.[1]

A generalized version of Bogoliubov's quasiaverages makes use of symmetry-breaking fields with a size-dependent amplitude $H^{(L)}$, which tends to zero simultaneously with the unlimited increase of the linear size L of the system. For example, one may set $H^{(L)} \propto L^{-\alpha}$ as $L \rightarrow \infty$, with some $\alpha > 0$. When the thermodynamic limit is taken at fixed density of the number N of particles, i.e., for a d-dimensional system in a space domain L^d, the ratio N/L^d=const as $L \rightarrow \infty$, one may set alternatively $H^{(N)} \propto N^{-\alpha/d}$. The generalized quasiaverage approach has been suggested in Ref. 2 and used to explore the set of zero-field-limit Gibbs states of some exactly solvable models: the Curie-Weiss-Ising ferromagnet,[2] the n-vector Curie-Weiss model,[3] and the spherical model with nearest-neighbor interaction.[4]

It has been realized[4,5] that the generalized quasiaverage approach, with field amplitudes vanishing according to a suitably chosen power law, provides a constructive procedure for the explicit calculation of finite-size scaling functions at both second-order and first-order phase transitions. In the case of a second-order phase transition, one has to consider the system at temperatures $T^{(L)}$ which approach the critical temperature T_c simultaneously with $L \rightarrow \infty$; the appropriate choice, predicted by the finite-size scaling theory,[6-8] is $T^{(L)}/T_c - 1 \propto L^{-\nu}$, where ν is the critical exponent of the correlation length.

Most of the works on finite-size scaling (see Ref. 8 and references therein) have focused on the case of uniform external fields (sources) which break rotational (gauge) symmetries. Hypotheses are most readily tested on the example of the mean spherical model,[9] for which a variety of analytical results has been obtained (see the recent Refs. 10–12 and references therein). Vanishing uniform fields have been applied in that model to study the scaling behavior with respect to the magnetic variable.[13,14] Bulk and surface fields have been used in a detailed investigation of the surface properties, in particular the variation of the susceptibility with the distance from the surface.[15]

Inhomogeneous fields, switched off after the thermodynamic limit, appeared to be useful tools for investigating phase separation and surface and interface phenomena. For example, a steplike inhomogeneous external field, which breaks the translational invariance in one space dimension, has been applied in a study of the problem of phase separation in the mean spherical model.[16] The spherical model in a magnetic field with the same spatial dependence, but with an amplitude vanishing simultaneously with $L \rightarrow \infty$, has been considered by Patrick.[17] Interesting phenomena have been found to occur in the regime of moderate rate of decrease of the amplitude $H^{(L)} \propto L^{-2}$: the leading $O(L^{-2})$ correction term of the free-energy density exhibits a new singularity with respect to the temperature at $T=T_c^*$, where $0<T_c^*<T_c$; below T_c^* there appears a "frozen" (temperature-independent), smooth magnetization profile. Qualitatively similar phenomena were shown to appear under the action of surface magnetic fields.[18]

The aim of the present work is to study the validity of finite-size scaling[6-8] in systems subjected to inhomogeneous external fields. Obviously, the problem is a part of the more general investigations on finite-size effects in spatially inhomogeneous systems.

In the present work we consider the mean spherical

0163-1829/94/50(5)/2970(8)/$06.00

model with nearest-neighbor interaction on a fully finite domain Λ of the three-dimensional simple cubic lattice. The spatial dependence of the external field is chosen as in Refs. 16 and 17: it changes sign stepwise along the first coordinate r_1, being positive in one half of Λ, $1 \le r_1 < L/2$, and negative in the other half, $L/2+1 < r_1 \le L$ (distances are measured in units of the lattice constant and L is assumed even). The amplitude of the field $H^{(L)}$ vanishes in the thermodynamic limit according to the finite-size scaling prediction[7,8] $H^{(L)} \propto L^{-\Delta/\nu}$ as $L \to \infty$, where $\Delta/\nu = \frac{5}{2}$. Different boundary conditions in the direction of broken translational invariance are considered: (i) periodic, (ii) free, and (iii) fixed (we adhere to the terminology of Gelfand and Fisher[19]); in the remaining dimensions the lattice is assumed periodic.

The paper is organized as follows. In Sec. II we give the definition of the model and present the necessary starting expressions for further investigation. The mean spherical constraint, under the above-mentioned boundary conditions and in two critical regimes with respect to the temperature, is analyzed in Sec. III. The exact results for the magnetization profile and its critical finite-size asymptotic behavior are given in Sec. IV. The paper closes with a discussion of the extended finite-size scaling behavior in Sec. V.

II. THE MODEL

Consider the ferromagnetic mean spherical model (see, e.g., the review, Ref. 9), on a finite d-dimensional hypercubic lattice $\Lambda = L \times \cdots \times L \in \mathbb{Z}^d$ of $L^d = N$ sites. The Hamiltonian of the model in the presence of an inhomogeneous magnetic field $h(\mathbf{r})$, $\mathbf{r} \in \Lambda$, is

$$\beta \mathcal{H}_\Lambda^{(\tau)}[\{\sigma(\mathbf{r}), \mathbf{r} \in \Lambda\}] = -\frac{1}{2} K \sum_{\mathbf{r},\mathbf{r}' \in \Lambda} Q_\Lambda^{(\tau)}(\mathbf{r}-\mathbf{r}')\sigma(\mathbf{r})\sigma(\mathbf{r}') - \sum_{\mathbf{r} \in \Lambda} h(\mathbf{r})\sigma(\mathbf{r}) . \tag{2.1}$$

