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Finite-size effects in the spherical model of finite thickness

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Abstract

A detailed analysis of the finite-size effects on the bulk critical behaviour of the d-dimensional mean spherical model confined to a film geometry with finite thickness L is reported. Along the finite direction different kinds of boundary conditions are applied: periodic (p), antiperiodic (a) and free surfaces with Dirichlet (D), Neumann (N) and a combination of Neumann and Dirichlet (ND) on both surfaces. A systematic method for the evaluation of the finite-size corrections to the free energy for the different types of boundary conditions is proposed. The free energy density and the equation for the spherical field are computed for arbitrary d. It is found, for $2 < d < 4$, that the singular part of the free energy has the required finite-size scaling form at the bulk critical temperature only for (p) and (a). For the remaining boundary conditions the standard finite-size scaling hypothesis is not valid. At $d = 3$, the critical amplitude of the singular part of the free energy (related to the so-called Casimir amplitude) is estimated. We obtain $\Delta^{(p)} = -2\zeta(3)/(5\pi) = -0.153\,051\ldots$, $\Delta^{(a)} = 0.274\,543\ldots$ and $\Delta^{(ND)} = 0.019\,22\ldots$, implying a fluctuation-induced attraction between the surfaces for (p) and repulsion in the other two cases. For (D) and (N) we find a logarithmic dependence on L.

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1. Introduction

Over the last 30 years there has been an increasing interest in the critical behaviour of systems (fluids, magnets . . .) confined between two infinite parallel plates i.e. films. Such systems can be regarded as d-dimensional generalization of two $(d-1)$-dimensional walls separated

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by matter of thickness L. The so-called thermodynamic Casimir effect related to fluctuation-induced long-ranged forces between the plates was, and still is, the central theme of these investigations both experimentally and theoretically[2]. This effect was first predicted by Fisher and de Gennes (1978) in their investigation on a confined critical binary liquid at its bulk demixing point. They showed that the reduced free-energy per unit area contains a term of the form $\Delta^{(\tau)}L^{-d+1}$, where $\Delta^{(\tau)}$ is the so-called Casimir amplitude by analogy with the Casimir effect in vacuum fluctuations of the electromagnetic field between two metallic plates (Casimir 1948). It is a universal quantity that depends on the bulk universality class and the boundary conditions (τ) imposed on the confining walls (Privman and Fisher 1984, Singh and Pathria 1985a). The different types of boundary conditions are in turn related to distinct universality classes of surface critical behaviour depending on the behaviour of the order parameter at the surfaces bounding the system and some additional surface properties (Diehl 1997).

In general, according to Privman and Fisher (1984), Singh and Pathria (1985a) the singular part of the free energy density of a finite (in one or more directions) d-dimensional system with linear size L, near the bulk critical point T_c, may be expressed in the form

$$f_{s,d}^{(\tau)}(t,h;L) \approx L^{-d}Y^{(\tau)}(c_1tL^{1/\nu}, c_2hL^{\Delta/\nu}), \tag{1.1}$$

where t and h are related to the temperature, T, and the external magnetic field, H, via

$$t = \frac{T-T_c}{T_c}, \qquad h = \frac{H}{k_BT}. \tag{1.2}$$

The arguments of $Y^{(\tau)}(x_1,x_2)$ are appropriate scaled variables, ν and Δ are the usual critical exponents, while all the details of the system are incorporated in the non-universal quantities c_1 and c_2. Then the function $Y^{(\tau)}(x_1,x_2)$ is a universal scaling function, whose exact expression depends upon the number of finite directions, the bulk universality class and the boundary conditions (τ) to which the system is subjected. For a system confined to a film geometry, at $T = T_c$, the Casimir amplitude coincides with the critical amplitude of the singular part of the free energy density, i.e.

$$\Delta^{(\tau)} = Y^{(\tau)}(0,0). \tag{1.3}$$

The spherical model of Berlin and Kac (1952) was initially designed to mimic the critical properties of the Ising model. It has been obtained by requiring the spins to be continuous variables subject to a global constraint (the sum of the squares of spins at each lattice site is equal to the total number of sites N) rather than a local one (the square of the spin at each site is exactly 1). Later it was shown that the free energy of this model can be obtained as a limiting case of that of the Heisenberg model with infinite number of spin components (Stanley 1968). The equivalence between the Heisenberg model with infinite spin components and the spherical model remains valid for finite systems, as long as one considers boundary conditions that preserve the translational invariance of the lattice (Knops 1973). Lewis and Wannier (1952) proposed to simplify the spherical model by requiring the global constraint of Berlin and Kac to be obeyed in the sense of an ensemble average. This model is generally known as the *mean spherical model*.

