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Daniel M Dantchev[1,2,3] **and Jordan G Brankov**[1]

[1] Institute of Mechanics, Bulgarian Academy of Sciences, Acado G Bonchev St bl 4, 1113 Sofia, Bulgaria
[2] Max-Planck-Institut für Metallforschung, Heisenbergstrasse 3, D-70569 Stuttgart, Germany
[3] Institut für Theoretische und Angewandte Physik, Universität Stuttgart, Pfaffenwaldring 57, D-70569 Stuttgart, Germany

E-mail: daniel@imbm.bas.bg and brankov@imbm.bas.bg

Abstract
Exact results of the finite-size behaviour of the susceptibility in three-dimensional mean spherical model films under Dirichlet–Dirichlet, Dirichlet–Neumann and Neumann–Neumann boundary conditions are presented. The corresponding scaling functions are explicitly derived and their asymptotics close to, above and below the bulk critical temperature T_c are obtained. The results can be incorporated in the framework of the finite-size scaling theory where the exponent λ characterizing the shift of the finite-size critical temperature with respect to T_c is smaller than $1/\nu$, with ν being the critical exponent of the bulk correlation length.

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1. Introduction

The basic ideas of the phenomenological finite-size scaling theory at criticality have been suggested by Fisher [1] and Fisher and Barber [2] (for more recent reviews consult [3–5]). According to the phenomenological theory, rounding and shifting of the anomalies in the thermodynamic functions set in when the bulk correlation length ξ_∞ becomes comparable to the characteristic linear size L of the system. More specifically, it is predicted that finite-size effects are controlled by the ratio L/ξ_∞. Here we recall some fundamental notions and facts of that theory.

Let us start with a system having the geometry $L^{d-d'} \times \infty^{d'}$, with $d' > d_l$, where d_l is the lower critical dimension of the corresponding class of bulk systems. Then, under boundary conditions τ imposed across the finite dimensions of the system, the *finite-size* system exhibits a phase transition at a temperature $T = T_{c,L}^{(\tau)}$, and the corresponding infinite

system at $T = T_{c,\infty}^{(\tau)} \equiv T_c$. The so-called *fractional shift*, characterizing the shift of the critical temperature of the finite-size system, is defined as

$$\varepsilon_L^{(\tau)} = \left(T_c - T_{c,L}^{(\tau)}\right)\big/T_c \simeq b^{(\tau)} L^{-\lambda} \tag{1.1}$$

where the expected asymptotic behaviour for $L \gg 1$ is given by the shift exponent λ.

Let us now consider the susceptibility χ (per spin) which in the bulk (infinite) system has a critical-point divergence of the type

$$\chi_\infty(T) \simeq A t^{-\gamma} \qquad t \to 0^+ \tag{1.2}$$

where $\gamma = \gamma(d)$ is the d-dimensional critical exponent and $t = (T - T_c)/T_c$. On approaching the finite-size critical temperature from above at fixed L one should have

$$\chi_L^{(\tau)}(T) \simeq \dot{A}_L^{(\tau)} \dot{t}^{-\dot{\gamma}} \qquad \dot{t} \to 0^+ \tag{1.3}$$

where $\dot{t} = \left(T - T_{c,L}^{(\tau)}\right)\big/T_c = \varepsilon_L^{(\tau)} + t$ and $\dot{\gamma} = \gamma(d')$ (in general, $\gamma \neq \dot{\gamma}$). Let $T_{*,L}^{(\tau)}$ denote the temperature at which the considered finite-size property $\chi_L^{(\tau)}(T)$ first shows significant (of the relative order of unity) deviation from its bulk limit $\chi_\infty(T)$. Then one defines the *fractional rounding* [2] $\delta_L^{(\tau)} = \left(T_{*,L}^{(\tau)} - T_c\right)\big/T_c \simeq c^{(\tau)} L^{-\theta}$, $L \gg 1$. The 'rounding' measures the region of crossover from bulk d-dimensional to d'-dimensional critical behaviour.

The basic assertions of the 'orthodox' *phenomenological finite-size scaling* are that (i) the only relevant variable on which the properties of the finite-size system depend in the neighbourhood of T_c is $L/\xi_\infty(T) \sim L t^\nu$, and (ii) the rounding occurs when $\xi_\infty(T) \simeq L$.

It is easy to see that assumption (ii) leads directly to the conclusion that $\theta = 1/\nu$ and, from (i), it immediately follows that

$$\chi_L^{(\tau)}(T) \simeq L^{\gamma/\nu} \tilde{X}^{(\tau)}\left(L/\xi_\infty(T)\right) \tag{1.4}$$

or, equivalently,

$$\chi_L^{(\tau)}(T) \simeq L^{\gamma/\nu} X^{(\tau)}(t L^{1/\nu}). \tag{1.5}$$

Here $X^{(\tau)}(x)$ is the universal *finite-size scaling function* describing the critical behaviour of χ, where, in order to reproduce the behaviour described by equations (1.2) and (1.3), one should have

$$X^{(\tau)}(x) \simeq X_\infty x^{-\gamma} \qquad \text{as} \quad x \to \infty \tag{1.6}$$

and

$$X^{(\tau)}(x) \simeq X_0^{(\tau)} x^{-\dot{\gamma}} \qquad \text{as} \quad x \to 0^+. \tag{1.7}$$

It has been considered, see [1–3], that a more general formulation of the finite-size scaling hypothesis is given by the equation

$$\chi_L^{(\tau)}(T) \simeq L^{\gamma/\nu} X^{(\tau)}(\dot{t} L^{1/\nu}). \tag{1.8}$$

Apart from the allowed shift of T_c from $T_{c,L}$, equations (1.5) and (1.8) are equivalent if ξ_∞ diverges algebraically with exponent $\nu \geqslant 1/\lambda$.

We emphasize that the use of the shifted temperature variable $\dot{t}$ in the above finite-size scaling hypotheses allows for any L-dependence of the shift $\varepsilon_L^{(\tau)}$, i.e. the shift exponent λ remains arbitrary. The assertion that the only criterion determining the finite-size scaling effects in the critical region is $\xi_\infty(T) \simeq L$ leads to the equalities $\lambda = \theta = 1/\nu$. This result follows from the renormalization group derivation of finite-size scaling [3, 6] (see also [7]). Except in some special cases (ideal Bose gas and spherical model with a film geometry and Dirichlet–Dirichlet [8, 9, 11, 12] or Neumann–Neumann boundaries [10], when one has a logarithmic shift of the type $\pm \ln L/L$ for $d = 3$ and $\lambda = 1$ in *all* other dimensions $d > 2$), this relation seems to be quite generally valid. We stress, nevertheless, that the relationship $\lambda = 1/\nu$ is *not* [2] a necessary condition for the finite-size scaling to hold in general.

1.1. Phenomenological finite-size scaling for systems with large critical shift

Let us now consider in a bit more detail what will be the consequences if the shift is asymptotically large, i.e. when $1/\nu > \lambda$. From equation (1.8) one then has

$$\chi_L^{(\tau)}(T) \simeq L^{\gamma/\nu} X^{(\tau)}(t L^{1/\nu} + b^{(\tau)} L^{1/\nu - \lambda}). \tag{1.9}$$

Obviously, in order to make explicit statements, we have to consider the two possibilities (i) $b^{(\tau)} > 0$ and (ii) $b^{(\tau)} < 0$ separately.

Case (i): $b^{(\tau)} > 0$
From equation (1.6) it immediately follows that at T_c

$$\chi_L^{(\tau)}(T_c) \simeq X_\infty [b^{(\tau)}]^{-\gamma} L^{\gamma \lambda} \tag{1.10}$$

i.e., the divergence of the susceptibility at T_c with respect to L will be reduced in comparison with the 'standard' behaviour

$$\chi_L^{(\tau)}(T_c) \simeq X^{(\tau)}(0) L^{\gamma/\nu} \tag{1.11}$$

predicted by equation (1.5).

An example of a model with large positive shift of the critical temperature is the spherical model under Neumann–Neumann boundary conditions [10] (see below). For $d = 3$ the shift in the dimensionless critical coupling is equal to $\ln L/(4\pi L)$. For such a shift one immediately obtains that

$$\chi_L^{(\tau)}(T_c) \simeq X_\infty \left[\frac{4\pi L}{\ln L} \right]^\gamma. \tag{1.12}$$

Case (ii): $b^{(\tau)} < 0$
Then, at T_c one has $i L^{1/\nu} = b^{(\tau)} L^{1/\nu - \lambda} \to -\infty$ when $L \to \infty$. Obviously, in order to give a general answer what will be the behaviour of the susceptibility in this case, one needs to know the asymptotics of the scaling function $X^{(\tau)}(x)$ for $x \to -\infty$.