Here $\beta = 1/k_B T$ is the inverse temperature, K is the dimensionless coupling, $\sigma(\mathbf{r}) \in \mathbb{R}$ is the dynamical variable (scalar continuous spin) at site $\mathbf{r} = \{r_1, \ldots, r_d\} \in \Lambda$, and the coordinates $r_\nu \in \{1, \ldots, L\}$, $\nu = 1, \ldots, d$, are measured in units of the lattice spacing. The dependence on the boundary conditions imposed along the first coordinate axis is denoted by a superscript (τ), $\tau = p$ for periodic, 0 for free, and 1 for fixed boundaries; in the remaining $d-1$ spatial dimensions periodic boundary conditions are assumed. We consider the case of nearest-neighbor ferromagnetic interactions, when $Q_\Lambda^{(\tau)}$ is the adjacency matrix: $Q_\Lambda^{(\tau)}(\mathbf{r}-\mathbf{r}') = 1$ if and only if sites $\mathbf{r}$ and $\mathbf{r}'$ are nearest neighbors (under the assumed boundary conditions) and $Q_\Lambda^{(\tau)}(\mathbf{r}-\mathbf{r}') = 0$ otherwise.

The partition function for the Gaussian model corresponding to Hamiltonian (2.1) is given by

$$Z_\Lambda^{(\tau)}(K, \{h(\mathbf{r}), \mathbf{r} \in \Lambda\}; s) = \int_{\mathbb{R}^N} \prod_{\mathbf{r} \in \Lambda} d\sigma(\mathbf{r}) \exp\{-\beta \mathcal{H}_\Lambda^{(\tau)}[\{\sigma(\mathbf{r}), \mathbf{r} \in \Lambda\}] - s \sum_{\mathbf{r} \in \Lambda} \sigma(\mathbf{r})\sigma(\mathbf{r})\} , \tag{2.2}$$

where s is a parameter. The quadratic form in the exponent in the right-hand side of (2.2) can be diagonalized by performing a unitary transformation of the dynamical variables:

$$\bar{x}(\mathbf{k}) = \sum_{\mathbf{r} \in \Lambda} \sigma(\mathbf{r}) U_\Lambda^{(\tau)}(\mathbf{r}, \mathbf{k}) , \qquad x(\mathbf{k}) = \sum_{\mathbf{r} \in \Lambda} \sigma(\mathbf{r}) \bar{U}_\Lambda^{(\tau)}(\mathbf{r}, \mathbf{k}) , \tag{2.3}$$

where $\bar{x}$ denotes the complex conjugate of x and $\mathbf{k} = \{k_1, \ldots, k_d\}$ with $k_\nu \in \{1, \ldots, L\}$. The transformation matrix in (2.3) reads

$$U_\Lambda^{(\tau)}(\mathbf{r}, \mathbf{k}) = U_L^{(\tau)}(r_1, k_1) \prod_{\nu=2}^{d} U_L^{(p)}(r_\nu, k_\nu) , \tag{2.4}$$

where

$$U_L^{(p)}(r_\nu, k_\nu) = L^{-1/2} \exp(-2\pi i r_\nu k_\nu / L) , \quad \nu = 1, \ldots, d , \tag{2.5a}$$

$$U_L^{(0)}(r_1, k_1) = \begin{cases} L^{-1/2} , & k_1 = 1 , \\ (2/L)^{1/2} \cos[\pi(r_1 - \frac{1}{2})(k_1 - 1)/L] , & k_1 = 2, \ldots, L , \end{cases} \tag{2.5b}$$

$$U_L^{(1)}(r_1, k_1) = [2/(L+1)]^{1/2} \sin[\pi r_1 k_1 / (L+1)] . \tag{2.5c}$$

The transformed interaction matrix can be written in the diagonal form

$$\sum_{\mathbf{r},\mathbf{r}' \in \Lambda} \bar{U}_\Lambda^{(\tau)}(\mathbf{r}, \mathbf{k}) Q_\Lambda^{(\tau)}(\mathbf{r}-\mathbf{r}') U_\Lambda^{(\tau)}(\mathbf{r}', \mathbf{k}') = \delta_{\mathbf{k},\mathbf{k}'}[2d - \omega_\Lambda^{(\tau)}(\mathbf{k})] , \tag{2.6}$$

where

$$\omega_\Lambda^{(p)}(\mathbf{k}) = 2d - 2 \sum_{\nu=1}^{d} \cos(2\pi k_\nu / L) , \tag{2.7a}$$

$$\omega_\Lambda^{(0)}(\mathbf{k}) = 2d - 2\cos[\pi(k_1 - 1)/L] - 2 \sum_{\nu=2}^{d} \cos(2\pi k_\nu / L) , \tag{2.7b}$$

$$\omega_\Lambda^{(1)}(\mathbf{k})=2d-2\cos[\pi k_1/(L+1)]-2\sum_{\nu=2}^{d}\cos(2\pi k_\nu/L) . \quad (2.7c)$$

In terms of the new variables (2.3) the exponent of the integrand in the right-hand side of (2.2) reads

$$\tfrac{1}{2}K\sum_{\mathbf{k}\in\Lambda}[\phi+\omega_\Lambda^{(\tau)}(\mathbf{k})]\bar{x}(\mathbf{k})x(\mathbf{k}) -\tfrac{1}{2}\sum_{\mathbf{k}\in\Lambda}[\bar{h}^{(\tau)}(\mathbf{k})x(\mathbf{k})+h^{(\tau)}(\mathbf{k})\bar{x}(\mathbf{k})] , \quad (2.8)$$

where, instead of the spherical field s, we have introduced the parameter

$$\phi=2s/K-2d , \quad (2.9)$$

and the transformed magnetic field is given by

$$\bar{h}^{(\tau)}(\mathbf{k})=\sum_{\mathbf{r}\in\Lambda}h(\mathbf{r})U_\Lambda^{(\tau)}(\mathbf{r},\mathbf{k}) , \qquad h^{(\tau)}(\mathbf{k})=\sum_{\mathbf{r}\in\Lambda}h(\mathbf{r})\bar{U}_\Lambda^{(\tau)}(\mathbf{r},\mathbf{k}) . \quad (2.10)$$

