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New surface critical exponents in the spherical model

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Abstract. The three-dimensional mean spherical model with a L-layer film geometry, under Neumann–Neumann and Neumann–Dirichlet boundary conditions is considered. Surafce fields h_1 and h_L are supposed to act at the surfaces bounding the system. In the case of Neumann boundary conditions a new surface critical exponent $\Delta_1^{\mathrm{sb}} = \frac{3}{2}$ is found. It is argued that this exponent corresponds to a special (surface–bulk) phase transition in the model. The Privman–Fisher scaling hypothesis for the free energy is verified and the corresponding scaling functions for both the Neumann–Neumann and Neumann–Dirichlet boundary conditions are explicitly derived. If the layer field is applied at some distance from the Dirichlet boundary, a family of critical exponents emerges: their values depend on the exponent defining how the distance scales with the finite size of the system, and interpolate continuously between the extreme cases $\Delta_1^{\mathrm{o}} = \frac{1}{2}$ and $\Delta_1^{\mathrm{sb}} = \frac{3}{2}$.

1. Introduction

It is well known that in statistical mechanical systems with surfaces a variety of surface phase transitions can take place, depending on the imposed boundary conditions, the enhancement of the surface couplings and on the (magnetic) fields applied at the boundaries (for a general review see, e.g., [1–3]). If the surface coupling enhancement and the dimensionality are large enough, the surface orders at some temperature T_{s} larger than the bulk critical one, T_{c}, of the corresponding infinite system. The lowering of the temperature leads then to the so-called extraordinary transition, when the bulk orders at T_{c} in the presence of an already ordered surface. In the opposite case, where the surface enhancement is not sufficient to compensate the effect of missing neighbours at the surface (in the most familiar case of the so-called 'free boundary conditions'), the surface critical behaviour will be driven by the bulk: this is the ordinary phase transition. The borderline case between these two types is termed the special, or surface–bulk, surface phase transition. To characterize the singular behaviour of the different surface-introduced quantities, e.g., the surface magnetization, a variety of surface critical exponents has been defined for each class of surface phase transitions. It is well established fact now that for the ordinary phase transition there is only one independent surface critical exponent (in addition of the bulk ones). In the extraordinary surface universality class all the surface exponents can be expressed in terms of the bulk ones. The special phase transition, being a borderline case and hence a multicritical phase transition, is characterized by two new independent critical exponents. In this case one additional crossover exponent Φ appears, which describes how in the phase diagram the line of surface phase transitions joins the line of extraordinary transitions.

In the present paper we will be interested in the finite-size scaling behaviour of a three-dimensional hypercubic lattice system with a film geometry $L \times \infty^2$. Across the finite dimension of extent L Neumann–Neumann or Neumann–Dirichlet boundary conditions will be imposed. Surface fields h_1 and h_L are supposed to act at the surfaces bounding the system. The concrete consideration will be done on the example of the mean spherical model.

Under Dirichlet boundary conditions for a lattice spin system we mean here the case where the interaction of the system with the 'surrounding world' is modelled by setting the spin configuration outside the system to zero. Under Neumann boundary conditions this interaction is modelled by setting the surrounding spins to be equal to their nearest neughbours inside the system. (A precise mathematical definition of the boundary conditions will be given in section 2.) In the literature on lattice spin systems the terms 'free' and 'fixed' boundary conditions have both been used instead of Dirichlet boundary conditions (see, e.g., [4–6]) and for what we call Neumann boundary conditions the term 'free' boundary conditions has also been used [6]. To avoid misunderstanding, we use here the corresponding classical terminology stemming from continuous models.

The mean spherical model has been extensively studied with respect to both the finite-size scaling theory and (relatively less) the theory of surface phase transitions (see, e.g., [1, 4, 7, 8] for a review). Nevertheless, the situation with its surface critical exponents, especially those for the special phase transition, is not completely clear. The d-dimensional L-layer model with Dirichlet boundary conditions, in the presence of an external homogeneous magnetic field h and a surface field h_1 acting on the first layer, was considered in [9]. For $d = 3$ it has been found that the singular part of the free energy density of the system (per $k_B T$ and per spin) is of the form

$$f_L\left(T, h, h_1\right) = L^{-d} X\left(a\dot{t}L^{1/\nu}, bhL^{\Delta/\nu}, ch_1 L^{\Delta_1/\nu}\right). \tag{1.1}$$

Here $\nu = 1$, $\Delta = \frac{5}{2}$, $\Delta_1 = \frac{1}{2}$ are the scaling exponents for $d = 3$, $\dot{t}$ is the shifted reduced critical temperature $\dot{t} = (T - T_c)/T_c + \varepsilon(L)$, where $\varepsilon(L)$ is the shift obeying $\lim_{L\to\infty} \varepsilon(L) = 0$ and a, b, c are some (non-universal) metric factors. Actually, the functional dependence given by this equation is expected to be fulfilled for any system undergoing an ordinary phase transition. The only independent new surface critical exponent in this case is $\Delta_1 = \Delta_1^{\mathrm{o}}$.

As is well known, the infinite translational invariant spherical model is equivalent to the $n \to \infty$ limit of such a n-component system [10, 11], but the spherical model with free surfaces (or, more generally, without translation-invariant symmetry) is in fact *not* such a limit [12]. The last becomes apparent if one investigates surface phase transitions for an $O(n)$ model in the limit $n \to \infty$. In that case one obtains [1] $\Delta_1 = 1/(d-2)$ (i.e. $\Delta_1 = 1$ for $d = 3$) for ordinary and $\Delta_1 = 2/(d-2)$ for special phase transitions. An attempt to clarify the situation with the special and extraordinary phase transitions within the spherical model has been made in [13, 14], where the spherical model with Dirichlet boundary conditions and an enhancement of the surface coupling $K_s = K(1+w)$ (K being the bulk coupling and $w > 0$) has been considered. It turns out that if, as usual, only one global mean spherical constraint is imposed, the model predicts quite unphysically the existence of an extraordinary phase transition [13] when $w > 1/(2d-2)$ for $d \geqslant 3$ (in [13] only integer dimensionalities were considered). But, if an additional constraint is involved to ensure the proper behaviour of the surface spins, one obtains [14], as is to be expected, that for any $w > 0$ there is no other critical temperature except the bulk one, provided $d \leqslant 3$. This is in agreement with the results for the $O(n)$ model in the limit $n \to \infty$, for which the crossover exponent $\Phi = (d-3)/(d-2)$. The critical exponent $\gamma_{1,1}$ for the local surface susceptibility

$$\chi_{1,1}(T) = \frac{1}{2} \lim_{L\to\infty} \left[-L\partial^2 f_L\left(T, h, h_1\right)/\partial h_1^2\right]\Big|_{h=h_1=0} \tag{1.2}$$

has been found to be $\gamma_{1,1}^{\mathrm{o}} = -1$ for the $d = 3$ spherical model. In the present paper we will show that the singular part of the free energy density of the spherical model with Neumann–Neumann boundary conditions for $d = 3$ can be represented in the form (1.1) with $\Delta_1 = \Delta_1^{\mathrm{sb}} = \frac{3}{2}$. According to the general theory of finite-size scaling, this is consistent with the expected form of the singular part of the free energy for a finite system undergoing special phase transition in the case where $\Phi = 0$ [8]. The corresponding scaling function X depends, of course, on the boundary conditions. Finally, in the case of Neumann–Dirichlet boundary conditions, with surface fields h_1 and h_2, respectively, it will be demonstrated that ($d = 3$)

$$f_L(T, h_1, h_L) = L^{-3} X\left(atL^{1/\nu}, c_1 h_1 L^{\Delta_1^{\mathrm{sb}}/\nu}, c_L h_L L^{\Delta_1^{\mathrm{o}}/\nu}\right). \tag{1.3}$$

The paper is organized as follows. In section 2 we describe the model and present convenient starting expressions for the mean spherical constraint and the free energy density. Our main results on the finite-size scaling behaviour of the free energy density in the critical region are given in section 3, for Neumann–Neumann boundary conditions, and in section 4, for Neumann–Dirichlet boundary conditions. The interseting case of a localized field acting on the lth layer in a system with Neumann–Dirichlet boundary conditions is considered in section 5. It is shown that a continuous family of layer critical exponents $\Delta_1(l)$ emerges then, depending on the power of L which scales the distance from the Dirichlet boundary. The paper closes with a short discussion given in section 6.