Generally speaking, when $x = t L^{1/\nu} \to -\infty$ takes place, the behaviour of the zero-field susceptibility in a $O(n)$ model depends on the fact whether $n = 1$, or $n > 1$, and on the geometry of the system. Then, under periodic boundary conditions, summarizing the results of [13–15] for the Ising-type models and those of [6, 15–19] for $O(n), n \geqslant 2$ models, one has

$$\chi_L^{(p)}(T < T_c) \sim \begin{cases} L^d & d' = 0 \\ L \exp[L^{d-1}\sigma(T)/k_B T] & d' = 1 \quad n = 1 \\ L^{2(d-1)} & d' = 1 \quad n \geqslant 2 \\ L^2 \exp[cL^{d-2}\Upsilon(T)/k_B T] & d' = 2 \quad n \geqslant 2 \\ \infty & \begin{array}{l} \text{if } d' > 1 \quad \text{and} \quad n = 1 \\ \text{or } d' > 2 \quad \text{and} \quad n \geqslant 2 \end{array} \end{cases} \tag{1.13}$$

where $\sigma(T)$ is the interfacial (or surface) tension in the Ising model, $\Upsilon(T)$ is its analogue—the helicity modulus—for an $O(n), n \geqslant 2$ system, and c is a constant. For other than periodic boundary conditions the situation is not so clear and detailed information for the behaviour of the zero-field finite-size susceptibility is still to be established, but one can hope that the leading-order behaviour will remain unchanged (eventually, the power of L in front of the exponential terms may change when $d' = d_l$).

We shall demonstrate the consequences of the shift on the finite-size behaviour of the susceptibility for a fully finite and a film geometry only. The interested reader can easily complete the list of all possible geometries.

1.1.1. The fully finite geometry. In order to reproduce the size dependence of the susceptibility at $T < T_c$, one should have $X^{(\tau)}(x) \simeq X_-^{(\tau)} x^{d\nu-\gamma}$. Then at T_c one obtains

$$\chi_L^{(\tau)}(T_c) \simeq X_- |b^{(\tau)}|^{d\nu-\gamma} L^{d-\lambda\nu(d-2+\eta)}. \tag{1.14}$$

For the spherical model under Dirichlet boundary conditions, taking into account that $\lambda = 1, \eta = 0$ and $\nu = 1/(d-2)$ (for $2 < d < 4$) one derives

$$\chi_L^{(\tau)}(T_c) \simeq A L^{d-1} \tag{1.15}$$

where A is a constant. This is exactly the result recently reported in [12].

1.1.2. The film geometry. Similarly to the above, one can write again the general expressions, but since they are rather cumbersome, we shall consider only the case of a film geometry on the example of the three-dimensional spherical model. Taking into account that then $\beta\Upsilon(T) = K - K_c$ [11, 20], where K is the dimensionless coupling in the system, and that $\varepsilon_L^{(D)} = -\ln L/(4\pi L)$, $c = 4\pi$ [8, 9, 11, 12], we obtain

$$\chi_L^{(\tau)}(T_c) \sim L^2 \exp(c \ln L/4\pi) \sim L^3 \tag{1.16}$$

which is exactly the result recently reported in [12] (see also below). Note that now $\chi_L^{(\tau)}$ diverges at T_c faster than in the case of the 'standard' finite-size scaling prediction given by equation (1.11) (we recall that $\gamma = 2/(d-2)$ for the spherical model, i.e. $\gamma/\nu = 2$). It is clear that when $d' = 2$, but $d > 3$, one will have $\chi_L^{(\tau)}(T_c) \sim L^2 \exp(\tilde{c}L^{d-3})$, where $\tilde{c}$ is a constant, and we have taken into account that $\lambda = 1$ for all $d > 2$.

Before finishing this overview of the general form of the phenomenological finite-size scaling theory and its consequences, let us just remind the reader what the finite-size behaviour in the case of geometry $L^{d-d'} \times \infty^{d'}$ with $d' \leqslant d_l$ is. Then, in the finite-size system there is no phase transition of its own, therefore, $\dot\gamma \equiv 0$. The hypotheses stated above still hold, provided we set $\dot\gamma = 0$ and replace $T_{c,L}^{(\tau)}$ by appropriately defined *pseudocritical* temperature $T_{m,L}^{(\tau)}$. The latter can be defined, for example, as the temperature at which the susceptibility reaches its maximum. Then, in the case of an algebraic bulk singularity of the type (1.2), one has, e.g., $\chi_L^{(\tau)}(T_{m,L}^{(\tau)}) \simeq X_0^{(\tau)} L^{\gamma/\nu}$, $L \gg 1$. This asymptotic behaviour is exploited in one of the basic methods for evaluation of bulk critical exponents from finite-size data. Here we would like to stress that $T_{m,L}^{(\tau)}$ depends on which physical quantity has been used for its definition, since the maxima of the susceptibility and, say, the specific heat take place at, generally speaking, different temperatures.

In the next sections we will present exact results for the finite-size behaviour of the zero-field susceptibility of the mean spherical model with a film geometry when Dirichlet–Dirichlet, Neumann–Dirichlet and Neumann–Neumann boundary conditions are applied at the surfaces of the film. The corresponding scaling functions $X^{(\tau)}$ will be derived and their asymptotic behaviour will be analysed. We will demonstrate the important role of the shift when it is asymptotically larger than $L^{-1/\nu}$.

The structure of the paper is as follows. In section 2 we briefly present the model and the basic facts needed for the analytical treatment of the free energy and the susceptibility for a fully finite system. Section 3 contains the corresponding modifications of these expressions in the case of a film geometry. The finite-size critical behaviour of the susceptibility is analysed in section 4. The paper closes with a discussion of the results obtained and their eventual generalization. Some technical details needed for evaluation of different sums are described in the appendix.

2. The model

We consider a d-dimensional mean spherical model with nearest-neighbour ferromagnetic interactions on a simple cubic lattice. At each lattice site $\vec{r} = (r_1, r_2, \ldots, r_d) \in \mathbf{Z}^d$ there is a random (spin) variable $\sigma(\vec{r}) \in \mathbf{R}$ and $\sigma_\Lambda = \{\sigma(\vec{r}), \vec{r} \in \Lambda\}$ is the configuration in a finite region $\Lambda \subset \mathbf{Z}^d$, containing $|\Lambda|$ sites. The boundary conditions (to be denoted by the superscript τ) define the interaction of the spins in the region Λ with a specified configuration $\{\sigma(\vec{r}), \vec{r} \in \Lambda^c\}$ in the complement $\Lambda^c = \mathbf{Z}^d \backslash \Lambda$. In the remainder we take Λ to be the parallelepiped $\Lambda = \mathcal{L}_1 \times \mathcal{L}_2 \times \cdots \times \mathcal{L}_d$, with $\mathcal{L}_i = \{1, \ldots, L_i\}$, and explicitly study the case of film geometry which results in the limit $L_2, \ldots, L_d \to \infty$ at finite values of $L_1 = L$. In the finite r_1 direction it suffices to specify the values of $\sigma(0, r_2, \ldots, r_d)$ and $\sigma(L + 1, r_2, \ldots, r_d)$ for all $(r_2, \ldots, r_d) \in \mathcal{L}_2 \times \cdots \times \mathcal{L}_d$.

The finite-size scaling behaviour of the mean spherical model has been studied so far under periodic, antiperiodic, Dirichlet, [8, 9, 21, 22], Neumann [10, 23] and Neumann–Dirichlet [10] boundary conditions (for a review see, e.g., [5]). For lattice systems under Dirichlet boundary conditions we mean that

$$\sigma(0, r_2, \ldots, r_d) = \sigma(L + 1, r_2, \ldots, r_d) = 0 \tag{2.1}$$

under Neumann boundary conditions that

$$\sigma(0, r_2, \ldots, r_d) = \sigma(1, r_2, \ldots, r_d) \qquad \sigma(L + 1, r_2, \ldots, r_d) = \sigma(L, r_2, \ldots, r_d) \tag{2.2}$$

and, under Neumann–Dirichlet boundary conditions that

$$\sigma(0, r_2, \ldots, r_d) = \sigma(1, r_2, \ldots, r_d) \qquad \sigma(L + 1, r_2, \ldots, r_d) = 0. \tag{2.3}$$

Obviously, the terminology Dirichlet and Neumann boundary conditions is justified by analogy with the continuum limit. The case of free surfaces in a system of film geometry (in the limit $L_2, \ldots, L_d \to \infty$), considered in the literature [8, 9, 21, 22], corresponds to Dirichlet boundary conditions ($\tau \equiv D$). When a fully finite system is envisaged, we always assume periodic boundary conditions with respect to the coordinates $r_2, \ldots, r_d$, i.e., for all $\vec{r} \in \Lambda$ and all integers $m_2, \ldots, m_d$, we set $\sigma(r_1, r_2 + m_2 L_2, \ldots, r_d + m_d L_d) = \sigma(r_1, r_2, \ldots, r_d)$.