Thus, by performing the integration in the partition function (2.2) at $\phi>-\min_{\mathbf{k}}\omega_\Lambda^{(\tau)}(\mathbf{k})$, for the free-energy density of the Gaussian model one obtains

$$\beta a_\Lambda^{(\tau)}(K,\{h(\mathbf{r}),\mathbf{r}\in\Lambda\};\phi)\equiv -N^{-1}\ln Z_\Lambda^{(\tau)}[K,\{h(\mathbf{r}),\mathbf{r}\in\Lambda\};\tfrac{1}{2}K(\phi+2d)]$$
$$=\text{const}+(2N)^{-1}\sum_{\mathbf{k}\in\Lambda}\ln[\phi+\omega_\Lambda^{(\tau)}(\mathbf{k})]-(2KN)^{-1}\sum_{\mathbf{k}\in\Lambda}[\phi+\omega_\Lambda^{(\tau)}(\mathbf{k})]^{-1}\bar{h}^{(\tau)}(\mathbf{k})h^{(\tau)}(\mathbf{k}) . \quad (2.11)$$

The free-energy density of the finite-size mean spherical model is defined by the Legendre transformation

$$\beta f_\Lambda^{(\tau)}(K,\{h(\mathbf{r}),\mathbf{r}\in\Lambda\})=\sup_\phi[\beta a_\Lambda^{(\tau)}(K,\{h(\mathbf{r}),\mathbf{r}\in\Lambda\};\phi) -\tfrac{1}{2}K(\phi+2d)] . \quad (2.12)$$

The supremum in (2.12) is attained at the solution of the mean spherical constraint on ϕ:

$$N^{-1}\sum_{\mathbf{k}\in\Lambda}[\phi+\omega_\Lambda^{(\tau)}(\mathbf{k})]^{-1} -(\partial/\partial\phi)P_\Lambda^{(\tau)}(K,\{h(\mathbf{r}),\mathbf{r}\in\Lambda\};\phi)=K , \quad (2.13)$$

with a field-dependent term

$$P_\Lambda^{(\tau)}(K,\{h(\mathbf{r}),\mathbf{r}\in\Lambda\};\phi) =(KN)^{-1}\sum_{\mathbf{k}\in\Lambda}[\phi+\omega_\Lambda^{(\tau)}(\mathbf{k})]^{-1}\bar{h}^{(\tau)}(\mathbf{k})h^{(\tau)}(\mathbf{k}) . \quad (2.14)$$

Here we will consider the case of an inhomogeneous external field which depends on the first coordinate only and has the steplike form

$$h(\mathbf{r})=h_L\operatorname{sgn}[(L+1)/2-r_1] , \quad (2.15)$$

with an amplitude $h_L\to 0$ as $L\to\infty$ which will be specified below. Under the field (2.15) and the boundary conditions $\tau=p,0$, and 1, the term (2.14) can be evaluated exactly with the aid of a "contour summation" technique (see Refs. 17 and 18). By using Eqs. (2.4), (2.5), (2.7), (2.10), and (2.15), and setting

$$z=\ln\{1+\phi/2+[(1+\phi/2)^2-1]^{1/2}\} , \quad (2.16)$$

we obtain that (2.14) reduces to (assuming L even)

$$P_L^{(p)}(K,h_L;\phi)=(4h_L^2/KL^2)\sum_{m=1}^{L/2}\frac{1}{\{1-\cos[2\pi(2m-1)/L]\}\{1+\phi/2-\cos[2\pi(2m-1)/L]\}}$$
$$=(h_L^2/\phi K)\left\{1-\frac{4}{z}\tanh(\tfrac{1}{4}Lz)/[L\sinh(z)]\right\} ; \quad (2.17a)$$

$$P_L^{(0)}(K,h_L;\phi)=(2h_L^2/KL^2)\sum_{m=1}^{L/2}\frac{1}{\{1-\cos[\pi(2m-1)/L]\}\{1+\phi/2-\cos[\pi(2m-1)/L]\}}$$
$$=(h_L^2/\phi K)\left\{1-\frac{2}{z}\tanh(\tfrac{1}{2}Lz)/[L\sinh(z)]\right\} ; \quad (2.17b)$$

$$P_L^{(1)}(K,h_L;\phi)=[2h_L^2/KL(L+1)]\sum_{m=1}^{L/2}\frac{\{(-1)^m-\cos[\pi m/(L+1)]\}^2}{\{1-\cos[2\pi m/(L+1)]\}\{1+\phi/2-\cos[2\pi m/(L+1)]\}}$$
$$=(h_L^2/\phi K)\left[\frac{L+2}{L+1}-\frac{4}{L\sinh(z)}\frac{\cosh[(L+1)z/2]-\cosh(z/2)}{\sinh[(L+1)z/2]}\right]$$
$$-(h_L^2/2K)\frac{\coth[(L+1)z/2]-(L+1)^{-1}\coth(z/2)}{L\sinh(z)} . \quad (2.17c)$$