2. The model

We consider explicitly the three-dimensional mean spherical model with nearest-neighbour ferromagnetic interactions on a simple cubic lattice. At each lattice site $\boldsymbol{r} = (r_1, r_2, r_3) \in \mathbb{Z}^3$ there is a random (spin) variable $\sigma(\boldsymbol{r}) \in \mathbb{R}$ and the energy of a configuration $\sigma_\Lambda = \{\sigma(\boldsymbol{r}), \boldsymbol{r} \in \Lambda\}$ in a finite region $\Lambda \subset \mathbb{Z}^3$, containing $|\Lambda|$ sites, is given by

$$\beta\mathcal{H}_\Lambda^{(\tau)}(\sigma_\Lambda|K, h_\Lambda; s) = -K\sum_{\boldsymbol{r},\boldsymbol{r}'\in\Lambda} Q_\Lambda(\boldsymbol{r}-\boldsymbol{r}')\sigma(\boldsymbol{r})\sigma(\boldsymbol{r}') - K\sum_{\boldsymbol{r}\in\Lambda,\boldsymbol{r}'\in\Lambda^{\mathrm{c}}} Q_\Lambda(\boldsymbol{r}-\boldsymbol{r}')\sigma(\boldsymbol{r})\sigma(\boldsymbol{r}')$$
$$+s\sum_{\boldsymbol{r}\in\Lambda}\sigma^2(\boldsymbol{r}) - \sum_{\boldsymbol{r}\in\Lambda} h(\boldsymbol{r})\sigma(\boldsymbol{r}). \tag{2.1}$$

Here $\beta = 1/k_{\mathrm{B}}T$ is the inverse temperature, $K = \beta J$ is the dimensionless coupling constant, $h_\Lambda = \{h(\boldsymbol{r}), \boldsymbol{r} \in \Lambda\}$, with $h(\boldsymbol{r}) \in \mathbb{R}$, is an external magnetic field, s is the spherical field which is to be determined from the mean spherical constraint (see equation (2.21) below), $Q_\Lambda(\boldsymbol{r} - \boldsymbol{r}')$, with $\boldsymbol{r}, \boldsymbol{r}' \in \mathbb{Z}^3$, is the adjacency matrix for the infinite cubic lattice: $Q_\Lambda(\boldsymbol{r} - \boldsymbol{r}') = 1$ if and only if $|\boldsymbol{r} - \boldsymbol{r}'| = 1$ and $Q_\Lambda(\boldsymbol{r} - \boldsymbol{r}') = 0$ otherwise. The first sum on the left-hand side of (2.1) describes the pairwise interaction between the spins in Λ, while the second sum is the boundary term which depends on the boundary conditions (denoted by the superscript τ): it describes the interaction of the spins in the region Λ with a specified configuration $\{\sigma(\boldsymbol{r}), \boldsymbol{r} \in \Lambda^{\mathrm{c}}\}$ in the complement $\Lambda^{\mathrm{c}} = \mathbb{Z}^3 \setminus \Lambda$. In the remainder we take Λ to be the parallelepiped $\Lambda = \mathcal{L}_1 \times \mathcal{L}_2 \times \mathcal{L}_3$, with $\mathcal{L}_i = \{1, \ldots, L_i\}$, and explicitly study the case of film geometry which results in the limit $L_2, L_3 \to \infty$ at finite values of $L_1 = L$. In the finite r_1 direction it suffices to specify the values of $\sigma(0, r_2, r_3)$ and $\sigma(L + 1, r_2, r_3)$ for all $(r_2, r_3) \in \mathcal{L}_2 \times \mathcal{L}_3$. The finite-size scaling behaviour of the mean spherical model in the presence of surface fields has been studied so far [5, 9, 13, 14], under periodic, antiperiodic and the following boundary conditions.

(a) Dirichlet boundary conditions:

$$\sigma(0, r_2, r_3) = \sigma(L+1, r_2, r_3) = 0. \tag{2.2}$$

Here we consider the following new cases.
(b) Neumann boundary conditions:

$$\sigma(0, r_2, r_3) = \sigma(1, r_2, r_3) \qquad \sigma(L+1, r_2, r_3) = \sigma(L, r_2, r_3). \tag{2.3}$$

(c) Neumann–Dirichlet boundary conditions:

$$\sigma(0, r_2, r_3) = \sigma(1, r_2, r_3) \qquad \sigma(L+1, r_2, r_3) = 0. \tag{2.4}$$

Obviously, the above terminology is justified by analogy with the continuum limit. The case of free surfaces in a system of film geometry (in the limit $L_2, L_3 \to \infty$), considered in the literature [5, 9, 13, 14], corresponds to Dirichlet boundary conditions ($\tau_1 = a$). To define the fully finite system, we assume periodic boundary conditions (p) in the r_2 and r_3 directions, i.e. for all $\boldsymbol{r} \in \Lambda$ and all $m, n \in \mathbb{Z}$ we set

$$\sigma(r_1, r_2 + mL_2, r_3 + nL_3) = \sigma(r_1, r_2, r_3). \tag{2.5}$$

It might be instructive to consider the configuration space $\Omega_\Lambda = \mathbb{R}^{|\Lambda|}$ as a 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 $\{(r_1, r_2, r_3) \in \Lambda\}$. Let $\sigma_\Lambda^\dagger$ be the corresponding transposed row vector and let the dot $(\cdot)$ denote matrix multiplication. Then, for given boundary conditions $\tau = (\tau_1, \tau_2, \tau_3)$, specified for each pair of opposite faces of Λ by some $\tau_i = p$ (periodic), a (Dirichlet), b (Neumann) or c (Neumann–Dirichlet), the energy function (2.1) takes the form

$$\beta\mathcal{H}_\Lambda^{(\tau)}(\sigma_\Lambda | K, h_\Lambda; s) = -K\sigma_\Lambda^\dagger \cdot Q_\Lambda^{(\tau)} \cdot \sigma_\Lambda + s\,\sigma_\Lambda^\dagger \cdot \sigma_\Lambda - h_\Lambda^\dagger \cdot \sigma_\Lambda. \tag{2.6}$$

Here the $|\Lambda| \times |\Lambda|$ interaction matrix $Q_\Lambda^{(\tau)}$ can be written as

$$Q_\Lambda^{(\tau)} = (\Delta_1^{(\tau_1)} + 2\,E_1) \times (\Delta_2^{(\tau_2)} + 2\,E_2) \times (\Delta_3^{(\tau_3)} + 2\,E_3) \tag{2.7}$$

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 is given by

$$u_L^{(a)}(r, k) = [2/(L+1)]^{1/2} \sin\left[r\varphi_L^{(a)}(k)\right] \tag{2.8}$$

$$u_L^{(b)}(r, k) = \begin{cases} L^{-1/2} & \text{for } k = 1 \\ (2/L)^{1/2} \cos\left[(r - \frac{1}{2})\varphi_L^{(b)}(k)\right] & \text{for } k = 2, \ldots, L \end{cases} \tag{2.9}$$

$$u_L^{(c)}(r, k) = 2/(2L+1)^{1/2} \cos\left[(r - \tfrac{1}{2})\varphi_L^{(c)}(k)\right] \tag{2.10}$$

$$u_L^{(p)}(r, k) = L^{-1/2} \exp\left[-\mathrm{i}r\varphi_L^{(p)}(k)\right] \tag{2.11}$$

where

$$\varphi_L^{(a)}(k) = \frac{\pi k}{L+1} \qquad \varphi_L^{(b)}(k) = \frac{\pi(k-1)}{L}$$
$$\varphi_L^{(c)}(k) = \frac{\pi(2k-1)}{2L+1} \qquad \varphi_L^{(p)}(k) = \frac{2\pi k}{L}. \tag{2.12}$$