Because of its exact solubility the ferromagnetic mean spherical model has been extensively used to gain insights into the critical properties of finite (in one or more directions) systems[3]. Periodic boundary conditions, implying ferromagnetic interactions of spins belonging to both boundaries on the finite directions, have been by far the most used

[2] The literature on the thermodynamic Casimir effect can be found in Grüneberg and Diehl (2008) and references therein.

[3] For an extensive list of literature see (Barber and Fisher 1973, Singh and Pathria 1985a, Privman 1990, Chamati *et al* 1998, Brankov *et al* 2000) and references therein.

boundary conditions. These allow for analytic treatment of problems related to the finite-size scaling theory (Privman *et al* 1991, Brankov *et al* 2000). In addition to periodic boundary conditions, antiperiodic boundary conditions have also been used (Barber and Fisher 1973, Singh and Pathria 1985b) to investigate the finite-size scaling properties of the ferromagnetic mean spherical model. The aforementioned boundary conditions do not break the translational invariance of the model in the absence of a magnetic field. Much less has been achieved in the case of nonperiodic (free) boundary conditions. These are believed to be more relevant to real systems, especially to systems confined between parallel plates. The ferromagnetic mean spherical model of finite thickness has been investigated in the case of Dirichlet boundary conditions by Barber and Fisher (1973), Barber (1974), Danchev *et al* (1997), Chen and Dohm (2003), Dantchev and Brankov (2003) and Neumann boundary conditions in Barber *et al* (1974), Danchev *et al* (1997), Dantchev and Brankov (2003). Barber and Fisher (1973), and Barber (1974) investigated the scaling properties of the mean spherical model with finite thickness using a method originally devised by Barber and Fisher (1973). They obtained explicit forms of the equation for the spherical field at three, four and five dimensions, separately. The method was extended to the study of the finite-size effects in the case of Neumann and Neumann–Dirichlet boundary conditions by Danchev *et al* (1997). Chen and Dohm (2003) argued that the results of Barber and Fisher (1973), Barber (1974) for Dirichlet boundary conditions were incorrect at three dimensions far from the critical point. Later, the equation for the spherical field of Barber and Fisher (1973) was rederived by Dantchev and Brankov (2003). It should be mentioned, however that the derivation of Dantchev and Brankov (2003) is based on an improved method of Barber and Fisher (1973). On the other hand, in Barber and Fisher (1973), Barber (1974), Danchev *et al* (1997), Dantchev and Brankov (2003) the free energy density for the different kinds of boundary conditions was obtained by integrating the equation for the spherical field leading to complicated integral representations.

In the present paper we propose a different method to treat the finite size effects in the mean spherical model of finite thickness. The method is a generalization of that devised by Singh and Pathria (1985a) for periodic boundary conditions. It applies to antiperiodic, Dirichlet, Neumann boundary conditions imposed on both surfaces bounding the system and a combination of Dirichlet and Neumann boundary conditions on each surface. The method is quite general and is used for arbitrary dimension. Furthermore, the finite-size contributions to the free energy density are obtained directly form the corresponding general expression rather than through integration of the equation for the spherical field. We anticipate here that from our results we recover the particular cases of Barber and Fisher (1973), Barber (1974), Danchev *et al* (1997), Dantchev and Brankov (2003) but not the results of Chen and Dohm (2003). We will return to these points later in the paper.

The rest of the paper is structured as follows: in section 2 we define the model and present the expressions for the free energy density and the equation for the spherical field for the different kinds of boundary conditions. In section 3 we present in detail how the method applies to the case of periodic boundary conditions and compare our results with those available in the literature. In sections 4 through 7 we extend the method for arbitrary dimensions to the other boundary conditions and compare with the results obtained by other authors using different methods. Finally in section 8 we summarize our results.