The field-dependent finite-size terms (2.17) are regular functions of ϕ at $\phi=0$. By expanding the above expressions in power series of ϕ, one obtains

$$P_L^{(p)}(K,h_L;\phi)\cong(h_L^2/48K)\times[L^2+8-\tfrac{1}{40}(L^4+10L^2+64)\phi]\ , \quad (2.18a)$$

$$P_L^{(0)}(K,h_L;\phi)\cong(h_L^2/12K)\times[L^2+2-\tfrac{1}{10}(L^4+5L^2/2+4)\phi]\ , \quad (2.18b)$$

$$P_L^{(1)}(K,h_L;\phi)\cong[h_L^2(L+2)/48K(L+1)]\times\{L^2+2L+8-\tfrac{1}{40}[(L+1)^4+6(L+1)^2+25]\phi\}\ . \quad (2.18c)$$

In general, when $\phi\to 0$ the field-dependent term in Eq. (2.13) can be written in the form

$$-(\partial/\partial\phi)P_L^{(\tau)}(K,h_L;\phi)=(h_L^2L^4/K)[G_0^{(\tau)}(\phi L^2)+L^{-1}G_1^{(\tau)}(\phi L^2)+\cdots]\ , \quad (2.19)$$

where $G_k^{(\tau)}(x)$, $k=1,2,\ldots$, are regular functions of x at $x=0$. From (2.18) we conclude that $G_0^{(\tau)}(0)>0$, $G_1^{(p)}(0)=G_1^{(0)}(0)=0$, and $G_1^{(1)}(0)>0$. In the next section we will obtain the asymptotic behavior of this term in the different finite-size scaling regimes.

III. THE MEAN SPHERICAL CONSTRAINT

In the absence of external magnetic fields, the finite-size scaling regimes of the mean spherical constraint have been studied in detail under general periodic, open, and fixed boundary conditions;[11] antiperiodic boundary conditions have been taken into account too.[12] Here we will study the asymptotic behavior of the solution $\phi=\phi_L$ of Eq. (2.13) in the presence of the steplike inhomogeneous field (2.15), with an amplitude vanishing as $L\to\infty$ in such a way that

$$x_2=h_LL^{5/2}K^{-1/2}=O(1)\ . \quad (3.1)$$

Previous studies[11] have shown that in the case of nonperiodic boundaries one has to distinguish between two different finite-size scaling regimes of approach to the critical coupling: when $K\to K_c$ as $L\to\infty$ either

$$x_1=(K_c-K)L=O(1)\ , \quad (3.2a)$$

or

$$\mathring{x}_1=(K_{c,L}^{(\tau)}-K)L=O(1)\ , \quad (3.2b)$$

where $K_{c,L}^{(\tau)}$ is the pseudocritical (or shifted critical) value of the coupling K [see (3.21) and (3.26) below]. Depending on the regime, the solution $\phi=\phi_L$ of the mean spherical constraint may approach the limiting value zero in different ways: $\phi_LL^2\to\infty$, $\phi_LL^2=O(1)$, or $\phi_LL^2\to 0$.

Consider first the possible asymptotic behavior of the field-dependent term $-(\partial/\partial\phi)P_L^{(\tau)}(K,h;\phi)$ in (2.13). Whenever $\phi_LL^2=O(1)$, or $\phi_LL^2\to 0$, as $L\to\infty$, the leading-order estimate of that term follows from (2.19):

$$-(\partial/\partial\phi)P_L^{(\tau)}(K,h_L;\phi)\cong(h_L^2L^4/K)G_0^{(\tau)}(\phi L^2)\ . \quad (3.3)$$

On the other hand, when $\phi_L\to 0$ and $L\to\infty$, so that $\phi_LL^2\to\infty$, from (2.16) we obtain

$$z=\phi^{1/2}[1+O(\phi)]\to 0\ ,$$
$$Lz=L\phi^{1/2}[1+O(\phi)]\to\infty\ , \quad (3.4)$$

and, as is readily seen from (2.17),

$$P_L^{(\tau)}(K,h_L;\phi)=(h_L^2/\phi K)[1-O(1/L\phi^{1/2})]\ . \quad (3.5)$$

Therefore, when $\phi_LL^2\to\infty$ as $\phi_L\to 0$ and $L\to\infty$, the leading-order estimate of the field-dependent term in (2.13) is

$$-(\partial/\partial\phi)P_L^{(\tau)}(K,h_L;\phi)\cong h_L^2L^4/(\phi_L^2L^4K)\ . \quad (3.6)$$

The asymptotic behavior of the first term in the left-hand side of Eq. (2.13),

$$W_{L,d}^{(\tau)}(\phi)=N^{-1}\sum_{\mathbf{k}\in\Lambda}[\phi+\omega_\Lambda^{(\tau)}(\mathbf{k})]^{-1}\ , \quad (3.7)$$

is known (see Ref. 11 and references therein). In the thermodynamic limit, when $L\to\infty$ at a fixed value of $\phi>0$, the term (3.7) tends to the d-dimensional Watson integral,[19]

$$\lim_{L\to\infty}W_{L,d}^{(\tau)}(\phi)=W_d(\phi)\ . \quad (3.8)$$

The leading finite-size corrections in (3.7) depend both on the boundary conditions (τ) and on the asymptotic regime of ϕL^2 as $\phi\to 0$ and $L\to\infty$. Here we summarize the relevant results at $d=3$.[11]