The corresponding eigenvalues are

$$\lambda_L^{(\tau)}(k) = -2 + 2\cos\varphi_L^{(\tau)}(k) \qquad k = 1, \ldots, L. \tag{2.13}$$

The eigenfunctions of the interaction matrix (2.7) have the form

$$u_\Lambda^{(\tau)}(\boldsymbol{r}, \boldsymbol{k}) = u_{L_1}^{(\tau_1)}(r_1, k_1)\, u_{L_2}^{(\tau_2)}(r_2, k_2)\, u_{L_3}^{(\tau_3)}(r_3, k_3) \qquad \boldsymbol{k} \in \Lambda \tag{2.14}$$

and the corresponding eigenvalues are

$$\mu_\Lambda^{(\tau)}(\boldsymbol{k}) = 2\sum_{\nu=1}^{3}\cos\varphi_{L_\nu}^{(\tau_\nu)}(k_\nu) \qquad \boldsymbol{k} \in \Lambda. \tag{2.15}$$

In order to ensure positivity of all the eigenvalues $-K\mu_\Lambda^{(\tau)}(\boldsymbol{k}) + s$, $\boldsymbol{k} \in \Lambda$, of the quadratic form in $\beta\mathcal{H}_\Lambda^{(\tau)}(\sigma_\Lambda|K, h_\Lambda; s)$ (see equations (2.1), (2.6)), the spherical field s must satisfy the inequality

$$s > K\max_{\boldsymbol{k}\in\Lambda}\mu_\Lambda^{(\tau)}(\boldsymbol{k}) := K\mu_\Lambda^{(\tau)}(\boldsymbol{k}_0). \tag{2.16}$$

In view of this condition, it is convenient to introduce a shifted and rescaled spherical field $\phi > 0$ by setting $s = s(\phi)$, where

$$s(\phi) := K\left[\phi + \mu_\Lambda^{(\tau)}(\boldsymbol{k}_0)\right]. \tag{2.17}$$

The joint probability distribution of the random variables $\sigma_\Lambda = \{\sigma(\boldsymbol{r}), \boldsymbol{r} \in \Lambda\}$ depends on the boundary conditions τ, the coupling parameter K, spherical field ϕ, and external field $h_\Lambda = \{h(\boldsymbol{r}), \boldsymbol{r} \in \Lambda\}$; it is given by the Gibbs measure

$$\mathrm{d}\mu_\Lambda^{(\tau)}(\sigma_\Lambda|K, h_\Lambda; \phi) = \exp\left[-\beta\mathcal{H}_\Lambda^{(\tau)}(\sigma_\Lambda|K, h_\Lambda; s(\phi))\right]\prod_{\boldsymbol{r}\in\Lambda}\mathrm{d}\sigma(\boldsymbol{r})/Z_\Lambda^{(\tau)}(K, h_\Lambda; \phi) \tag{2.18}$$

where $\mathrm{d}\sigma(\boldsymbol{r})$ is the Lebesgue measure on $\mathbb{R}$ and

$$Z_\Lambda^{(\tau)}(K, h_\Lambda; \phi) = \int_{\mathbb{R}^{|\Lambda|}}\exp\left[-\beta\mathcal{H}_\Lambda^{(\tau)}(\sigma_\Lambda|K, h_\Lambda; s(\phi))\right]\prod_{\boldsymbol{r}\in\Lambda}\mathrm{d}\sigma(\boldsymbol{r}) \tag{2.19}$$

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 shperical model in a finite region Λ is given by the Legendre transformation

$$\beta f_\Lambda^{(\tau)}(K, h_\Lambda) := \sup_\phi\left\{-|\Lambda|^{-1}\ln Z_\Lambda^{(\tau)}(K, h_\Lambda; \phi) - s(\phi)\right\}. \tag{2.20}$$

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

$$|\Lambda|^{-1}\sum_{\boldsymbol{r}\in\Lambda}\langle\sigma^2(\boldsymbol{r})\rangle_\Lambda^{(\tau)}(K, h_\Lambda; \phi) = 1 \tag{2.21}$$

where $\langle\cdots\rangle_\Lambda^{(\tau)}(K, h_\Lambda; \phi)$ denotes expectation value with respect to the measure (2.18).

By direct evaluation of the integrals in the partition function (2.19), one obtains

$$\beta f_\Lambda^{(\tau)}(K, h_\Lambda) = \tfrac{1}{2}\ln(K/\pi) - K\mu_\Lambda^{(\tau)}(\boldsymbol{k}_0) + \tfrac{1}{2}U_\Lambda^{(\tau)}(\phi_\Lambda^{(\tau)}) - \tfrac{1}{2}P_\Lambda^{(\tau)}(K, h_\Lambda; \phi_\Lambda^{(\tau)}) - K\phi_\Lambda^{(\tau)}. \tag{2.22}$$

Here we have introduced the function

$$U_\Lambda^{(\tau)}(\phi) = |\Lambda|^{-1}\sum_{\boldsymbol{k}\in\Lambda}\ln\left[\phi + \omega_\Lambda^{(\tau)}(\boldsymbol{k})\right] \tag{2.23}$$

which describes the contribution of the spin-spin interaction (to be called the 'interaction term'), where $\omega_\Lambda^{(\tau)}(\boldsymbol{k}) := \mu_\Lambda^{(\tau)}(\boldsymbol{k}_0) - \mu_\Lambda^{(\tau)}(\boldsymbol{k})$, and the function

$$P_\Lambda^{(\tau)}(K, h_\Lambda; \phi) = (2K|\Lambda|)^{-1} \sum_{\boldsymbol{k}\in\Lambda} \frac{|\hat{h}_\Lambda^{(\tau)}(\boldsymbol{k})|^2}{\phi + \omega_\Lambda^{(\tau)}(\boldsymbol{k})} \tag{2.24}$$

which represents the 'field term'. In equation (2.24) $\hat{h}_\Lambda^{(\tau)}(\boldsymbol{k})$ denotes the projection of the magnetic field configuration h_Λ on the eigenfunction $\bar{u}_\Lambda^{(\tau)}(\boldsymbol{r}, \boldsymbol{k})$:

$$\hat{h}_\Lambda^{(\tau)}(\boldsymbol{k}) = \sum_{\boldsymbol{r}\in\Lambda} h(\boldsymbol{r}) \bar{u}_\Lambda^{(\tau)}(\boldsymbol{r}, \boldsymbol{k}). \tag{2.25}$$

The mean spherical constraint (2.21) has the form

$$\frac{\mathrm{d}}{\mathrm{d}\phi} U_\Lambda^{(\tau)}(\phi) - \frac{\partial}{\partial\phi} P_\Lambda^{(\tau)}(K, h_\Lambda; \phi) = 2K. \tag{2.26}$$

Now we set $\tau_1 = \tau \in \{a, b, c\}$, $\tau_2 = \tau_3 = p$, note that for these boundary conditions $\boldsymbol{k}_0 = \{1, L_2, L_3\}$, and take the limit $L_2, L_3 \to \infty$ in expression (2.23) at fixed $L_1 = L$:

$$U_{L,3}^{(\tau)}(\phi) := \lim_{L_2, L_3\to\infty} U_\Lambda^{(\tau,p,p)}(\phi). \tag{2.27}$$