2. The model

We consider the mean spherical model on a d-dimensional lattice confined to a film geometry i.e. infinite in $d-1$ dimensions and of finite thickness L in the remaining dimension with volume $V = L \times \infty^{d-1}$. The linear size of the lattice is measured in units of the lattice constant, which will be taken equal to 1. The model is defined through

$$\mathcal{H} = -\frac{1}{2}\sum_{ij} J_{ij} s_i s_j - H\sum_i s_i + \frac{1}{2}\mu\sum_i s_i^2, \tag{2.1}$$

where $s_i \equiv s_i(\boldsymbol{r}, z)$, the spin at site i, is a continuous real variable ($-\infty \leqslant s_i \leqslant \infty$) with coordinates $\boldsymbol{r}$ in the $d-1$ infinite 'parallel' planes and z in the finite lateral direction. J_{ij} is the interaction matrix between spins at sites i and j, and H is an ordering external magnetic field. Finally the field μ is introduced so as to ensure the spherical constraint

$$\sum_i \left\langle s_i^2 \right\rangle = N, \tag{2.2}$$

where $\langle\cdots\rangle$ denotes standard thermodynamic averages computed with the Hamiltonian $\mathcal{H}$ and N the total number of spins on the lattice.

Along the finite z direction we impose different kinds of boundary conditions which we will denote collectively by τ. For a lattice system this means

(p) periodic: $s(\boldsymbol{r}, 1) = s(\boldsymbol{r}, L+1)$;
(a) antiperiperiodic: $s(\boldsymbol{r}, 1) = -s(\boldsymbol{r}, L+1)$;
(D) Dirichlet: $s(\boldsymbol{r}, 0) = s(\boldsymbol{r}, L+1) = 0$;
(N) Neumann: $s(\boldsymbol{r}, 0) = s(\boldsymbol{r}, 1)$ and $s(\boldsymbol{r}, L) = s(\boldsymbol{r}, L+1)$;
(ND) Neumann–Dirichlet: $s(\boldsymbol{r}, 0) = s(\boldsymbol{r}, 1)$ and $s(\boldsymbol{r}, L+1) = 0$.

For nearest neighbour interactions and under the above boundary conditions the Hamiltonian (2.1) may be diagonalized by plane waves parallel to the confining plates and appropriate eigenfunctions $\varphi_n^{(\tau)}(z)$ using the representation

$$s_i(\boldsymbol{r}, z) = \sum_n \int_0^{2\pi} \frac{\mathrm{d}q_1}{2\pi} \cdots \int_0^{2\pi} \frac{\mathrm{d}q_{d-1}}{2\pi} s_{\boldsymbol{q},n}\, \mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}} \varphi_n^{(\tau)}(z), \tag{2.3}$$

where the integrals over q_i s, the components of $\boldsymbol{q}$, are restricted to the first Brillouin zone of the hypercubic lattice of dimension $d-1$. The orthogonal eigenfunctions read

$$\varphi_n^{(p)}(z) = \frac{1}{\sqrt{L}} \exp\left[\mathrm{i}\frac{2\pi}{L} nz\right], \qquad n = 0, \ldots, L-1; \tag{2.4a}$$

$$\varphi_n^{(a)}(z) = \frac{1}{\sqrt{L}} \exp\left[\mathrm{i}\frac{2\pi}{L}\left(n + \frac{1}{2}\right) z\right], \qquad n = 0, \ldots, L-1; \tag{2.4b}$$

$$\varphi_n^{(D)}(z) = \sqrt{\frac{2}{L+1}} \sin\left[\frac{\pi}{L+1}(n+1)z\right], \qquad n = 0, \ldots, L-1; \tag{2.4c}$$

$$\varphi_n^{(N)}(z) = \begin{cases} L^{-1/2}, & n = 0, \\ \sqrt{\dfrac{2}{L}} \cos\left[\dfrac{\pi}{L} nz\right], & n = 1, \ldots, L-1; \end{cases} \tag{2.4d}$$

$$\varphi_n^{(ND)}(z) = \frac{2}{\sqrt{2L+1}} \cos\left[\frac{2\pi}{2L+1}\left(n + \frac{1}{2}\right) z\right]; \qquad n = 0, \ldots, L-1. \tag{2.4e}$$