(a) When $\phi L^2\to\infty$ as $\phi\to 0$ and $L\to\infty$, then

$$W_{L,3}^{(p)}(\phi)\cong W_3(\phi)+O(L^{-1})\ ; \quad (3.9a)$$

$$W_{L,3}^{(0)}(\phi)\cong W_3(\phi)+(1/2L)W_2(\phi)+O(L^{-1})\ ; \quad (3.9b)$$

$$W_{L,3}^{(1)}(\phi)\simeq 2W_3(\phi)-(1/2L)W_2(\phi)+O(L^{-1})\ . \quad (3.9c)$$

(b) When $\phi L^2=O(1)$ or $\phi L^2\to 0$ as $\phi\to 0^+$ and $L\to\infty$, then

$$W_{L,3}^{(p)}(\phi)\cong W_3(\phi)+(\phi L^3)^{-1}+L^{-1}R^{(p)}(\phi L^2)\ , \quad (3.10a)$$

$$W_{L,3}^{(0)}(\phi)\cong W_3(\phi)+(\phi L^3)^{-1}+\ln L/4\pi L+L^{-1}R^{(0)}(\phi L^2)\ , \quad (3.10b)$$

where $R^{(\tau)}(x)$, $\tau=p,0$, are some functions analytical at $x=0$.

In the case of fixed boundary conditions, one has to take into account that the finite-size gap parameter is $\lambda=\phi+\delta^{(\tau)}$, rather than ϕ, where

$$\delta_L^{(\tau)}=\min_{\mathbf{k}} \omega_\Lambda^{(\tau)}(\mathbf{k})=\begin{cases}0, & \tau=p,0,\\ 2-2\cos[\pi/(L+1)], & \tau=1\ .\end{cases} \tag{3.11}$$

Therefore, the different finite-size critical regimes $\lambda L^2=O(1)$ or $\lambda L^2\to 0$, as $\lambda\to 0^+$ and $L\to\infty$, both imply $\phi L^2=O(1)$ as $L\to\infty$. Note that since $\delta_L^{(1)}L^2\cong\pi^2$, the parameter ϕ is allowed to take negative values. Now the following asymptotic estimate holds:[11]

$$W_{L,3}^{(1)}(\lambda-\delta_L^{(1)})\cong W_3(\lambda)+(\lambda L^3)^{-1}-\ln L/4\pi L + L^{-1}R^{(1)}(\lambda L^2)\ , \tag{3.12}$$

where $R^{(1)}(x)$ is a function analytical at $x=0$.

It is convenient to make use of the asymptotic expansion

$$W_3(\lambda)=K_c-\lambda^{1/2}/4\pi+O(\lambda)\ ,\quad \lambda\to 0^+\ , \tag{3.13}$$

and rewrite the mean spherical constraint (2.13) in the general form

$$[W_{L,3}^{(\tau)}(\lambda-\delta_L^{(\tau)})-W_3(\lambda)]L - L(\partial/\partial\lambda)P_L^{(\tau)}(K,h_L;\lambda-\delta_L^{(\tau)}) =(K-K_c)L+\lambda^{1/2}L/4\pi+O(\lambda L)\ . \tag{3.14}$$

Finally, taking into account the asymptotic expansion of the two-dimensional Watson integral $W_2(\lambda)$ as $\lambda\to 0^+$,

$$W_2(\lambda)=(1/4\pi)\ln\lambda^{-1}+O(1)\ , \tag{3.15}$$

we will summarize the results of our asymptotic analysis of Eq. (3.14) under the considered boundary conditions.

(i) Under fully periodic boundary conditions, $\tau=p$, when $\phi L^2=O(1)$ or $\phi L^2\to 0$ as $\phi\to 0$ and $L\to\infty$, Eq. (3.14) becomes

$$(\phi L^2)^{-1}+R^{(p)}(\phi L^2)+x_2^2G_0^{(p)}(\phi L^2) =-x_1+\phi^{1/2}L/4\pi+O(\phi L)\ . \tag{3.16}$$

Therefore, when $x_1=O(1)$ the solution is $\phi_L=O(L^{-2})$ and depends analytically on both x_1 and x_2:

$$\phi_L\cong L^{-2}X^{(p)}(x_1,x_2)\quad \text{if } x_1=O(1)\ . \tag{3.17}$$

(ii) Under open boundary conditions in one space dimension, $\tau=0$, the mean spherical constraint has the following solutions.

(a) Assuming $\phi L^2\to\infty$ as $\phi\to 0$ and $L\to\infty$, Eq. (3.14) takes the form

$$(1/8\pi)\ln\phi^{-1}+O(1)=-x_1+\phi^{1/2}L/4\pi+O(\phi L)\ . \tag{3.18}$$

Therefore, when $x_1=O(1)$ the leading asymptotic form of the solution is

$$\phi_L\cong(\ln L/L)^2\quad \text{if } x_1=O(1)\ , \tag{3.19}$$

which agrees with the assumption $\phi_L L^2\to\infty$ and $\phi_L\to 0$ as $L\to\infty$. Note that this solution is independent of the scaled temperature (x_1) and field (x_2) variables.

(b) Assuming $\phi L^2=O(1)$ or $\phi L^2\to 0$ as $\phi\to 0$ and $L\to\infty$, Eq. (3.14) becomes

$$(\phi L^2)^{-1}+R^{(0)}(\phi L^2)+x_2^2G_0^{(0)}(\phi L^2) =-\mathring{x}_1+\phi^{1/2}L/4\pi+O(1)\ . \tag{3.20}$$

Therefore, when $\mathring{x}_1=O(1)$ [see (3.2b)], where the shifted critical coupling is given by

$$K_{c,L}^{(0)}=K_c+\ln L/4\pi L\ , \tag{3.21}$$

the solution has the order of magnitude $\phi_L=O(L^{-2})$ and depends analytically on both $\mathring{x}_1$ and x_2:

$$\phi_L\cong L^{-2}X^{(0)}(\mathring{x}_1,x_2)\quad \text{if } \mathring{x}_1=O(1)\ . \tag{3.22}$$

(iii) Under fixed boundary conditions in one space dimension, $\tau=1$, the analysis of the mean spherical constraint leads to the following conclusions.