Next we confine ourselves to the consideration of magnetic fields that are uniform in the r_2 and r_3 directions, $h(\boldsymbol{r}) = h_{\mathrm{surf}}(r_1)$, $\boldsymbol{r} \in \Lambda$, and by taking the same limit in (2.24) we obtain

$$\begin{aligned} P_L^{(\tau)}(K, h_{\mathrm{surf}}; \phi) &:= \lim_{L_2, L_3\to\infty} P_\Lambda^{(\tau,p,p)}(K, h_\Lambda; \phi) \\ &= \frac{1}{2KL} \sum_{k=1}^{L} \frac{[\hat{h}_{\mathrm{surf}}^{(\tau)}(k)]^2}{\phi + 2\cos\varphi_L^{(\tau)}(1) - 2\cos\varphi_L^{(\tau)}(k)} \end{aligned} \tag{2.28}$$

where

$$\hat{h}_{\mathrm{surf}}^{(\tau)}(k) := \sum_{r=1}^{L} h_{\mathrm{surf}}(r) u_L^{(\tau)}(r, k) \qquad \tau \in \{a, b, c\}. \tag{2.29}$$

Thus, the mean spherical constraint (2.26) can be written in the form

$$W_{L,3}^{(\tau)}(\phi) - \frac{\partial}{\partial\phi} P_L^{(\tau)}(K, h_{\mathrm{surf}}; \phi) = 2K \tag{2.30}$$

where

$$W_{L,3}^{(\tau)}(\phi) := \frac{1}{L} \sum_{k=1}^{L} W_2\left[\phi + 2\cos\varphi_L^{(\tau)}(1) - 2\cos\varphi_L^{(\tau)}(k)\right] \tag{2.31}$$

and

$$W_2(z) = (2\pi)^{-2} \int_0^{2\pi} \mathrm{d}\theta_1 \int_0^{2\pi} \mathrm{d}\theta_2 \left[z + 2\sum_{\nu=1}^{2}(1 - \cos\theta_\nu)\right]^{-1}. \tag{2.32}$$

Note that having evaluated $W_{L,3}^{(\tau)}(\phi)$, the corresponding interaction term $U_{L,3}^{(\tau)}(\phi_L^{(\tau)})$ in the singular (in the limit $L \to \infty$) part of the free energy density (see equation (2.22))

$$\beta f_{L,\mathrm{sing}}^{(\tau)}(K, h_{\mathrm{surf}}) = \tfrac{1}{2} U_{L,3}^{(\tau)}(\phi_L^{(\tau)}) - \tfrac{1}{2} P_L^{(\tau)}(K, h_{\mathrm{surf}}; \phi_L^{(\tau)}) - K\phi_L^{(\tau)} \tag{2.33}$$

can be obtained by integration:

$$U_{L,3}^{(\tau)}(\phi_L^{(\tau)}) = U_{L,3}^{(\tau)}(\phi_0) + \int_{\phi_0}^{\phi_L^{(\tau)}} W_{L,3}^{(\tau)}(\phi). \tag{2.34}$$

Here $\phi_L^{(\tau)} = \phi_L^{(\tau)}(K, h_{\rm surf})$ is the solution of equation (2.30), and $\phi_0 \geqslant 0$ is a suitably chosen constant.

Equations (2.28)–(2.34) provide the starting expressions for our further finite-size scaling analysis.

3. Finite-size scaling for Neumann–Neumann boundary conditions

In this section we study the finite-size scaling behaviour of the mean spherical constraint and the free energy density in the case of Neumann–Neumann boundary conditions. We consider external fields h_1 and h_L which act at the surfaces bounding the system:

$$h_{\rm surf}(r_1) = h_1\delta_{r_1,1} + h_L\delta_{r_1,L}. \tag{3.1}$$

From equation (2.28), assuming L even, we find that the field term takes the form

$$\begin{aligned} P_L^{(b)}(K, h_1, h_L; \phi) = {} & \frac{(h_1+h_L)^2}{2KL^2}\left[\frac{1}{\phi} - \frac{L}{4} + \frac{1}{2} + \left(1+\frac{\phi}{4}\right)\sum_{k=1}^{L/2-1}\left(1+\frac{\phi}{2} - \cos\frac{2k\pi}{L}\right)^{-1}\right] \\ & + \frac{(h_1-h_L)^2}{2KL^2}\left[-\frac{L}{4} + \left(1+\frac{\phi}{4}\right)\sum_{k=1}^{L/2}\left(1+\frac{\phi}{2} - \cos\frac{(2k-1)\pi}{L}\right)^{-1}\right]. \end{aligned} \tag{3.2}$$

Since $\phi > 0$, we set $1 + \frac{1}{2}\phi = \cosh x$, and by making use of the identities [15]

$$\sum_{k=1}^{n-1} \ln\left(2\cosh x - 2\cos\frac{k\pi}{n}\right) = \ln(\sinh nx) - \ln(\sinh x) \tag{3.3}$$

and

$$\sum_{k=1}^{n} \ln\left(2\cosh x - 2\cos\frac{(2k-1)\pi}{2n}\right) = \ln(2\cosh nx) \tag{3.4}$$

we obtain the exact expression

$$\begin{aligned} P_L^{(b)}(K, h_1, h_L; \phi) = {} & \frac{(h_1+h_L)^2}{4KL}\left[\phi^{-1/2}(1+\phi/4)^{1/2}\coth(Lx/2) - 1/2\right] \\ & + \frac{(h_1-h_L)^2}{4KL}\left[\phi^{-1/2}(1+\phi/4)^{1/2}\tanh(Lx/2) - 1/2\right]. \end{aligned} \tag{3.5}$$

Hence, in the limit

$$\phi \to 0 \qquad L \to \infty \qquad \text{so that } \phi^{1/2}L = O(1) \tag{3.6}$$

by taking into account that $x = \phi^{1/2}[1 + {\rm O}(\phi)]$, we obtain the asymptotic form of the field term

$$\begin{aligned} P_L^{(b)}(K, h_1, h_L; \phi) \simeq {} & -\frac{1}{4KL}(h_1^2 + h_L^2) + \frac{1}{4KL\phi^{1/2}}\left[(h_1+h_L)^2\coth(\tfrac{1}{2}L\phi^{1/2})\right. \\ & \left. + (h_1-h_L)^2\tanh(\tfrac{1}{2}L\phi^{1/2})\right] \end{aligned} \tag{3.7}$$

which holds up to corrections of ${\rm O}(\phi) = {\rm O}(L^{-2})$.

Next we evaluate the interaction term in the mean spherical constraint by using an improved version of the method developed by Barber and Fisher [5]. Following [5] we set

$$W_2(z) := -(1/4\pi)\ln z + (5/4\pi)\ln 2 + Q_2(z) \tag{3.8}$$

where $Q_2(z)$, defined by the above equation, has the asymptotic behaviour as $z \to 0$

$$Q_2(z) = \mathrm{O}(z \ln z) \qquad Q_2'(z) := \mathrm{d}Q_2/\mathrm{d}z = \mathrm{O}(\ln z). \tag{3.9}$$

Then the interaction term in equation (2.30) takes the form

$$\begin{aligned} W_{L,3}^{(b)}(\phi) &:= \frac{1}{L}\sum_{k=1}^{L} W_2\left(\phi + 2 - 2\cos\phi_L^{(b)}(k)\right) \\ &= g_1^{(b)}(\phi) + g_2^{(b)}(\phi) + (5/4\pi)\ln 2 \end{aligned} \tag{3.10}$$

where

$$g_1^{(b)}(\phi) = -\frac{1}{4\pi L}\sum_{k=0}^{L-1}\ln\left(2\cosh x - 2\cos\frac{\pi k}{L}\right) \tag{3.11}$$

and

$$g_2^{(b)}(\phi) = \frac{1}{L}\sum_{k=0}^{L-1} Q_2\left(\phi + 4\sin^2\frac{\pi k}{2L}\right). \tag{3.12}$$