For brevity of notation, we consider the configuration space $\Omega_\Lambda = \mathbf{R}^{|\Lambda|}$ as an Euclidean vector space in which each configuration is represented by a column-vector σ_Λ with components labelled according to the lexicographic order of the set $\{(r_1, r_2, \ldots, r_d) \in \Lambda\}$. Let $\sigma_\Lambda^\dagger$ be the corresponding transposed row-vector and let the dot ($\cdot$) denote matrix multiplication. Then, for given boundary conditions $\tau = (\tau_1, \tau_2, \ldots, \tau_d)$, specified for each pair of opposite faces of Λ by some $\tau_i = p$ (periodic), D (Dirichlet), N (Neumann), or ND (Neumann–Dirichlet), and given external magnetic field configuration $h_\Lambda = \{h(\vec{r}), \vec{r} \in \Lambda\}$, with $h(\vec{r}) \in \mathbf{R}$, the Hamiltonian of the model takes the form

$$\beta \mathcal{H}_\Lambda^{(\tau)}(\sigma_\Lambda | K, h_\Lambda; s) = -\tfrac{1}{2} K \sigma_\Lambda^\dagger \cdot Q_\Lambda^{(\tau)} \cdot \sigma_\Lambda + s\, \sigma_\Lambda^\dagger \cdot \sigma_\Lambda - h_\Lambda^\dagger \cdot \sigma_\Lambda. \tag{2.4}$$

Here $\beta = 1/k_B T$ is the inverse temperature; $K = \beta J$ is the dimensionless coupling constant; s is the spherical field which is to be determined from the mean spherical constraint, see equation (2.19) below; the $|\Lambda| \times |\Lambda|$ interaction matrix $Q_\Lambda^{(\tau)}$ can be written as

$$Q_\Lambda^{(\tau)} = \left(\Delta_1^{(\tau_1)} + 2\, E_1\right) \times \cdots \times \left(\Delta_d^{(\tau_d)} + 2\, E_d\right) \tag{2.5}$$

where $\times$ denotes the outer product of the corresponding matrices, $\Delta_i^{(\tau_i)}$ is the $L_i \times L_i$ discrete Laplacian under boundary conditions τ_i and E_i is the $L_i \times L_i$ unit matrix.

As is well known, the complete set of orthonormal eigenfunctions, $\{u_L^{(\tau)}(r, k), k = 1, \ldots, L\}$, of the one-dimensional discrete Laplacian for periodic, Dirichlet, Neumann and Neumann–Dirichlet boundary conditions is given by

$$u_L^{(p)}(r, k) = L^{-1/2} \exp\left[-\mathrm{i}\, r \varphi_L^{(p)}(k)\right] \tag{2.6}$$

$$u_L^{(D)}(r, k) = [2/(L+1)]^{1/2} \sin\left[r\varphi_L^{(D)}(k)\right] \tag{2.7}$$

$$u_L^{(N)}(r, k) = \begin{cases} L^{-1/2} & \text{for} \quad k = 1 \\ (2/L)^{1/2} \cos\left[(r - \tfrac{1}{2})\varphi_L^{(N)}(k)\right] & \text{for} \quad k = 2, \dots, L \end{cases} \tag{2.8}$$

and

$$u_L^{(ND)}(r, k) = 2(2L+1)^{-1/2} \cos\left[(r - \tfrac{1}{2})\,\varphi_L^{(ND)}(k)\right] \tag{2.9}$$

where

$$\varphi_L^{(p)}(k) = \frac{2\pi k}{L} \qquad \varphi_L^{(D)}(k) = \frac{\pi k}{L+1} \tag{2.10}$$

$$\varphi_L^{(N)}(k) = \frac{\pi(k-1)}{L} \qquad \varphi_L^{(ND)}(k) = \frac{\pi(2k-1)}{2L+1}. \tag{2.11}$$

The corresponding eigenvalues are

$$\lambda_L^{(\tau)}(k) = -2 + 2\cos\varphi_L^{(\tau)}(k) \qquad k = 1, \dots, L. \tag{2.12}$$

The eigenfunctions of the interaction matrix (2.5) have the form

$$u_\Lambda^{(\tau)}(\vec{r}, \vec{k}) = u_{L_1}^{(\tau_1)}(r_1, k_1)\, u_{L_2}^{(\tau_2)}(r_2, k_2) \cdots u_{L_d}^{(\tau_d)}(r_d, k_d) \qquad \vec{k} \in \Lambda \tag{2.13}$$

and the corresponding eigenvalues are

$$\mu_\Lambda^{(\tau)}(\vec{k}) = 2 \sum_{\nu=1}^{d} \cos\varphi_{L_\nu}^{(\tau_\nu)}(k_\nu) \qquad \vec{k} \in \Lambda. \tag{2.14}$$

In order to ensure positivity of all the eigenvalues $-\frac{1}{2}K\mu_\Lambda^{(\tau)}(\vec{k}) + s, \vec{k} \in \Lambda$, of the quadratic form in $\beta\mathcal{H}_\Lambda^{(\tau)}(\sigma_\Lambda | K, h_\Lambda; s)$, see equation (2.4), it is convenient to introduce a shifted and rescaled spherical field $\phi > 0$ by setting

$$s = s(\phi) := \tfrac{1}{2}K\left[\phi + \mu_\Lambda^{(\tau)}(\vec{k}_0)\right] \tag{2.15}$$

where $\vec{k}_0$ is a vector $\vec{k} \in \Lambda$ at which $\mu_\Lambda^{(\tau)}(\vec{k})$ attains maximum value.

The joint probability distribution of the random variables $\sigma_\Lambda = \{\sigma(\vec{r}), \vec{r} \in \Lambda\}$ is given by the Gibbs measure

$$d\rho_\Lambda^{(\tau)}(\sigma_\Lambda | K, h_\Lambda; \phi) = \exp\left[-\beta\mathcal{H}_\Lambda^{(\tau)}(\sigma_\Lambda | K, h_\Lambda; s(\phi))\right] \prod_{\vec{r} \in \Lambda} d\sigma(\vec{r}) \Big/ Z_\Lambda^{(\tau)}(K, h_\Lambda; \phi) \tag{2.16}$$

where $d\sigma(\vec{r})$ is the Lebesgue measure on $\mathbf{R}$ and

$$Z_\Lambda^{(\tau)}(K, h_\Lambda; \phi) = \int_{\mathbf{R}^{|\Lambda|}} \exp\left[-\beta\mathcal{H}_\Lambda^{(\tau)}(\sigma_\Lambda | K, h_\Lambda; s(\phi))\right] \prod_{\vec{r} \in \Lambda} d\sigma(\vec{r}) \tag{2.17}$$

is the partition function of the Gaussian model. The latter is finite for all $\phi > 0$ and equals $+\infty$ for $\phi \leqslant 0$. The free-energy density of the mean spherical model in a finite region Λ is given by the Legendre transformation

$$\beta f_\Lambda^{(\tau)}(K, h_\Lambda) := \sup_\phi \left\{-|\Lambda|^{-1} \ln Z_\Lambda^{(\tau)}(K, h_\Lambda; \phi) - s(\phi)\right\}. \tag{2.18}$$

Here the supremum is attained at the solution $\phi = \phi_\Lambda^{(\tau)}(K, h_\Lambda)$ (for brevity denoted by $\phi_\Lambda^{(\tau)}$) of the mean spherical constraint

$$|\Lambda|^{-1} \sum_{\vec{r} \in \Lambda} \langle \sigma^2(\vec{r}) \rangle_\Lambda^{(\tau)}(K, h_\Lambda; \phi) = 1 \tag{2.19}$$

where $\langle \cdots \rangle_\Lambda^{(\tau)}(K, h_\Lambda; \phi)$ denotes expectation value with respect to the measure (2.16).