(a) Assuming $\lambda L^2\to\infty$ as $\lambda\to 0$ and $L\to\infty$, which is equivalent to $\phi L^2\to\infty$ as $\phi\to 0$ and $L\to\infty$, Eq. (3.14) takes the form

$$-(1/8\pi)\ln\phi^{-1}+O(1)=-x_1+\phi^{1/2}L/4\pi+O(\phi L)\ . \tag{3.23}$$

Thus, if $x_1=O(1)$, the mean spherical constraint has no solution $\phi=\phi_L\to 0$ with the property $\phi_L L^2\to\infty$ as $L\to\infty$.

(b) Assuming $\lambda L^2=O(1)$ or $\lambda L^2\to 0$ as $\lambda\to 0$ and $L\to\infty$, Eq. (3.14) takes the form

$$(\lambda L^2)^{-1}+R^{(1)}(\lambda L^2)+x_2^2G_0^{(1)}(\lambda L^2-\pi^2) =-x_1+(1/4\pi)\ln L+\lambda^{1/2}L/4\pi+O(1)\ . \tag{3.24}$$

Therefore we reach the following conclusions.

(1) If $x_1=O(1)$, the solution of the above equation is $\lambda=\lambda_L\cong 4\pi/L^2\ln L$. Since $\lambda_L L^2\to 0$ as $L\to\infty$, then the leading asymptotic form of ϕ_L is [see (3.11)]

$$\phi_L\cong-(\pi/L)^2\quad \text{if } x_1=O(1)\ , \tag{3.25}$$

and does not depend on the scaled temperature (x_1) and field (x_2) variables.

(2) If $\mathring{x}=O(1)$, with shifted critical coupling

$$K_{c,L}^{(1)}=K_c-\ln L/4\pi L\ , \tag{3.26}$$

then Eq. (3.24) has a solution $\lambda=\lambda_L=O(L^{-2})$ which is an analytical function of the scaled temperature $(\mathring{x}_1)$ and field (x_2) variables:

$$\phi_L\cong L^{-2}X^{(1)}(\mathring{x}_1,x_2)\quad \text{if } \mathring{x}_1=O(1)\ . \tag{3.27}$$

IV. FINITE-SIZE SCALING FOR THE MAGNETIZATION

The mean spherical model permits one to obtain exact finite-size expressions for the magnetization profile. By inverting the transformation (2.3),

$$\sigma(\mathbf{r})=\sum_{\mathbf{k}\in\Lambda}U_\Lambda^{(\tau)}(\mathbf{r},\mathbf{k})x(\mathbf{k})\ , \tag{4.1}$$

and evaluating the average values of the dynamical variables $x(\mathbf{k})$, one obtains the general expression

$$\langle\sigma(\mathbf{r})\rangle^{(\tau)}=K^{-1}\sum_{\mathbf{k}\in\Lambda}U_\Lambda^{(\tau)}(\mathbf{r},\mathbf{k})\times[\phi+\omega_\Lambda^{(\tau)}(\mathbf{k})]^{-1}h^{(\tau)}(\mathbf{k}) , \quad (4.2)$$

where $\langle\cdots\rangle^{(\tau)}$ denotes a Gibbs canonical average with the Hamiltonian (2.1). In the case under consideration the right-hand side of (4.2) depends on the coordinate r_1 only. Upon shifting the origin of the coordinate system by setting $r_1=L/2+j$, and performing the summations which appear in the expression for the magnetization profile,

$$m_L^{(\tau)}(K,h,j)=\langle\sigma(\{r_1=L/2+j,r_2,\ldots,r_d\})\rangle^{(\tau)} , \quad (4.3)$$

we obtain the explicit results

$$m_L^{(p)}(K,h,j)=-(h_L/KL)\sum_{m=1}^{L/2}\frac{\sin[2\pi(2m-1)(j-\frac{1}{2})/L]}{\sin[\pi(2m-1)/L]\{1+\phi/2-\cos[2\pi(2m-1)/L]\}}$$
$$=(h_L/4K)\frac{\mathrm{sgn}(\frac{1}{2}-j)}{\sinh^2(z/2)}\left[1-\frac{\cosh[(L/4-|j-\frac{1}{2}|)z]}{\cosh(Lz/4)\cosh(z/2)}\right] ; \quad (4.4a)$$

$$m_L^{(0)}(K,h,j)=-(h_L/KL)\sum_{m=1}^{L/2}\frac{\sin[\pi(2m-1)(j-\frac{1}{2})/L]}{\sin[\pi(2m-1)/2L]\{1+\phi/2-\cos[\pi(2m-1)/L]\}}$$
$$=(h_L/4K)\frac{\mathrm{sgn}(\frac{1}{2}-j)}{\sinh^2(z/2)}\left[1-\frac{\cosh[(L/2-|j-\frac{1}{2}|)z]}{\cosh(Lz/2)\cosh(z/2)}\right] ; \quad (4.4b)$$

$$m_L^{(1)}(K,h,j)=-[h_L/K(L+1)]\sum_{m=1}^{L/2}\frac{\{1-(-1)^m\cos[\pi m/(L+1)]\}\sin[2\pi m(j-\frac{1}{2})/(L+1)]}{\sin[\pi m/(L+1)]\{1+\phi/2-\cos[2\pi m/(L+1)]\}}$$
$$=(h_L/4K)\frac{\mathrm{sgn}(\frac{1}{2}-j)}{\sinh^2(z/2)}\left[1-\frac{\cosh[(j-\frac{1}{2})z]}{\cosh(z/2)}+\left[\frac{\cosh[(L+1)z/2)]}{\cosh(z/2)}-1\right]\frac{\sinh(|j-\frac{1}{2}|z)}{\sinh[(L+1)z/2)]}\right] . \quad (4.4c)$$