From equation (3.3) at $n = L$ we obtain

$$g_1^{(b)}(\phi) = -\frac{1}{4\pi L}\left[\ln\phi + \ln(\sinh Lx) - \ln(\sinh x)\right]. \tag{3.13}$$

In the limit (3.6) the above expression yields

$$g_1^{(b)}(\phi) = \frac{\ln L}{4\pi L} - \frac{1}{4\pi L}\ln\left[L\phi^{1/2}\sinh(L\phi^{1/2})\right] + \mathrm{O}(L^{-3}). \tag{3.14}$$

By using the Poisson summation formula for the sum in (3.12), $g_2^{(b)}(\phi)$ can be written as

$$\begin{aligned} g_2^{(b)}(\phi) = {}& \frac{1}{\pi}\int_0^{\pi} Q_2(\phi + 4\sin^2\theta)\mathrm{d}\theta + \frac{1}{2L}\left[Q_2(\phi) - Q_2(\phi+4)\right] \\ & + \frac{2}{\pi}\sum_{q=1}^{\infty}\int_0^{\pi} Q_2(\phi + 4\sin^2\theta)\cos(4Lq\theta)\mathrm{d}\theta. \end{aligned} \tag{3.15}$$

Integration by parts, with the aid of (3.9), yields the result that the last term in equation (3.15) is $\mathrm{O}(L^{-2})$. Thus

$$\begin{aligned} g_2^{(b)}(\phi) = {}& W_3(\phi) + (1/4\pi)\ln\left[1 + \tfrac{1}{2}\phi + \phi^{1/2}(1+\phi/4)^{1/2}\right] + \frac{1}{2L}\left[Q_2(\phi) - Q_2(\phi+4)\right] \\ & -(5/4\pi)\ln 2 + \mathrm{O}(L^{-2}) \end{aligned} \tag{3.16}$$

where

$$W_3(z) := \frac{1}{(2\pi)^3}\int_0^{2\pi}\int_0^{2\pi}\int_0^{2\pi}\frac{\mathrm{d}\theta_1\mathrm{d}\theta_2\mathrm{d}\theta_3}{z + 2\sum_{\nu=1}^{3}(1-\cos\theta_\nu)} \tag{3.17}$$

is the three-dimensional Watson integral.

When $\phi \to 0$, in view of (3.9) and the asymptotic expansion of $W_3(\phi)$ (see [5]), expression (3.16) simplifies to

$$g_2^{(b)}(\phi) = 2K_\mathrm{c} - (5/4\pi)\ln 2 - \frac{1}{2L}\left[W_2(4) - (3/4\pi)\ln 2 + \mathrm{O}(\phi\ln\phi)\right] + \mathrm{O}(\phi) + \mathrm{O}(L^{-2}) \tag{3.18}$$

where $K_\mathrm{c} = \frac{1}{2}W_3(0)$ is the bulk critical coupling.

Therefore, from equations (3.10), (3.14) and (3.18), in the limit (3.6) we obtain the following asymptotic form of the interaction term:

$$W_{L,3}^{(b)}(\phi) = 2K_{\mathrm{c}} + \frac{\ln L}{4\pi L} - \frac{1}{L}\left[\frac{1}{4\pi}\ln\left[L\phi^{1/2}\sinh(L\phi^{1/2})\right] - \frac{3\ln 2}{8\pi} + \frac{1}{2}W_2(4)\right] + \mathrm{O}(L^{-2}). \tag{3.19}$$

Hence, by taking the derivative of (3.7) with respect to ϕ and ignoring the $\mathrm{O}(L^{-2})$ corrections, the mean spherical constraint (2.30) gives the finite-size scaling form

$$\frac{1}{4\pi}\ln(y\sinh y) - \frac{(\eta_1+\eta_L)^2}{16y^2}\left[\frac{2}{y}\coth\frac{1}{2}y + \frac{1}{\sinh^2\frac{1}{2}y}\right] - \frac{(\eta_1-\eta_L)^2}{16y^2}\left[\frac{2}{y}\tanh\frac{1}{2}y - \frac{1}{\cosh^2\frac{1}{2}y}\right] = 2\tau. \tag{3.20}$$

Here we have introduced the scaled spherical field

$$y = \phi^{1/2}L = O(1) \tag{3.21}$$

and scaled variables

$$\tau = (K_{\mathrm{c},L}^{(b)} - K)L \qquad \eta_1 = K^{-1/2}h_1L^{3/2} \qquad \eta_L = K^{-1/2}h_LL^{3/2}. \tag{3.22}$$

where $K_{\mathrm{c},L}^{(b)}$ is the shifted critical coupling

$$K_{\mathrm{c},L}^{(b)} = K_{\mathrm{c}} + \frac{1}{8\pi L}\left[\ln L + \tfrac{3}{2}\ln 2 - 2\pi W_2(4)\right]. \tag{3.23}$$

The free energy density for Neumann–Neumann boundary conditions can be found from equations (2.22), (3.7), and (3.19):

$$\beta f_L^{(b)}(K,h_1,h_L) = \tfrac{1}{2}\ln(K/\pi) - 6K + \tfrac{1}{2}U_L^{(b)}(0) + \frac{1}{8KL}(h_1^2+h_L^2)$$
$$-L^{-3}\left\{\frac{1}{4\pi}\int_0^{y_L^{(b)}} x\ln(\sinh x)\mathrm{d}x + \frac{1}{8\pi}(y_L^{(b)})^2(\ln y_L^{(b)} - \tfrac{1}{2})\right.$$
$$\left. + \frac{1}{8y_L^{(b)}}\left[(\eta_1+\eta_L)^2\coth\tfrac{1}{2}y_L^{(b)} + (\eta_1-\eta_L)^2\tanh\tfrac{1}{2}y_L^{(b)}\right] - (y_L^{(b)})^2\tau\right\}$$
$$+\mathrm{O}(L^{-4}). \tag{3.24}$$

Here $y_L^{(b)} = y_L^{(b)}(\tau,\eta_1,\eta_L)$ is the solution of the mean spherical constraint (3.20) in the neighbourhood of the critical point defined by

$$\tau = O(1) \qquad \eta_1 = O(1) \qquad \eta_L = O(1). \tag{3.25}$$

Thus, for a three-dimensional L-layer spherical model equation (3.24) predicts that the finite-size scaling form of the singular (in the thermodynamic limit) part of the free energy density under Neumann–Neumann boundary conditions is

$$f_{L,\,\mathrm{sing}}^{(b)}(K,h_1,h_L) = L^{-3}X\left(a\dot{t}L^{1/\nu}, bh_1L^{\Delta_1^{\mathrm{sb}}/\nu}, bh_LL^{\Delta_1^{\mathrm{sb}}/\nu}\right) \tag{3.26}$$

where $\dot{t} := (K_{\mathrm{c},L}^{(b)} - K)$ is the shifted coupling, $\nu = 1$ and $\Delta_1^{\mathrm{sb}} = \frac{3}{2}$ are the scaling exponents at $d = 3$, and the metric factor is $b = K^{-1/2}$.

4. Finite-size scaling for Neumann–Dirichlet boundary conditions

In this case the corresponding field term (2.28) in the free energy density can be written in the form

$$P_L^{(c)}(K, h_1, h_L; \phi) = \frac{1}{2KL(2L+1)} \left\{ h_1^2 \left[C_L(\phi, 0) + C_L(\phi, 1) \right] \right.$$
$$\left. + 2h_1 h_L \left[C_L(\phi, L-1) - C_L(\phi, L+1) \right] + h_L^2 \left[C_L(\phi, 0) - C_L(\phi, 2) \right] \right\} \quad (4.1)$$

where

$$C_L(\phi, q) = \sum_{k=1}^{L} \frac{\cos q\varphi_L^{(c)}(k)}{\frac{1}{2}\phi + \cos\varphi_L^{(c)}(1) - \cos\varphi_L^{(c)}(k)}. \quad (4.2)$$

The summation on the right-hand side of (4.2) can be performed exactly by using the techniques suggested by Patrick [16]. The resulting analytic expression depends on the fact whether $\frac{1}{2}\phi + \cos\varphi_L^{(c)}(1)$ is greater than, or less than 1.