By direct evaluation of the integrals in the partition function (2.17), one obtains

$$\beta f_\Lambda^{(\tau)}(K, h_\Lambda) = \tfrac{1}{2}\big\{ \ln(K/2\pi) - K\mu_\Lambda^{(\tau)}(\vec{k}_0) + U_\Lambda^{(\tau)}(\phi_\Lambda^{(\tau)}) - P_\Lambda^{(\tau)}(K, h_\Lambda; \phi_\Lambda^{(\tau)}) - K\phi_\Lambda^{(\tau)}\big\}.$$

(2.20)

Here we have introduced the function

$$U_\Lambda^{(\tau)}(\phi) = |\Lambda|^{-1} \sum_{\vec{k}\in\Lambda} \ln\big[\phi + \omega_\Lambda^{(\tau)}(\vec{k})\big]$$

(2.21)

which describes the contribution of the spin–spin interaction (called 'interaction term'), where

$$\omega_\Lambda^{(\tau)}(\vec{k}) := \mu_\Lambda^{(\tau)}(\vec{k}_0) - \mu_\Lambda^{(\tau)}(\vec{k})$$

(2.22)

is the normalized excitation spectrum, and the function

$$P_\Lambda^{(\tau)}(K, h_\Lambda; \phi) = \frac{1}{K|\Lambda|} \sum_{\vec{k}\in\Lambda} \frac{\big|\hat{h}_\Lambda^{(\tau)}(\vec{k})\big|^2}{\phi + \omega_\Lambda^{(\tau)}(\vec{k})}$$

(2.23)

represents the 'field term'. In (2.23) $\hat{h}_\Lambda^{(\tau)}(\vec{k})$ denotes the projection of the magnetic field configuration h_Λ on the eigenfunction $\bar{u}_\Lambda^{(\tau)}(\vec{r}, \vec{k})$:

$$\hat{h}_\Lambda^{(\tau)}(\vec{k}) = \sum_{\vec{r}\in\Lambda} h(\vec{r})\bar{u}_\Lambda^{(\tau)}(\vec{r}, \vec{k}).$$

(2.24)

The mean spherical constraint (2.19) has the form

$$\frac{\mathrm{d}}{\mathrm{d}\phi} U_\Lambda^{(\tau)}(\phi) - \frac{\partial}{\partial\phi} P_\Lambda^{(\tau)}(K, h_\Lambda; \phi) = K.$$

(2.25)

Its solution $\phi = \phi_\Lambda^{(\tau)}(K, h_\Lambda)$ depends on the lattice region Λ, the dimensionless coupling constant K and the external magnetic field configuration h_Λ.

3. The finite system with a film geometry

Hereafter we consider only boundary conditions $\tau = \{\tau_1, p, \ldots, p\}$, with $\tau_1 = D, N, ND$ for, respectively, Dirichlet–Dirichlet, Neumann–Neumann and Neumann–Diriclet boundary conditions, when $\vec{k}_0 = \{1, L_2, \ldots, L_d\}$. By taking the limit $L_2, \ldots, L_d \to \infty$ in expression (2.21) at fixed $L_1 = L$ we obtain

$$U_{L,d}^{(\tau_1)}(\phi) := \lim_{L_2,\ldots,L_d\to\infty} U_\Lambda^{(\tau_1, p, \ldots, p)}(\phi).$$

(3.1)

Next we confine ourselves to the consideration of uniform magnetic fields, $h(\vec{r}) = h, \vec{r} \in \Lambda$. By taking the limit of a film geometry in (2.23), we obtain

$$P_L^{(\tau)}(K, h; \phi) := \lim_{L_2,\ldots,L_d\to\infty} P_\Lambda^{(\tau, p, p)}(K, h_\Lambda; \phi)$$

$$= \frac{1}{KL} \sum_{k=1}^{L} \frac{[\hat{h}^{(\tau)}(k)]^2}{\phi + 2\cos\varphi_L^{(\tau)}(1) - 2\cos\varphi_L^{(\tau)}(k)}$$

(3.2)

where

$$\hat{h}^{(\tau)}(k) := h \sum_{r=1}^{L} u_L^{(\tau)}(r, k) \qquad \tau \in \{D, N, ND\}.$$

(3.3)

From equations (2.7)–(2.11) we obtain explicitly

$$\hat{h}^{(D)}(k) = \begin{cases} h\sqrt{\frac{2}{L+1}} \cot\left[\frac{\pi k}{2(L+1)}\right] & k \quad \text{odd} \\ 0 & k \quad \text{even} \end{cases}$$

(3.4)

$$\hat{h}^{(N)}(k) = \begin{cases} hL^{1/2} & k = 1 \\ -h\sqrt{\frac{2}{L}}\cos\left[\frac{\pi(k-1)}{2L}\right] & k = 2, \ldots, L \end{cases} \tag{3.5}$$

and

$$\hat{h}^{(ND)}(k) = \frac{h}{\sqrt{2L+1}}(-1)^{k-1}\cot\left[\frac{\pi(2k-1)}{2(2L+1)}\right]. \tag{3.6}$$

We just mention that for periodic boundary conditions the well-known result is $P_L^{(p)}(K, h; \phi) = h^2/K\phi$.

Note that due to the field dependence of the solution of the mean spherical constraint for the spherical field $\phi_L(K, h)$, one has to distinguish between two kinds of susceptibilities. The 'fluctuation part' of the susceptibility

$$k_B T \, \chi_{L,\text{fluct}}^{(\tau)}(K, h) := -\frac{\partial^2}{\partial h^2}\left[\beta f_L^{(\tau)}(K, h)\right]\Big|_{\phi_L^{(\tau)}=\text{const}}$$

$$= \frac{1}{2}\frac{\partial^2}{\partial h^2}\left[P_L^{(\tau)}(K, h; \phi)\right]\Big|_{\phi=\phi_L^{(\tau)}(K,h)} \tag{3.7}$$

measures the fluctuations of the magnetization in the limit of layer geometry (more precisely, the variance of a properly normalized block-spin in the corresponding limit Gibbs state) and satisfies the fluctuation–dissipation theorem. On the other hand, by differentiating twice the free energy density with respect to the magnetic field, taking into account the implicit dependence on h through the solution $\phi_L^{(\tau)}(K, h)$ of the mean spherical constraint, one obtains the *total* magnetic susceptibility per spin,

$$k_B T \, \chi_{L,\text{tot}}^{(\tau)}(K, h) := -\frac{d^2}{dh^2}\left[\beta f_L^{(\tau)}(K, h)\right] = k_B T \, \chi_{L,\text{fluct}}^{(\tau)}(K, h)$$

$$- \frac{1}{2}\frac{\partial^2}{\partial\phi\partial h}\left[P_L^{(\tau)}(K, h; \phi)\right]\Big|_{\phi=\phi_L^{(\tau)}(K,h)}\frac{d\phi_L^{(\tau)}(K, h)}{dh}. \tag{3.8}$$

These two susceptibilities coincide in the zero-field case when there is no spontaneous magnetization in the system.

For the system with a film geometry the mean spherical constraint (2.19) takes the form

$$W_{L,d}^{(\tau)}(\phi) - \frac{\partial}{\partial\phi}P_L^{(\tau)}(K, h; \phi) = K \tag{3.9}$$

where

$$W_{L,d}^{(\tau)}(\phi) := \frac{1}{L}\sum_{k=1}^{L}W_{d-1}\left[\phi + 2\cos\varphi_L^{(\tau)}(1) - 2\cos\varphi_L^{(\tau)}(k)\right] \tag{3.10}$$

and

$$W_{d-1}(z) = (2\pi)^{-(d-1)}\int_0^{2\pi}d\theta_1\int_0^{2\pi}\cdots d\theta_{d-1}\left[z + 2\sum_{\nu=1}^{d-1}(1-\cos\theta_\nu)\right]^{-1}. \tag{3.11}$$

After the evaluation of $W_{L,d}^{(\tau)}(\phi)$, the corresponding interaction term $U_{L,d}^{(\tau)}(\phi_L^{(\tau)})$ in the singular (in the limit $L \to \infty$) part of the free energy density, see (2.20),

$$\beta f_{L,\text{sing}}^{(\tau)}(K, h) = \frac{1}{2}\left\{U_{L,d}^{(\tau)}(\phi_L^{(\tau)}) - P_L^{(\tau)}(K, h; \phi_L^{(\tau)}) - K\phi_L^{(\tau)}\right\} \tag{3.12}$$

can be obtained by integration:

$$U_{L,d}^{(\tau)}(\phi_L^{(\tau)}) = U_{L,d}^{(\tau)}(\phi_0) + \int_{\phi_0}^{\phi_L^{(\tau)}}d\phi\,W_{L,d}^{(\tau)}(\phi). \tag{3.13}$$

Here $\phi_L^{(\tau)} = \phi_L^{(\tau)}(K, h)$ is the solution of equation (3.9), and $\phi_0 \geqslant 0$ is a suitably chosen constant.