According to the finite-size scaling hypothesis,[7,8] the magnetization $m_L(K,h)$ of a system with linear size $L\gg1$, placed in a uniform magnetic field h (in units of k_BT), should have the following leading asymptotic form in the neighborhood of a second-order critical point ($h=0,t=0$):

$$m_L^{(\tau)}(K,h)\cong C_2L^{-\beta/\nu}Y^{(\tau)}(C_1tL^{1/\nu},C_2hL^{\Delta/\nu}) . \quad (4.5)$$

Here $t=T/T_c-1$; β,ν, and $\Delta=\beta+\gamma$ are the standard critical exponents; $Y^{(\tau)}(\cdots)$ is a universal scaling function which may depend on the boundary conditions (τ); and C_1 and C_2 are nonuniversal metric factors. For the three-dimensional spherical model with short-range interactions one has

$$\beta=\tfrac{1}{2} , \quad \nu=1 , \quad \Delta=\tfrac{5}{2} , \quad C_1=K_c , \quad C_2=K_c^{-1/2} . \quad (4.6)$$

Here we will check if the coordinate-dependent magnetization profile $m_L^{(\tau)}(K,h,j)$ obeys some extended version of the finite-size scaling, which is expected to include an additional dependence on the coordinate j through the ratio j/L. Consider first the finite-size scaling regime $\mathring{x}_1=O(1)$, when [see (3.17), (3.22), and (3.27)]

$$\phi_L\cong L^{-2}X^{(\tau)}(\mathring{x}_1,x_2) , \quad \tau=p,0,1 . \quad (4.7)$$

Note that under periodic boundary conditions ($\tau=p$) the finite-size shift in the critical temperature is $O(L^{-1})$;[7,8] therefore the variables $\mathring{x}_1$ and x_1 are equivalent (differing by a constant). From (2.16) and (4.7) it follows that

$$z\cong L^{-1}[X^{(\tau)}(\mathring{x}_1,x_2)]^{1/2}\equiv L^{-1}y_\tau(\mathring{x}_1,x_2) . \quad (4.8)$$

Therefore in this case the exact expressions (4.4) for the magnetization profile reduce to

$$m_L^{(p)}(K,h,j)\cong\mathrm{sgn}(h)\frac{C_2x_2L^{-1/2}}{y_p^2(\mathring{x}_1,x_2)}\left[1-\frac{\cosh[(\frac{1}{4}-|j/L|)y_p(\mathring{x}_1,x_2)]}{\cosh[y_p(x_1,x_2)/4]}\right] ; \quad (4.9a)$$

$$m_L^{(0)}(K,h,j)\cong\mathrm{sgn}(h)\frac{C_2x_2L^{-1/2}}{y_0^2(\mathring{x}_1,x_2)}\left[1-\frac{\cosh[(\frac{1}{2}-|j/L|)y_0(\mathring{x}_1,x_2)]}{\cosh[y_0(\mathring{x}_1,x_2)/2]}\right] ; \quad (4.9b)$$

$$m_L^{(1)}(K,h,j)\cong\mathrm{sgn}(h)\frac{C_2x_2L^{-1/2}}{y_1^2(\mathring{x}_1,x_2)}\left[1-\frac{\cosh[(\frac{1}{4}-|j/L|)y_1(\mathring{x}_1,x_2)]}{\cosh[y_1(\mathring{x}_1,x_2)/4]}\right] . \quad (4.9c)$$

Consider next the asymptotic regime $x_1=O(1)$ in the case of open boundary conditions, $\tau=0$. From (3.4) and (3.19) it follows that $z\cong\ln L/L$, and after substitution in the right-hand side of (4.4b) we obtain

$$m_L^{(0)}(K,h,j)\cong\mathrm{sgn}(h)(C_2x_2L^{-1/2}/\ln^2 L)\times\{1-\exp[-|j|\ln L/L\} . \quad (4.10)$$

Finally, under fixed boundary conditions, $\tau=1$, the regime $x_1=O(1)$ leads to $z\cong i\pi/L$ [see (2.16) and (3.25)], and after substitution in the right-hand side of (4.4c) we obtain

$$m_L^{(1)}(K,h,j)\cong\mathrm{sgn}(h)(C_2x_2L^{-1/2}/\pi^2)\times[\cos(\pi j/L)+\sin(\pi|j|/L)-1] . \quad (4.11)$$

An independent derivation of (4.11) can be given by applying the mathematical technique of Barber and Fisher[20] to sum in the right-hand side of the first equality (4.4c). Thus, by setting $\lambda_L L^2\propto(L/\xi_L)^2=0$, which implies $1+\phi_L/2=\cos[\pi/(L+1)]$, and considering $j/L\equiv\rho=O(1)$, one arrives at the evaluation of the leading-order sum

$$\sum_{k=1}^{[(L+2)/4]}\frac{\cos[\pi(2k-1)/2L]\sin[2\pi\rho(2k-1)]}{\sin[\pi(2k-1)/2L][\cos(\pi/L)-\cos[2\pi(2k-1)/L]}\cong 8(L/\pi)^3\sum_{k=1}^{\infty}\frac{\sin[2\pi\rho(2k-1)]}{(4k-1)(4k-2)(4k-3)}$$
$$=(L^3/\pi^2)[\cos(\pi\rho)+\sin(\pi|\rho|)-1] . \quad (4.12)$$

Taking into account the factor $-h_L/KL$, one recovers exactly (4.11).