The eigenmodes associated with the above eigenfunctions are given by

$$\omega_n^{(p)} = -2 + 2\cos\left[\frac{2\pi}{L} n\right]; \tag{2.5a}$$

$$\omega_n^{(a)} = -2 + 2\cos\left[\frac{2\pi}{L}\left(n + \frac{1}{2}\right)\right]; \tag{2.5b}$$

$$\omega_n^{(D)} = -2 + 2\cos\left[\frac{\pi}{L+1}(n+1)\right]; \tag{2.5c}$$

$$\omega_n^{(N)} = -2 + 2\cos\left[\frac{\pi}{L}n\right]; \tag{2.5d}$$

$$\omega_n^{(DN)} = -2 + 2\cos\left[\frac{2\pi}{2L+1}\left(n + \frac{1}{2}\right)\right]. \tag{2.5e}$$

Those corresponding to the diagonalized interaction matrix are $\lambda_n^{(\tau)} = 2 + \omega_0^{(\tau)}$.

At zero field, the free energy density of the mean spherical model under the above boundary conditions imposed along the finite lateral size has the general expression (obtained via the Legendre transformation)

$$\beta F_d^{(\tau)}(T, L; \phi) = \frac{1}{2}\ln K + \frac{1}{2L}\sum_{n=0}^{L-1} U_{d-1}\left(\phi + \omega_0^{(\tau)} - \omega_n^{(\tau)}\right) - \frac{1}{2}K\left(\phi + \omega_0^{(\tau)}\right) - K, \tag{2.6}$$

where $K = \beta J = J/k_B T$ and

$$U_d(z) = \int_0^{2\pi}\frac{\mathrm{d}\theta_1}{2\pi}\cdots\int_0^{2\pi}\frac{\mathrm{d}\theta_d}{2\pi}\ln\left[z + 2\sum_{i=1}^{d}(1 - \cos\theta_i)\right]. \tag{2.7}$$

In (2.6), the shifted spherical field, defined by

$$\phi = \mu/J - \lambda_0^{(\tau)},$$

is the solution of the spherical constraint

$$K = \frac{1}{L}\sum_{n=0}^{L-1} W_{d-1}\left(\phi + \omega_0^{(\tau)} - \omega_n^{(\tau)}\right), \tag{2.8}$$

with the bulk function

$$W_d(z) = \int_0^{2\pi}\frac{\mathrm{d}\theta_1}{2\pi}\cdots\int_0^{2\pi}\frac{\mathrm{d}\theta_d}{2\pi}\frac{1}{z + 2\sum_{i=1}^{d}(1 - \cos\theta_i)}, \tag{2.9}$$

whose asymptotic behaviour has been studied in considerable detail for $z \in \mathbb{C}$ in Barber and Fisher (1973).

The bulk limit is obtained from (2.8) by letting the lateral size L go to infinity. This allows us to investigate the thermodynamics of the ferromagnetic mean spherical model in the thermodynamic limit. Here we shall not enter into the investigation of the thermodynamic properties (the interested reader may refer to Pathria (1996)). It is worth mentioning that the present model undergoes a continuous phase transition at a bulk critical point determined by

$$K_{c,d} = W_d(0), \tag{2.10}$$

for $d > 2$. On the other hand for $d > 4$ the model exhibits mean-field-like critical behaviour. Recently an efficient method to estimate the Watson integral $W_d(0)$ and the associated logarithmic integral for d-dimensional hypercubic lattice has been proposed by Joyce and Zucker (2001).

Before embarking into the investigation of the finite-size effects for the different boundary conditions a few comments are in order:

(1) For the evaluation of the finite-size contributions to the bulk expressions of the free energy and the equation for the spherical field the case of periodic boundary conditions is the

simplest. A powerful method to treat these sums was proposed in Singh and Pathria (1985a). It was found that in this case the correlation length ξ_L of the finite system is given by $\xi_L = \phi^{-1/2}$ (Singh and Pathria 1987).