Equations (3.2)–(3.13) provide the starting expressions for our further finite-size scaling analysis.

4. Critical behaviour of a three-dimensional film

At $d = 3$ and nonperiodic boundary conditions $\tau = D, N, ND$ at the surfaces of the film, the interaction term (3.10) in the mean spherical constraint (3.9) takes the form

$$W_{L,3}^{(\tau)}(\phi) := \frac{1}{L} \sum_{k=1}^{L} W_2 \left[\phi + 2 \cos \varphi_L^{(\tau)}(1) - 2 \cos \varphi_L^{(\tau)}(k) \right]. \tag{4.1}$$

This term has been evaluated by using an improved version [10] of the method developed by Barber and Fisher [8, 24]. Following [8] we set

$$W_2(z) := -(1/4\pi) \ln z + (5/4\pi) \ln 2 + Q_2(z) \tag{4.2}$$

where $Q_2(z)$ is defined by the above equation. The asymptotic behaviour of $Q_2(z)$ as $z \to 0$ follows from the well-known one of the Watson integral $W_2(z)$:

$$Q_2(z) = -\frac{1}{32\pi} z \ln z + O(z). \tag{4.3}$$

Now expression (4.1) can be identically rewritten as

$$W_{L,3}^{(\tau)}(\phi) = g_1^{(\tau)}(\phi) + g_2^{(\tau)}(\phi) + (5/4\pi) \ln 2 \tag{4.4}$$

where

$$g_1^{(\tau)}(\phi) = -\frac{1}{4\pi L} \sum_{k=1}^{L} \ln \left(\phi + 2 \cos \varphi_L^{(\tau)}(1) - 2 \cos \varphi_L^{(\tau)}(k) \right) \tag{4.5}$$

and

$$g_2^{(\tau)}(\phi) = \frac{1}{L} \sum_{k=1}^{L} Q_2 \left(\phi + 2 \cos \varphi_L^{(\tau)}(1) - 2 \cos \varphi_L^{(\tau)}(k) \right). \tag{4.6}$$

We remark that for the boundary conditions under consideration, the function (4.5) can be calculated *exactly*, and the function (4.6) can be readily evaluated with the aid of the Poisson summation formula. Here we present the final results.

4.1. Dirichlet–Dirichlet boundary conditions

We are interested in the critical regime when $\phi \to 0^+$ and $L \to \infty$, so that $\phi/2 + \cos \varphi_L^{(D)}(1) < 1$. Then we set

$$x = \arccos \left[\frac{\phi}{2} + \cos \left(\frac{\pi}{L+1} \right) \right] \cong \left[\frac{\pi^2}{(L+1)^2} - \phi \right]^{1/2}. \tag{4.7}$$

Under the above substitution, the function $g_1^{(D)}(\phi)$, defined by equation (4.5) for $\tau = D$, reads

$$g_1^{(D)}(\phi) = -\frac{1}{4\pi L} \sum_{k=1}^{L} \ln \left[2 \cos x - 2 \cos \left(\frac{k\pi}{L+1} \right) \right]. \tag{4.8}$$

The sum in the right-hand side can be calculated exactly by making use of the identity, see [25],

$$\cos(nx) - \cos(ny) = (\cos x - \cos y) \prod_{k=1}^{n-1} [2\cos x - 2\cos(y + 2k\pi/n)] \quad (4.9)$$

setting here $y = 0$, $n = 2(L + 1)$, and making simple transformations of the product using the periodicity of the cosine. Thus one obtains

$$g_1^{(D)}(\phi) = -\frac{1}{4\pi L} \ln \left[\frac{\sin(L+1)x}{\sin x} \right]. \quad (4.10)$$

Now we pass to the evaluation of the function $g_2^{(D)}(\phi)$, defined by equation (4.6) at $\tau = D$. Under the substitution (4.7) it explicitly reads

$$g_2^{(D)}(\phi) = \frac{1}{L} \sum_{k=1}^{L} Q_2 \left(2\cos x - 2\cos \frac{\pi k}{L+1} \right)$$

$$= \frac{1}{2L} \sum_{k=1}^{2L+1} Q_2 \left(2\cos x - 2\cos \frac{\pi k}{L+1} \right) - \frac{1}{2L} Q_2(2\cos x + 2). \quad (4.11)$$

In deriving the second equality we have used the periodicity of the cosine. For $\phi < \pi^2/(L+1)^2 \to 0^+$ as $L \to \infty$ the last term obviously yields $Q_2(4)/2L + O(L^{-2})$. By applying the Poisson summation formula to the sum in the right-hand side of the last equality in equation (4.11), changing the integration variable and using the periodicity of the integrand, we obtain

$$g_2^{(D)}(\phi) = \frac{L+1}{L\pi} \int_{\pi/(L+1)}^{\pi} d\theta \, Q_2(2\cos x - 2\cos \theta)$$

$$- \frac{1}{2L} [Q_2(4) - Q_2(\phi)] + \Delta g_2^{(D)}(\phi) + O(L^{-2}) \quad (4.12)$$

where

$$\Delta g_2^{(D)}(\phi) = 2\frac{L+1}{L\pi} \sum_{q=1}^{\infty} \int_{\pi/(L+1)}^{\pi} d\theta \, \cos[2q(L+1)\theta] Q_2(2\cos x - 2\cos \theta). \quad (4.13)$$

Consider first the integral in the right-hand side of equation (4.12). Its lower limit cannot be extended to 0, since we consider the regime when

$$2\cos x = \phi + 2\cos[\pi/(L+1)] \cong 2 - x^2 < 2 \quad (4.14)$$

and the function Q_2 is not defined for negative arguments, see equation (4.2). That is why we approximate the integrand by

$$Q_2(2\cos x - 2\cos \theta) \cong Q_2(\phi + 2 - 2\cos \theta) - \left[\frac{\pi}{L+1} \right]^2 Q_2'(\phi + 2 - 2\cos \theta) \quad (4.15)$$

and note that the resulting integrals converge when the lower limit tends to zero. Then, by expressing Q_2 in terms of W_2 through the definition (4.2), and taking the integral

$$\frac{1}{4\pi^2} \int_0^{\pi} d\theta \, \ln(\phi + 2 - 2\cos \theta) = \frac{1}{4\pi} \ln \left\{ 1 + \phi/2 + [\phi(1 + \phi/4)]^{1/2} \right\}$$

$$= \frac{\phi^{1/2}}{4\pi} + O(\phi) \quad (4.16)$$

we obtain

$$\frac{1}{\pi} \int_{\pi/(L+1)}^{\pi} d\theta \, Q_2(2\cos x - 2\cos \theta) \cong W_3(\phi) - \frac{5\ln 2}{4\pi} + \frac{\phi^{1/2}}{4\pi} + O(L^{-2}). \quad (4.17)$$

The integral in the right-hand side of equation (4.13) can be evaluated by twofold integration by parts. Since the resulting three terms are $\propto q^{-2}$, the sum over q in equation (4.13) converges and we conclude that

$$\Delta g_2^{(D)}(\phi) = O(L^{-2}). \tag{4.18}$$

By combining equations (4.12), (4.17), (4.18), and taking into account the small argument asymptotic form of W_3 and Q_2 we obtain

$$g_2^{(D)}(\phi) = K_{c,3} - \frac{5\ln 2}{4\pi} + \frac{1}{L}\left[K_{c,3} - \frac{1}{2}W_2(4) - \frac{7\ln 2}{8\pi}\right] + O(L^{-2}). \tag{4.19}$$

Finally, by substitution of equations (4.10) and (4.19) into equation (4.4), and taking into account equation (4.7), we obtain the zero-field mean spherical constraint in the form

$$\ln\left[\frac{\sin(\pi^2 - L^2\phi)^{1/2}}{(\pi^2 - L^2\phi)^{1/2}}\right] + \ln L = 4\pi L(K_{c,3} - K) + 4\pi\left[K_{c,3} - \frac{1}{2}W_2(4) - \frac{7\ln 2}{8\pi}\right] + O(L^{-1}). \tag{4.20}$$

This equation coincides (up to a factor of 2, due to the different choice of the coupling constant in the Hamiltonian) with the analytical continuation of equation (7.12) in [8], or equation (22) in [9], from the domain $L^2\phi > \pi^2$ to the domain $L^2\phi < \pi^2$. In that work the focus was on the finite-size scaling behaviour and the $\ln L$ term on the left-hand side of equation (4.20) was attributed to the finite-size shift of the critical coupling

$$K_{m,L}^{(D)} = K_{c,3} - \frac{\ln L}{4\pi L} + \frac{1}{L}\left[K_{c,3} - \frac{1}{2}W_2(4) - \frac{7\ln 2}{8\pi}\right]. \tag{4.21}$$

Then, in terms of the variables $L^2\phi$ and $L(K_{m,L}^{(D)} - K)$ the mean spherical constraint (4.20) takes the expected finite-size scaling form (in [8] the difference $K_{m,L}^{(D)} - K$ is denoted by $\Delta\dot{K}$).