Case 1. When $\frac{1}{2}\phi + \cos\varphi_L^{(c)}(1) > 1$ we set

$$\tfrac{1}{2}\phi + \cos\varphi_L^{(c)}(1) = \cosh x \quad (4.3)$$

and for any integer $q \in \{0, \ldots, 2L\}$ obtain

$$C_L(\phi, q) = (L + \tfrac{1}{2}) \frac{\sinh(L - q + \frac{1}{2})x}{\sinh x \cosh(L + \frac{1}{2})x} - \frac{(-1)^q}{2(1 + \cosh x)}. \quad (4.4)$$

In this case the field term (4.1) becomes

$$P_L^{(c)}(K, h_1, h_L; \phi) = \frac{1}{2KL\cosh(L + \frac{1}{2})x} \left[h_1^2 \sinh Lx \cosh\tfrac{1}{2}x / \sinh x + 2h_1 h_L \cosh\tfrac{1}{2}x \right.$$
$$\left. + h_L^2 \cosh(L - \tfrac{1}{2})x \right]. \quad (4.5)$$

In the limit

$$\phi \to 0 \qquad L \to \infty \qquad \text{so that } \; y := \phi^{1/2} L = O(1) \quad (4.6)$$

equation (4.3) yields the result that for any fixed $y > \pi/2$

$$x = (y^2 - \pi^2/4)^{1/2} L^{-1} + \mathrm{O}(L^{-2}). \quad (4.7)$$

Therefore, the asymptotic behaviour of (4.5) is

$$P_L^{(c)}(K, h_1, h_L; \phi) = \frac{h_L^2}{2KL} + \frac{1}{2KL^3} [h_1^2 L^3 Y_1(y) + 2h_1 h_L L^2 Y_2(y) + h_L^2 L Y_3(y)]$$
$$\times \left[1 + \mathrm{O}(L^{-1}) \right] \quad (4.8)$$

where

$$Y_1(y) = \frac{\tanh(y^2 - \pi^2/4)^{1/2}}{(y^2 - \pi^2/4)^{1/2}}$$
$$Y_2(y) = \frac{1}{\cosh(y^2 - \pi^2/4)^{1/2}} \quad (4.9)$$
$$Y_3(y) = -(y^2 - \pi^2/4)^{1/2} \tanh(y^2 - \pi^2/4)^{1/2}.$$

The interaction term in the mean spherical constraint can be derived along the same lines as in section 3, by using, instead of the identity (3.4), the identity [15]

$$\prod_{k=0}^{L-1} 2\left(\cosh x - \cos\frac{\pi(2k+1)}{2L+1}\right) = \frac{\cosh(L+\frac{1}{2})x}{\cosh\frac{1}{2}x}. \tag{4.10}$$

We obtain

$$W_{L,3}^{(c)}(\phi) = 2K_{c,L}^{(c)} - \frac{1}{4\pi L}\ln\left[\cosh(y^2-\pi^2/4)^{1/2}\right] + \mathrm{O}(L^{-2}) \tag{4.11}$$

where

$$K_{c,L}^{(c)} = K_c + \frac{1}{2L}\left[K_c - \frac{1}{2}W_2(4) - \frac{\ln 2}{4\pi}\right] \tag{4.12}$$

is the shifted critical coupling.

Finally, by combining (4.11), and the derivative of (4.8) with respect to ϕ, after ignoring the $\mathrm{O}(L^{-2})$ corrections, the mean spherical constraint (2.30) takes the finite-size scaling form

$$\frac{1}{4\pi}\ln\left[\cosh(y^2-\pi^2/4)^{1/2}\right] + \frac{1}{4y}\left[\eta_1^2 Y_1'(y) + 2\eta_1\eta_L Y_2'(y) + \eta_L^2 Y_3'(y)\right] = 2\tau \tag{4.13}$$

where $Y_i'(y) = \mathrm{d}Y_i(y)/\mathrm{d}y$, $i = 1, 2, 3$, and the scaled variables are given by

$$\tau = (K_{c,L}^{(c)} - K)L \qquad \eta_1 = K^{-1/2}h_1 L^{3/2} \qquad \eta_L = K^{-1/2}h_L L^{1/2}. \tag{4.14}$$

The free energy density for Neumann–Dirichlet boundary conditions in the limit (4.6) can be found from (2.22), (4.8) and (4.11). By choosing the integration constant $\phi_0 = 2 - 2\cos\varphi_L^{(c)}(1)$, and setting $y_0 := \phi_0^{1/2}L = \pi/2 + \mathrm{O}(L^{-1})$, we obtain

$$\begin{aligned}\beta f_L^{(c)}(K, h_1, h_2) = {} & \frac{1}{2}\ln(K/\pi) - \left[4 + 2\cos\varphi_L^{(c)}(1)\right]K + \frac{1}{2}U_L^{(c)}(\phi_0) - \frac{h_L^2}{4KL} - \frac{1}{L^2}K_{c,L}^{(c)}y_0^2 \\ & -L^{-3}\left\{\frac{1}{4\pi}\int_{\pi/2}^{y_L^{(c)}} x\ln\left[\cosh(x^2-\pi^2/4)^{1/2}\right]\mathrm{d}x - (y_L^{(c)})^2\tau \right.\\ & \left. +\frac{1}{4}\left[\eta_1^2 Y_1(y_L^{(c)}) + 2\eta_1\eta_L Y_2(y_L^{(c)}) + \eta_L^2 Y_3(y_L^{(c)})\right]\right\} + \mathrm{O}(L^{-4}).\end{aligned} \tag{4.15}$$

Here $y_L^{(c)} = y_L^{(c)}(\tau, \eta_1, \eta_L)$ is the solution of the mean spherical constraint (4.13) in the neighbourhood of the critical point defined by

$$\tau = O(1) \qquad \eta_1 = O(1) \qquad \eta_L = O(1). \tag{4.16}$$

Case 2. When $\frac{1}{2}\phi + \cos\varphi_L^{(c)}(1) < 1$ we set

$$\tfrac{1}{2}\phi + \cos\varphi_L^{(c)}(1) = \cos x \tag{4.17}$$

and for any integer $q \in \{0, \ldots, 2L\}$ obtain

$$C_L(\phi, q) = (L+\tfrac{1}{2})\frac{\sin(L-q+\frac{1}{2})x}{\sin x\cos(L+\frac{1}{2})x} - \frac{(-1)^q}{2(1+\cos x)}. \tag{4.18}$$

In this case the field term (4.1) in the free energy density is given by equation (4.5) with the hyperbolic functions replaced by the corresponding trigonometric ones. Now in the limit (4.6) equation (4.17) yields the result that for any fixed $0 \leqslant y < \pi/2$

$$x = (\pi^2/4 - y^2)^{1/2}L^{-1} + \mathrm{O}(L^{-2}). \tag{4.19}$$

Therefore, the asymptotic behaviour of the field term (4.1) is given by equation (4.8) where the functions $Y_i(y), i = 1, 2, 3$ should be replaced by their analytical continuation to the domain $0 \leqslant y^2 \leqslant \pi^2/4$.