The results (4.9) are in full conformity with the extended finite-size scaling hypothesis

$$m_L(K,h,j)\cong C_2L^{-1/2}Z^{(\tau)}(\mathring{x}_1,x_2,j/L) , \quad (4.13)$$

where $\mathring{x}_1,x_2$ are the scaling variables (3.1), (3.2b); expression (4.11) agrees with it apart from the fact that the magnetization profile is frozen, i.e., independent of the scaled temperature variable. Obviously, expression (4.10) contains terms logarithmic in L which violate (4.13).

V. DISCUSSION

In the critical regime $\mathring{x}_1=O(1)$ the finite-size correlation length ξ_L, defined in terms of the gap parameter λ_L as $\xi_L=\lambda_L^{-1/2}$, increases proportionally to the linear size L of the system, i.e., $\xi_L\propto L$. That fact ensures the proper scaling of the dependence on the coordinate j as $j/\xi_L\propto j/L$, which is observed in our explicit results (4.9). The profile under periodic boundary conditions (4.9a) has been obtained by Patrick[17] in the case of the spherical model of Berlin and Kac.[9] To our knowledge, the results for nonperiodic boundaries (4.9b) and (4.9c) are new. Rather surprising is the symmetry and similarity of these expressions. The symmetry of the magnetization profile in the mean spherical model under fixed boundary conditions has been noticed by Abraham and Robert,[16] and interpreted as a physically interesting decoupling effect in their study of the phase separation problem in a bulk inhomogeneous field. Expression (4.9c) clearly manifests that the magnetization profile near a boundary at which the spin value is fixed to zero, $|j/L|=\pm\frac{1}{2}$, is the same as the one near the boundary $|j/L|=0$, at which one half of the system is in contact with the other half, subject to the opposite field. That decoupling effect explains the identical form of the profiles under periodic and fixed boundary conditions [compare (4.9a) and (4.9c)].

In the low-temperature region, when $\mathring{x}_1\to-\infty$ as $L\to\infty$, the finite-size scaling functions (4.7) attain the universal asymptotic form

$$X^{(\tau)}(\mathring{x}_1,x_2)\cong|\mathring{x}_1|^{-1} \quad (\mathring{x}_1\to-\infty) \quad (5.1)$$

and the magnetization profile freezes [see (4.8) and (4.9)]. The corresponding temperature-independent scaling functions are

$$Z^{(\tau)}|(\mathring{x}_1,x_2,j/L)=\mathrm{sgn}(h)(x_2/2)\times\left[\left[\frac{1}{4}-\left|\frac{j}{L}\right|\right]^2-(\tfrac{1}{4})^2\right] , \quad (5.2a)$$

for $\tau=p,1$, and

$$Z^{(0)}(\mathring{x}_1,x_2,j/L)=\mathrm{sgn}(h)(x_2/2)\times\left[\left[\frac{1}{2}-\left|\frac{j}{L}\right|\right]^2-(\tfrac{1}{2})^2\right] . \quad (5.2b)$$

for $\tau=0$. The shape of (5.2a) repeats the frozen profile found in Ref. 17.

The presence of nonperiodic boundaries changes the asymptotic behavior of the correlation length near the bulk critical temperature, where $x_1=O(1)$, so that two different macroscopic length scales L and ξ_L appear. In the case of open boundaries ξ_L increases more slowly than L, since $\xi_L/L\propto 1/\ln L\to 0$ [see (3.19)], and the logarithmic corrections break the standard finite-size scaling. In a system with finite correlation length one would expect an exponential dependence on the coordinate j of the type

$$m_L^{(0)}(K,h,j)\propto 1-\exp(-|j|/\xi_L) . \quad (5.3)$$

From (4.10) one may conclude that the observed spatial behavior resembles that of a weakly correlated system in which distances scale with the finite-size correlation length rather than with the size L. However, since $\xi_L\to\infty$ as $L\to\infty$, one may adopt the alternative finite-size scaling form,

$$m_L^{(\tau)}(K,h,j)\cong C_2\xi_L^{-\beta/\nu}Z^{(\tau)}(C_1t\xi_L^{1/\nu},C_2h\xi_L^{\Delta/\nu},j/\xi_L) , \quad (5.4)$$

which has been discussed in the context of the correlation function in the presence of long-range interactions.[10,21] The hypothesis (5.4) explains why the profile (4.10) is frozen: in conformity with the standard finite-size scaling we have assumed that $x_1 \cong C_1 t L^{1/\nu} = O(1)$, but since now $\xi_L / L \to 0$ as $L \to \infty$ we obtain that $C_1 t \xi_L^{1/\nu} \to 0$.

The fixed boundary conditions have the opposite effect of abnormally large fluctuations (see also Ref. 16) when $\xi_L / L \propto (\ln L)^{1/2} \to \infty$ as $L \to \infty$. From the finite-size scaling form (5.4) one would expect in this case the spatial dependence to disappear in the limit $L \to \infty$, due to the fact that $|j|$ is bounded from above by $L/2$. However, expression (4.11) exhibits a smooth dependence on $|j|/L$. The problem why in this case the magnetization profile scales with L, instead of ξ_L, remains open.

ACKNOWLEDGMENTS

This work was supported by the Bulgarian National Foundation for Scientific Research, Grant No. F-23/91.

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