However, Chen and Dohm [12] have noted that at the bulk critical temperature, when $K = K_{c,3}$, equation (4.20) has a leading-order solution $\phi_L^{(D)}(K_{c,3}, 0) \sim L^{-3}$. This behaviour follows by assuming $L^2\phi \to 0$ as $L \to \infty$ and expanding the left-hand side of the mean spherical constraint up to the leading order:

$$\ln\phi + 3\ln L = 4\pi L(K_{c,3} - K) + O(1). \tag{4.22}$$

Note that, if $K_{c,3} > K$, i.e. $L(K_{c,3} - K) \to \infty$, the solution of the above equation is

$$\phi \simeq L^{-3}\,e^{-4\pi L(K_{c,3} - K) + O(1)}. \tag{4.23}$$

To relate the above fact to the critical behaviour of the model, we start from the exact result for the zero-field susceptibility per spin under Dirichlet–Dirichlet boundary conditions, see equation (A.10),

$$\chi_L^{(D)}(K, 0) = \frac{1}{2J}\left\{\frac{\cot^2(x/2)\sin[(L+1)x]}{L\sin x[1 + \cos(L+1)x]} - \frac{L+1}{2L\sin^2(x/2)}\right\}. \tag{4.24}$$

By expanding the right-hand side for $L^2\phi \to 0$ as $L \to \infty$, we obtain

$$\chi_L^{(D)}(K, 0) = \frac{4}{J\pi^2\phi} + O((\phi L)^{-1}) + O(L^{-2}). \tag{4.25}$$

Hence, at the *bulk* critical temperature one recovers the leading-order result of [12]

$$\chi_L^{(D)}(K_{c,3}, 0) \sim L^3 \tag{4.26}$$

in full accordance with the predictions of the phenomenological finite-size scaling, see equation (1.16). For $K_{c,3} > K$ one has $\chi_L^{(D)}(K < K_{c,3}, 0) \sim L^3\exp[4\pi L(K_{c,3} - K)]$,

i.e. the susceptibility diverges then exponentially, which agrees with equation (1.13) in the case $d' = 2$.

To understand this anomalous behaviour at T_c, we recall that the 'standard' finite-size scaling regime takes place when $L(K_{m,L}^{(D)} - K) = O(1)$, or equivalently, at

$$K = K_{c,3} - \frac{\ln L}{4\pi L} - \frac{x_1}{L} \qquad x_1 = O(1) \tag{4.27}$$

i.e., in a narrow temperature interval of width $O(L^{-1})$ (note that in the three-dimensional spherical model $\nu = 1/(d-2) = 1$) which is shifted by $O(\ln L/L)$ *above* the bulk critical temperature $T_{c,3}$. Thus, the change to the behaviour $\chi_L \sim L^3$, which takes place at the bulk critical point, occurs in a temperature region of the same width shifted by $O(\ln L/L)$ *below* the finite-size scaling one.

We emphasize that the result $\chi_L^{(D)}(K_{c,3}, 0) \sim L^3$ is characteristic of the layer geometry with *two* free surfaces. To show that we consider below the cases of Neumann–Dirichlet and Neumann–Neumann boundary conditions.

4.2. Neumann–Dirichlet boundary conditions

In the critical regime when $\phi \to 0^+$ and $L \to \infty$, so that $\phi/2 + \cos \varphi_L^{(ND)}(1) < 1$, we set

$$x = \arccos\left[\frac{\phi}{2} + \cos\left(\frac{\pi}{2L+1}\right)\right] \cong \left[\frac{\pi^2}{(2L+1)^2} - \phi\right]^{1/2}. \tag{4.28}$$

In this case the exact expression for the function $g_1^{(ND)}(\phi)$, defined by equation (4.5), follows from the identity (4.20) in [10]:

$$g_1^{(ND)}(\phi) = -\frac{1}{4\pi L} \ln\left[\frac{\cos(L+1/2)x}{\cos(x/2)}\right] \tag{4.29}$$

where x is given by equation (4.28). The evaluation of $g_2^{(ND)}(\phi)$ goes along the same lines as in the previous case with the result

$$g_2^{(ND)}(\phi) = K_{c,3} - \frac{5\ln 2}{4\pi} + \frac{1}{2L}\left[K_{c,3} - W_2(4) - \frac{\ln 2}{2\pi}\right] + O(L^{-2}). \tag{4.30}$$

Now the zero-field mean spherical constraint takes the form (see equation (4.22) in [10] at zero surface fields and replace there $2K \to K$)

$$\ln\left[\cos(\pi^2/4 - L^2\phi)^{1/2}\right] = 4\pi L(K_{c,3} - K) + 2\pi\left[K_{c,3} - W_2(4) - \frac{\ln 2}{2\pi}\right] + O(L^{-1}\ln L). \tag{4.31}$$

Comparing the above equation with the analogous equation (4.20), we see that now there is no $\ln L/L$ finite-size shift of the critical temperature:

$$K_{m,L}^{(ND)} = K_{c,3} + \frac{1}{2L}\left[K_{c,3} - W_2(4) - \frac{\ln 2}{2\pi}\right]. \tag{4.32}$$

The mean spherical constraint (4.31) takes the expected finite-size scaling form in terms of the variables $L^2\phi$ and $L(K_{m,L}^{(ND)} - K)$. Even in the regime $L^2\phi \to 0$ as $L \to \infty$, by expanding its left-hand side one obtains in the leading order

$$\ln \phi + 2\ln L = 4\pi L(K_{c,3} - K) + O(1). \tag{4.33}$$

Therefore, at the bulk critical temperature one has the standard finite-size behaviour $\phi_L^{(ND)}(K_{c,3}, 0) \sim L^{-2}$. Note that below T_c, when $L(K_{c,3} - K) \to \infty$, the solution of the spherical field equations is

$$\phi \simeq L^{-2} e^{-4\pi L(K_{c,3} - K) + O(1)} \tag{4.34}$$

i.e. it is similar (only the power of L in front of the exponential term differs) to that of Dirichlet–Dirichlet boundary conditions, see equation (4.23).

The critical behaviour of the zero-field susceptibility per spin under Neumann–Dirichlet boundary conditions follows from the exact result, see equation (A.19),

$$\chi_L^{(ND)}(K,0) = \frac{1}{J}\left\{4\cot^2(x/2)\left[\frac{\tan[(L+1/2)x]}{L\sin x}\right.\right.$$
$$\left.\left.- \frac{1}{2L(2L+1)\cos^2(x/2)}\right] - \frac{L+1}{2(2L+1)\sin^2(x/2)}\right\} \tag{4.35}$$

where x is given by equation (4.28). By expanding the right-hand side of the above equation for $x \ll 1$, we obtain to the leading order

$$\chi_L^{(ND)}(K,0) \cong \frac{L^2}{J(\pi^2/4 - L^2\phi)}\left[\frac{\tan(\pi^2/4 - L^2\phi)^{1/2}}{(\pi^2/4 - L^2\phi)^{1/2}} - 1\right]. \tag{4.36}$$

From equation (4.31) it is clear that for any finite value of $L(K_{c,3} - K)$ the susceptibility diverges as L^2 when $L \to \infty$. Note that $(\pi^2/4 - L^2\phi)^{1/2} \to 0^+$ only when $L(K_{m,L}^{(ND)} - K) \to 0$. Therefore, at the shifted critical temperature one obtains the simple result

$$\chi_L^{(ND)}(K_{m,L}^{(ND)},0) \cong \frac{L^2}{3J}. \tag{4.37}$$

Thus we conclude that in the presence of only one free (Dirichlet) surface the mean spherical model has the usual finite-size critical behaviour. It is instructive to see whether this behaviour will change in the presence of two equivalent surfaces with Neumann boundary conditions.