The interaction term in the mean spherical constraint can be obtained along the same lines as in case 1. Thus, by using the identity [15]

$$\prod_{k=0}^{L-1} 2\left(\cos x - \cos\frac{\pi(2k+1)}{2L+1}\right) = \frac{\cos(L+\frac{1}{2})x}{\cos\frac{1}{2}x} \tag{4.20}$$

we obtain the result that in the limit (4.6) the interaction term takes the asymptotic form

$$W_{L,3}^{(c)}(\phi) = 2K_{c,L}^{(c)} - \frac{1}{4\pi L}\ln\left[\cos(\pi^2/4 - y^2)^{1/2}\right] + O(L^{-2}). \tag{4.21}$$

Hence, ignoring the $O(L^{-2})$ corrections, the mean spherical constraint (2.30) takes the finite-size scaling form (see equation (4.13))

$$\frac{1}{4\pi}\ln\left[\cos(\pi^2/4 - y^2)^{1/2}\right] + \frac{1}{4y}\left[\eta_1^2 Y_1'(y) + 2\eta_1\eta_L Y_2'(y) + \eta_L^2 Y_3'(y)\right] = 2\tau \tag{4.22}$$

from which it follows (see equation (2.34)) that

$$\begin{aligned}\beta f_L^{(c)}(K, h_1, h_L) = {} & \frac{1}{2}\ln(K/\pi) - \left[4 + 2\cos\varphi_L^{(c)}(1)\right]K + \frac{1}{2}U_L^{(c)}(\phi_0) - \frac{h_L^2}{4KL} - \frac{1}{L^2}K_{c,L}^{(c)}y_0^2 \\ & -L^{-3}\left\{-\frac{1}{4\pi}\int_{y_L^{(c)}}^{\pi/2} x\ln\left[\cos(\pi^2/4 - x^2)^{1/2}\right]dx - (y_L^{(c)})^2\tau\right. \\ & \left. +\frac{1}{4}\left[\eta_1^2 Y_1(y_L^{(c)}) + 2\eta_1\eta_L Y_2(y_L^{(c)}) + \eta_L^2 Y_3(y_L^{(c)})\right]\right\} + O(L^{-4}). \end{aligned} \tag{4.23}$$

Here $y_L^{(c)} = y_L^{(c)}(\tau, \eta_1, \eta_L)$ is the solution of the mean spherical constraint (4.22) in the neighbourhood of the critical point defined by (4.16). Obviously, equation (4.23) is an analytical continuation of equation (4.15) from the domain $y_L^{(c)} > \pi/2$ to the domain $0 \leqslant y_L^{(c)} < \pi/2$.

Thus, for the three-dimensional L-layer mean spherical model equations (4.15) and (4.23) predict that the finite-size scaling form of the singular part of the free energy density under the Neumann–Dirichlet boundary conditions is

$$f_{L,\,\text{sing}}^{(c)}(K, h_1, h_L) \simeq L^{-3}X\left(a\dot{t}L^{1/\nu}, bh_1L^{\Delta_1^{sb}/\nu}, bh_LL^{\Delta_1^{o}/\nu}\right). \tag{4.24}$$

Here $\dot{t} := (K_{c,L}^{(c)} - K)$ is the shifted coupling, $\nu = 1$, $\Delta_1^{sb} = \frac{3}{2}$, and $\Delta_1^{o} = \frac{1}{2}$ are the scaling exponents at $d = 3$, and the metric factor is $b = K^{-1/2}$.

5. Layer field exponents under Neumann–Dirichlet boundary conditions

In the light of the results of section 4, one may naturally guess that the layer critical exponent $\Delta_1(l)$ for a magnetic field acting only on the lth layer, $1 \leqslant l \leqslant L$, should interpolate between the two extreme values: $\Delta_1^{sb} = \frac{3}{2}$ at the Neumann boundary ($l = 1$) and $\Delta_1^{o} = \frac{1}{2}$ at the Dirichlet boundary ($l = L$). In this section we prove that this is indeed the case, provided one takes into account the following important fact: we establish that the effective exponent $\Delta_1(l)$ depends not on l itself, but on the exponent which scales l with the finite size L.

Consider a field of strength h_l which acts on the lth layer, i.e. set

$$h_{\text{surf}} = h_l\delta_{l,r}. \tag{5.1}$$

Hence, the field term (2.28) takes the form

$$P_L^{(c)}(K, h_l; \phi) = \frac{h_l^2}{2KL(2L+1)} \left[C_L(\phi, 0) + C_L(\phi, 2l-1)\right] \tag{5.2}$$

where $C_L(\phi, q)$ has been defined in equation (4.2).

As in the previous section, we consider separately the two cases depending on whether the value of $\frac{1}{2}\phi + \cos\varphi_L^{(c)}(1)$ is greater than or less than 1.

Case 1. When $\frac{1}{2}\phi + \cos\varphi_L^{(c)}(1) > 1$, we use the substitution (4.3) and with the aid of (4.4) obtain the following exact expression for the field term:

$$P_L^{(c)}(K, h_l; \phi) = \frac{h_l^2}{2KL} \frac{\sinh(L-l+1)x \cosh(l-\frac{1}{2})x}{\sinh x \cosh(L+\frac{1}{2})x}. \tag{5.3}$$

Assume now that the distance l from the Neumann boundary scales with L as

$$l = \rho L^{\alpha} \qquad 0 \leqslant \alpha \leqslant 1. \tag{5.4}$$

If $\alpha = 1$ and $0 \leqslant \rho < 1$, with the aid of equation (4.7) we obtain in the limt (4.6) that the leading-order asymptotic behaviour of (5.3) is

$$P_L^{(c)}(K, h_l; \phi) \simeq \frac{h_l^2}{2K} \frac{\sinh\left[(1-\rho)(y^2-\pi^2/4)^{1/2}\right] \cosh\left[\rho(y^2-\pi^2/4)^{1/2}\right]}{(y^2-\pi^2/4)^{1/2} \cosh(y^2-\pi^2/4)^{1/2}}. \tag{5.5}$$

This implies that on the macroscopic scale $l = \rho L$, with $0 \leqslant \rho < 1$, the finite-size scaled field variable is

$$\eta_l = K^{-1/2} h_l L^{3/2} \tag{5.6}$$

i.e. $\Delta_1(l) = \frac{3}{2}$. From expression (5.3) it is evident that the case where $0 \leqslant \alpha < 1$ in (5.4) is equivalent to setting $\rho = 0$ in (5.5).

The situation may change qualitatively only when l is asymptotically close to the Dirichlet boundary ($l = L$). Indeed, let us assume

$$l = L - \rho L^{\alpha} \qquad 0 \leqslant \alpha < 1. \tag{5.7}$$

Then, in the limit (4.6) one obtains for $0 < \alpha < 1$

$$P_L^{(c)}(K, h_l; \phi) = \frac{h_l^2}{2K}\left[\rho L^{-(1-\alpha)} + L^{-1}\right] - \frac{h_l^2}{2K} L^{-2(1-\alpha)} \rho^2 (y^2-\pi^2/4)^{1/2} \tanh(y^2-\pi^2/4)^{1/2}$$
$$+ h_l^2 \mathrm{O}(L^{-2+\alpha}). \tag{5.8}$$

Since the first term on the right-hand side of the above equation is independent of y and must be attributed to the regular part of the free energy density, we conclude that the proper finite-size scaled field variable in this case is

$$\eta_l = K^{-1/2} h_l L^{1/2+\alpha} \tag{5.9}$$

i.e. there exists a continuous family of layer exponents $\Delta_1(l) = \frac{1}{2} + \alpha$ depending on the parameter α in (5.7). In particular, the layer critical exponent is the same for any fixed distance from the boundary.

For the sake of completeness, we give below the explicit finite-size scaling forms of the mean spherical constraint and the free energy density in this non-trivial case.

Since the interaction term is the same as in section 4, by combining (4.11) and the derivative of (5.8) with respect to ϕ, one obtains to leading order the finite-size scaling form of the mean spherical constraint:

$$\frac{1}{4\pi}\ln\left[\cosh(y^2-\pi^2/4)^{1/2}\right]-\frac{\rho^2}{4}\eta_l{}^2\left[Y_1(y)+Y_2^2(y)\right]=2\tau. \tag{5.10}$$

Similarly, for the singular part of the free energy density we obtain

$$\beta f^{(c)}_{L,\,\mathrm{sing}}(K,h_l)=-L^{-3}\left\{\frac{1}{4\pi}\int_{\pi/2}^{y_L^{(c)}}x\ln\left[\cosh(x^2-\pi^2/4)^{1/2}\right]\mathrm{d}x-(y_L^{(c)})^2\tau+\frac{\rho^2}{4}\eta_l{}^2Y_3(y)\right\}$$
$$+\,\mathrm{O}(L^{-3-\alpha}). \tag{5.11}$$

Here the $Y_i(y)$, $i=1,2,3$, are defined in (4.9), and τ is defined in (4.14), $y_L^{(c)}=y_L^{(c)}(\tau,\eta_l)$ is the solution of the mean spherical constraint (5.10) in the neighbourhood of the critical point defined by

$$\tau=O(1)\qquad \eta_l=O(1). \tag{5.12}$$

Case 2. When $\frac{1}{2}\phi+\cos\varphi_L^{(c)}(1)<1$, we use the substitution (4.17) and with the aid of (4.18) obtain

$$P_L^{(c)}(K,h_l;\phi)=\frac{h_l^2}{2KL}\frac{\sin(L-l+1)x\cos(l-\frac{1}{2})x}{\sin x\cos(L+\frac{1}{2})x}. \tag{5.13}$$

Under the assumption (5.4), with $\alpha=1$ and $0\leqslant\rho<1$, we obtain in the limt (4.6) that the leading-order asymptotic behaviour of the field term (5.13) is

$$P_L^{(c)}(K,h_l;\phi)\simeq\frac{h_l^2}{2K}\frac{\sin\left[(1-\rho)(\pi^2/4-y^2)^{1/2}\right]\cos\left[\rho(\pi^2/4-y^2)^{1/2}\right]}{(\pi^2/4-y^2)^{1/2}\cos(\pi^2/4-y^2)^{1/2}}. \tag{5.14}$$

This implies, as in case 1, that $\Delta_1(l)=\frac{3}{2}$.

Under the assumption (5.7) with $0<\alpha<1$, we find that in the limit (4.6)

$$P_L^{(c)}(K,h_l;\phi)=\frac{h_l^2}{2K}\left[\rho L^{-(1-\alpha)}+L^{-1}\right]+\frac{h_l^2}{2K}L^{-2(1-\alpha)}\rho^2(\pi^2/4-y^2)^{1/2}\tan(\pi^2/4-y^2)^{1/2}$$
$$+\,h_l^2\mathrm{O}(L^{-2+\alpha}). \tag{5.15}$$

Hence one easily derives the finite-size scaling forms of the mean spherical constraint

$$\frac{1}{4\pi}\ln\left[\cos(\pi^2/4-y^2)^{1/2}\right]-\frac{\rho^2}{4}\eta_l{}^2\left[Y_1(y)+Y_2^2(y)\right]=2\tau \tag{5.16}$$

and the singular part of the free energy density

$$\beta f^{(c)}_{L,\,\mathrm{sing}}(K,h_l)=-L^{-3}\left\{-\frac{1}{4\pi}\int_{y_L^{(c)}}^{\pi/2}x\ln\left[\cos(\pi^2/4-x^2)^{1/2}\right]\mathrm{d}x-(y_L^{(c)})^2\tau+\frac{\rho^2}{4}\eta_l{}^2Y_3(y)\right\}$$
$$+\,\mathrm{O}(L^{-3-\alpha}). \tag{5.17}$$

Here $y_L^{(c)}=y_L^{(c)}(\tau,\eta_l)$ is the solution of the mean spherical constraint (5.16) in the neighbourhood of the critical point defined by (5.12).

Thus, for the three-dimensional L-layer mean spherical model equations (5.11) and (5.17) predict that the finite-size scaling form of the singular part of the free energy density under assumption (5.7) is

$$f^{(c)}_{L,sing}(K,h_l)\simeq L^{-3}X\left(atL^{1/\nu},bh_lL^{\Delta_1(l)/\nu}\right). \tag{5.18}$$

Here $\nu = 1$ is the bulk correlation length exponent, and $\Delta_1(l) = \frac{1}{2} + \alpha$ is a family of layer critical exponents depending on the parameter α in (5.7).

6. Discussion

In the present paper the finite-size scaling behaviour of a three-dimensional system with a $L \times \infty^2$ film geometry has been investigated within the spherical model with Neumann–Neumann and Neumann–Dirichlet boundary conditions and surface fields h_1 and h_L acting at the boundaries. The corresponding main explicit results, given by equations (3.24), (4.15), and (4.23), respectively, verify the Privman–Fisher finite-size scaling hypothesis for the singular part of the free energy. These results imply the known exponent $\Delta_1^{\rm o} = \frac{1}{2}$ for the ordinary surface phase transition at a Dirichlet boundary, and the emergence of a new critical exponent $\Delta_1^{\rm sb} = \frac{3}{2}$, characterizing the Neumann boundary. We conjecture that the latter critical exponent corresponds to the special (surface–bulk) phase transition within the model. The last is consistent with the general expectation for the finite-size scaling form of the free energy for this type of phase transition if one also accepts that the crossover exponent $\Phi = 0$, as it is for the three-dimensional $O(n)$ models [1].

When the external magnetic field is applied at the lth layer under Neumann–Dirichlet boundary conditions, a family of l-dependent critical exponent $\Delta_1(l)$ appears. These exponents change continuously from $\Delta_1^{\rm sb} = \frac{3}{2}$ (at the Neumann surface) to $\Delta_1^{\rm o} = \frac{1}{2}$ (at the Dirichlet surface), see section 5. It is interesting to note that $\Delta_1(l)$ depends actually on the exponent which scales l with respect to L. For any layer at a finite distance apart from the nearest boundary $\Delta_1(l)$ is the same as for that boundary. This is in full conformity with the situation observed in [9] for the case of Dirichlet–Dirichlet boundary conditions. Only when $l = L - \rho L^\alpha$, with $0 < \alpha < 1$, the exponent $\Delta_1(l)$ depends continuously on α. Note that this result implies the existence of a family of critical exponents in the limit $L \to \infty$.

It should be emphasized that the spherical model under non-periodic 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. For example $\Delta_1^{\rm o} = 1$ and $\Delta_1^{\rm sb} = 2$ for the $O(\infty)$ model, but $\Delta_1^{\rm o} = \frac{1}{2}$ and $\Delta_1^{\rm sb} = \frac{3}{2}$ for the spherical model.

From equations (1.2) and (3.24) and it immediately follows that the critical exponent $\gamma_{1,1}^{\rm sb}$ for the local surface susceptibility $\chi_{1,1}$ is $\gamma_{1,1}^{\rm sb} = 1$. The same result was obtained for the spherical model with enhanced surface couplings under Dirichlet–Dirichlet boundary conditions [13]. Unfortunately, in that case the model quite unphysically predicts that the surface orders for sufficiently large enhancements even for $d = 3$ at some temperature above the bulk critical temperature. If one improves the model by introducing a second spherical constraint for the spins at the boundaries only [14] this is no longer the case, i.e. the only critical point for $d \leqslant 3$ remains the bulk one. Then for $d = 3$ the exponent $\gamma_{1,1}^{\rm o} = -1$, which is the corresponding critical exponent for the ordinary phase transition [1, 9]. In our considerations the bulk and surface couplings are equal, but the question if and how the behaviour will change when additional spherical constraints on the spins at the surfaces are introduced still remains open. We hope to return to this problem in a subsequent publication.

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