4.3. Neumann–Neumann boundary conditions

The interaction term (4.1) in this case has been treated completely and rigorously in [10]. Since $\cos\varphi_L^{(N)}(1) = 1$, see (2.11), we set

$$x = \cosh^{-1}(1 + \phi/2) \cong \phi^{1/2} \tag{4.38}$$

where $\cosh^{-1}$ denotes the inverse function of $\cosh$. The exact expression for the function $g_1^{(N)}(\phi)$ is given by equation (3.13) of [10]. It reads

$$g_1^{(N)}(\phi) = -\frac{1}{4\pi L}\left\{\ln\phi + \ln\left[\frac{\sinh Lx}{\sinh x}\right]\right\}. \tag{4.39}$$

In the critical regime $\phi \to 0$ as $L \to \infty$ the result for the function $g_2^{(N)}(\phi)$ is (see equation (3.18) in [10] under the replacement $2K_c \to K_c$)

$$g_2^{(N)}(\phi) = K_c - \frac{5\ln 2}{4\pi} - \frac{1}{2L}\left[W_2(4) - \frac{3\ln 2}{4\pi}\right] + O(L^{-2}). \tag{4.40}$$

Thus, by substitution of equations (4.39) and (4.40) into (4.4), in the limit $\phi \to 0$, $L \to \infty$, we obtain in the leading order the following finite-size scaling form of the zero-field mean spherical constraint:

$$\ln[L\phi^{1/2}\sinh(L\phi^{1/2})] = 4\pi L(K_{m,L}^{(N)} - K) \tag{4.41}$$

where $K_{m,L}^{(N)}$ is the shifted critical coupling,

$$K_{m,L}^{(N)} = K_{c,3} + \frac{\ln L}{4\pi L} - \frac{1}{2L}\left[W_2(4) - \frac{3\ln 2}{2}\right]. \tag{4.42}$$

Comparing equations (4.42) and (4.21) we see that under Neumann–Neumann boundary conditions the finite-size scaling region of width $O(L^{-1})$ is shifted *below* the bulk critical temperature $T_{c,3}$ by $O(\ln L/L)$. Since at the bulk critical point, when $K = K_{c,3}$, the right-hand side of equation (4.41) goes to plus infinity like $\ln L$ as $L \to \infty$, we conclude that $L\phi^{1/2} \to \infty$, although $\phi \to 0^+$. In this regime equation (4.41) simplifies to

$$\ln \phi^{1/2} + L\phi^{1/2} = O(1) \tag{4.43}$$

which yields

$$\phi_L^{(N)}(K_{c,3}) \sim (\ln L/L)^2. \tag{4.44}$$

Thus, at the bulk critical temperature, the finite-size critical behaviour of the spherical field under Neumann–Neumann boundary conditions becomes logarithmically modified. Note that below T_c, i.e. when $L(K_{c,3} - K) \to \infty$, the solution of the spherical field equation (4.41) is

$$\phi \simeq L^{-1} \, e^{-4\pi L(K_{c,3}-K)+O(1)} \tag{4.45}$$

i.e. the leading-order behaviour of ϕ again differs only in the power of L in front of the exponential term, compare with equations (4.23) and (4.34).

The corresponding critical behaviour of the zero-field susceptibility follows from the exact expression, see (A.27),

$$\chi_L^{(N)}(K, 0) = \frac{1}{J} \left\{ \frac{1}{\phi} + \frac{1 + \cosh x}{L^2 \sinh x} [L \coth(Lx) - \coth x] - \frac{L-1}{L^2} \right\} \tag{4.46}$$

where x is given by equation (4.38). By expanding this expression for $x \cong \phi^{1/2} \to 0^+$ and $Lx \cong L\phi^{1/2} \to \infty$, we obtain the following modified leading-order behaviour of the finite-size zero-field susceptibility at the bulk critical point:

$$\chi_L^{(N)}(K_{c,3}, 0) \cong \frac{1}{J\phi_L^{(N)}(K_{c,3})} \cong \frac{L^2}{J(\ln L)^2} \tag{4.47}$$

in a full accordance with equation (1.12).

We emphasize that the above behaviour takes place at the bulk critical temperature, in a temperature region of width $O(L^{-1})$ shifted by $O(\ln L/L)$ *above* the finite-size scaling one. It will be further modified, although not radically, if one considers the temperature interval located at $p > 0$ times the same shift above $T_{c,3}$. Then one obtains from equation (4.41), up to the leading order,

$$\phi_L^{(N)}(K_{L,p}) \sim [(1 + p) \ln L/L]^2 \tag{4.48}$$

and hence the corresponding reduction of the finite-size zero-field susceptibility (4.47) by a factor of $(1 + p)^{-2}$.

5. Discussion

In the current paper we have presented the predictions of the phenomenological finite-size scaling for systems with asymptotically large shift of the bulk critical temperature. We have shown that in such systems the behaviour of the zero-field susceptibility at the bulk critical point depends crucially on the sign of the shift—the positive shift leads to the reduction of the 'standard' divergence of $\chi_L^{(\tau)} \sim L^{\gamma/\nu}$, while the negative shift leads to a stronger divergence. We have verified our considerations on the example of the three-dimensional spherical model under Dirichlet–Dirichlet, Dirichlet–Neumann and Neumann–Neumann boundary conditions. A Dirichlet surface leads to a negative shift of the critical coupling, $-\ln L/(8\pi L)$, and a

Neumann surface to a positive one, $\ln L/(8\pi L)$ [11]. So, for a film geometry under Dirichlet–Dirichlet boundary condition the shift $\varepsilon_L^{(D)} = -\ln L/(4\pi L)$ leads to $\chi_L^{(D)}(K_{c,3}, 0) \sim L^3$ (see equation 4.26), in full accordance with our phenomenological predictions (see equations (1.13) and (1.16)). For Neumann–Neumann boundary conditions the shift is positive, i.e. $\varepsilon_L^{(N)} = \ln L/(4\pi L)$, wherefrom $\chi_L^{(N)}(T_c) \cong L^2/[J(\ln L)^2]$, in full agreement with the phenomenological prediction given by equation (1.12).

We emphasize that, in order to make concrete phenomenological prediction for the finite-size behaviour of the zero-field susceptibility in systems with asymptotically large shift of the critical temperature, use has been made of the size dependence of $\chi_L^{(p)}$ for $T < T_c$. We have supposed that the leading behaviour of $\chi_L^{(\tau)}$ will be the same under other boundary conditions. We have verified this assumption on the example of the spherical model. It is highly desirable to have the corresponding results for other models too.

One might ask why is the shift of the critical coupling in the spherical model positive under Neumann–Neumann and negative under Dirichlet–Dirichlet boundary conditions. Indeed, this contradicts the general expectations based on arguments such as that the missing neighbours in a ferromagnetic system should reduce its critical temperature. In order to understand the above facts, let us note that the observed behaviour is in agreement with the length of the spins near the boundary. This length is reduced near a Dirichlet boundary and enlarged near a Neumann one [23] (there $\langle\sigma^2\rangle \simeq 1.34$ [23]; similar estimation for the Dirichlet boundary gives $\langle\sigma^2\rangle \simeq 0.83$). Then, since the total length of all the spins is fixed, that leads to spins in the main part of the system being larger than 1 under Dirichlet and smaller than 1 under Neumann boundary conditions. As a result, an effective interaction is taking place with spins whose length is not equal to 1. In turn, this produces a shift in the 'critical temperature' of the finite system which is positive for Dirichlet and negative for Neumann boundary conditions, contrary to what one would expect for a system with a fixed length of the spins.

Finally, let us recall that the infinite translational invariant spherical model is equivalent to the $n \to \infty$ limit of the corresponding system of n-component vectors [26, 27], but the spherical model with surfaces (or, more generally, without translation-invariant symmetry) is in fact *not* such a limit [28]. In other words, the spherical model under nonperiodic boundary conditions is not in the same surface universality class as the corresponding $O(n)$ model in the limit $n \to \infty$, in contrast with the bulk universality classes. The last becomes apparent when one investigates surface phase transitions for an $O(n)$ model in the limit $n \to \infty$. In that case in the limit $n \to \infty$ one obtains [29] $\Delta_1^o = 1/(d-2)$ (i.e. $\Delta_1^o = 1$ for $d = 3$) for ordinary and $\Delta_1^{sb} = 2/(d-2)$ (i.e. $\Delta_1^{sb} = 2$ for $d = 3$) for special phase transitions, while $\Delta_1^o = 1/2$ and $\Delta_1^{sb} = 3/2$ [10, 23] for the three-dimensional spherical model. It is believed that the corresponding equivalence will be recovered if one imposes spherical constraints in a way which ensures that the mean square value of each spin of the system is the same [28] (unfortunately such a model is rather untractable analytically). The introduction of just one additional spherical field that fixes the mean square values of the spins at the boundaries changes the surface critical exponents [23], but is not enough to recover the correspondence to the $O(n)$ models. Unfortunately, the finite-size scaling properties even of that analytically tractable model have not been investigated.

Acknowledgments

Appendix A. Calculation of the field term

A.1. Dirichlet–Dirichlet boundary conditions

In uniform magnetic field h and in the regime when $\cos x := \phi/2 + \cos \varphi_L^{(D)}(1) < 1$, the field term equation (3.2) has the explicit form (assuming L odd)

$$P_L^{(D)}(K, h; \phi) = \frac{h^2}{K L(L+1)} \sum_{k=0}^{(L-1)/2} \frac{\cot^2 \frac{\pi(2k+1)}{2(L+1)}}{\cos x - \cos \frac{\pi(2k+1)}{L+1}}. \tag{A.1}$$

By making use of the elementary identity

$$\cot^2(\alpha/2) = \frac{2}{1 - \cos \alpha} - 1 \tag{A.2}$$

the above expression can be rewritten as

$$P_L^{(D)}(K, h; \phi) = \frac{h^2}{K} \left\{ \frac{2}{1 - \cos x} \left[S_L^{(D)}(x) - S_L^{(D)}(0) \right] - S_L^{(D)}(x) \right\} \tag{A.3}$$

where

$$S_L^{(D)}(x) = \frac{1}{L(L+1)} \sum_{k=0}^{(L-1)/2} \frac{1}{\cos x - \cos \frac{\pi(2k+1)}{L+1}}. \tag{A.4}$$

To calculate the sum $S_L^{(D)}(x)$, we use the identity (4.9) and set there $n = L+1$ and $y = \pi/(L+1)$. This yields

$$\prod_{k=0}^{L} \left[\cos x - \cos \frac{\pi(2k+1)}{L+1} \right] = 2^{-L}[\cos(L+1)x + 1]. \tag{A.5}$$

Since the left-hand side of the above identity equals

$$\left\{ \prod_{k=0}^{(L-1)/2} \left[\cos x - \cos \frac{\pi(2k+1)}{L+1} \right] \right\}^2 \tag{A.6}$$

we obtain

$$\prod_{k=0}^{(L-1)/2} \left[\cos x - \cos \frac{\pi(2k+1)}{L+1} \right] = 2^{-L/2}[\cos(L+1)x + 1]^{1/2}. \tag{A.7}$$

Next, by taking logarithm of both sides of equation (A.7) and differentiating the result with respect to x, we obtain

$$S_L^{(D)}(x) = \frac{\sin(L+1)x}{2L \sin x[1 + \cos(L+1)x]}. \tag{A.8}$$

Hence

$$S_L^{(D)}(0) = \lim_{x \to 0} S_L^{(D)}(x) = \frac{L+1}{4L}. \tag{A.9}$$

Finally, by inserting equations (A.8) and (A.9) into equation (A.3), and making elementary transformations based on the identity (A.2), we obtain the exact result

$$P_L^{(D)}(K, h; \phi) = \frac{h^2}{2K} \left\{ \frac{\cot^2(x/2) \sin[(L+1)x]}{L \sin x[1 + \cos(L+1)x]} - \frac{L+1}{2L \sin^2(x/2)} \right\}. \tag{A.10}$$

A.2. Neumann–Dirichlet boundary conditions

In uniform magnetic field h and in the regime when $\cos x := \phi/2 + \cos \varphi_L^{(ND)}(1) < 1$, the field term equation (3.2) has the following explicit form:

$$P_L^{(ND)}(K, h; \phi) = \frac{h^2}{KL(2L + 1)} \sum_{k=0}^{L-1} \frac{\cot^2 \frac{\pi(2k+1)}{2(2L+1)}}{\cos x - \cos \frac{\pi(2k+1)}{2L+1}}. \tag{A.11}$$

By making use of the elementary identity (A.2) the above expression can be rewritten as

$$P_L^{(ND)}(K, h; \phi) = \frac{h^2}{K} \left\{ \frac{2}{1 - \cos x} \left[S_L^{(ND)}(x) - S_L^{(ND)}(0) \right] - S_L^{(ND)}(x) \right\} \tag{A.12}$$

where

$$S_L^{(ND)}(x) = \frac{1}{2L(2L + 1)} \sum_{k=0}^{L-1} \frac{1}{\cos x - \cos \frac{\pi(2k+1)}{2L+1}}. \tag{A.13}$$

To calculate the sum $S_L^{(ND)}(x)$, we use the identity (4.9) and set there $n = 2L + 1$ and $y = \pi/(2L + 1)$. This yields

$$\prod_{k=0}^{2L} \left[\cos x - \cos \frac{\pi(2k + 1)}{2L + 1} \right] = 2^{-2L}[\cos(2L + 1)x + 1]. \tag{A.14}$$

Since the left-hand side of the above identity equals

$$(\cos x + 1) \left\{ \prod_{k=0}^{L-1} \left[\cos x - \cos \frac{\pi(2k + 1)}{2L + 1} \right] \right\}^2 \tag{A.15}$$

we obtain

$$\prod_{k=0}^{L-1} \left[\cos x - \cos \frac{\pi(2k + 1)}{2L + 1} \right] = 2^{-L} \left[\frac{\cos(2L + 1)x + 1}{\cos x + 1} \right]^{1/2}. \tag{A.16}$$

Next, by taking logarithm of both sides of equation (A.16) and differentiating the result with respect to x, we obtain

$$S_L^{(ND)}(x) = \frac{\sin(2L + 1)x}{4L \sin x[1 + \cos(2L + 1)x]} - \frac{1}{4L(2L + 1)(1 + \cos x)}. \tag{A.17}$$

Hence

$$S_L^{(ND)}(0) = \lim_{x \to 0} S_L^{(ND)}(x) = \frac{L + 1}{2(2L + 1)}. \tag{A.18}$$

Finally, by inserting equations (A.17) and (A.19) into equation (A.12), and making elementary transformations, we obtain the exact result

$$P_L^{(D)}(K, h; \phi) = \frac{h^2}{K} \left\{ 4 \cot^2(x/2) \left[\frac{\tan[(L + 1/2)x]}{L \sin x} - \frac{1}{2L(2L + 1)\cos^2(x/2)} \right] - \frac{L + 1}{2(2L + 1)\sin^2(x/2)} \right\}. \tag{A.19}$$

A.3. Neumann–Neumann boundary conditions

This case differs from the previous two ones in that now $\cos\varphi_L^{(N)}(1) = 1$ and we have to set $\cosh x := 1 + \phi/2 > 1$. In uniform magnetic field h, the field term equation (3.2) has the explicit form

$$P_L^{(N)}(K, h; \phi) = \frac{h^2}{K\phi} + \frac{2h^2}{K} S_L^{(N)}(x) \tag{A.20}$$

where

$$S_L^{(N)}(x) = \frac{1}{L^2} \sum_{k=1}^{L-1} \frac{\cos^2 \frac{\pi k}{2L}}{\cosh x - \cos(\pi k/L)}. \tag{A.21}$$

By making use of the elementary identity

$$\cos^2(\alpha/2) = \tfrac{1}{2}(1 + \cosh x) - \tfrac{1}{2}(\cosh x - \cos\alpha) \tag{A.22}$$

the above expression can be rewritten as

$$S_L^{(N)}(x) = \frac{1 + \cosh x}{2L^2} \sum_{k=1}^{L-1} \frac{1}{\cosh x - \cos(\pi k/L)} - \frac{L-1}{2L^2}. \tag{A.23}$$

To calculate the above sum, we start from the identity [25]

$$\prod_{k=1}^{n-1} \left[z^2 - 2z \cos \frac{\pi k}{n} + 1 \right] = \frac{z^{2n} - 1}{z^2 - 1}. \tag{A.24}$$

By setting here $z = \exp(x)$, $n = L$, and performing elementary transformations, we obtain

$$\prod_{k=1}^{L-1} \left[\cosh x - \cos \frac{\pi k}{L} \right] = 2^{-L+1} \frac{\sinh(Lx)}{\sinh x}. \tag{A.25}$$

Next, by taking the logarithm of both sides of equation (A.7) and differentiating the result with respect to x, we obtain

$$S_L^{(N)}(x) = \frac{1 + \cosh x}{2L^2 \sinh x}[L \coth(Lx) - \coth x] - \frac{L-1}{2L^2}. \tag{A.26}$$

Finally, by inserting equations (A.26) into equation (A.20), we obtain the exact result

$$P_L^{(N)}(K, h; \phi) = \frac{h^2}{K} \left\{ \frac{1}{\phi} + \frac{1 + \cosh x}{L^2 \sinh x} [L \coth(Lx) - \coth x] - \frac{L-1}{L^2} \right\}. \tag{A.27}$$

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