(2) The same method was successfully extended to the case of antiperiodic boundary conditions (Singh and Pathria 1985b). However, the calculations were done in the absence of the lowest mode $\omega_0^{(\tau)}$ in (2.6) and (2.8). Later by investigating the correlation function (Allen and Pathria 1993), it was found that the correlation length ξ_L and the root square of spherical field ϕ are no more connected by a simple relation as it is the case for periodic boundary conditions. It was suggested that the correlation length is in fact related to the solution of the equation for spherical field shifted by the asymptotic behaviour of $\omega_0^{(\tau)}$ i.e. $\frac{\pi^2}{L^2}$.

(3) The remaining boundary conditions have attracted less attention (Barber and Fisher 1973, Barber 1974, Barber *et al* 1974, Danchev *et al* 1997, Brankov *et al* 2000, Chen and Dohm 2003, Dantchev and Brankov 2003). Apart from the paper by Chen and Dohm (2003), all investigations were specialized to $d = 3$ using an approach based on Barber and Fisher (1973). For arbitrary d and Dirichlet boundary conditions, a recent work by Chen and Dohm (2003) proposed a different method and claimed that the results of Barber and Fisher (1973), obtained at $d = 3$, were incorrect.

Here we generalize the method of Singh and Pathria (1985a) for periodic boundary conditions to the other boundary conditions. We investigate the finite-size effects of the free energy density (2.6) and the equation for the spherical field (2.8) in each case for arbitrary dimension and comment on the results of the aforementioned papers.

3. Periodic boundary conditions

For the sake of completeness we will derive here the relevant expressions for the mean spherical model of finite thickness under periodic boundary conditions for arbitrary dimensionality. The derivation is adapted from Singh and Pathria (1985a) (see also Chamati *et al* (1998)). The explicit expressions for the free energy density (2.6) and the equation for the spherical field (2.8) are given by

$$\beta F_d^{(p)}(T, L) = \frac{1}{2}\ln K + \frac{1}{2L}\sum_{n=0}^{L-1} U_{d-1}\left(\phi + 2\left[1 - \cos\left(\frac{2\pi}{L}n\right)\right]\right) - \frac{1}{2}K\phi - K, \qquad (3.1a)$$

and

$$K = \frac{1}{L}\sum_{n=0}^{L-1} W_{d-1}\left(\phi + 2\left[1 - \cos\left(\frac{2\pi}{L}n\right)\right]\right), \qquad (3.1b)$$

respectively. In this case $\omega_0^{(p)} = 0$.

Using the integral representations

$$z^{-1} = \int_0^\infty e^{-zt} \qquad (3.2a)$$

and

$$\ln z = \int_0^\infty \frac{dt}{t}[e^{-t} - e^{-zt}] \qquad (3.2b)$$

we can separate the expressions for the free energy density (3.1a) and the equation for the spherical field (3.1b) into the corresponding bulk expressions and the associated finite-size contributions. Let us illustrate how this works for the equation for the spherical field. With the aid of (3.2*a*) the sum entering this equation can be written as

$$\mathcal{S}_{d,L}^{(p)}(\phi) = \sum_{n=0}^{L-1} W_{d-1}\left[\phi + 2\left(1-\cos\frac{2\pi}{L}n\right)\right]$$
$$= \int_0^{2\pi}\frac{\mathrm{d}\theta_1}{2\pi}\cdots\int_0^{2\pi}\frac{\mathrm{d}\theta_{d-1}}{2\pi}\int_0^{\infty}\mathrm{d}z\,\exp\left\{-z\left[\phi+2+2\sum_{i=1}^{d-1}(1-\cos\theta_i)\right]\right\}Q_L^{(p)}(2z), \tag{3.3}$$

with

$$Q_L^{(p)}(z) = \sum_{n=0}^{L-1}\exp\left[z\cos\frac{2\pi}{L}n\right]. \tag{3.4}$$

Note that the summand in (3.4) is a periodic function of period 2π. Further we use (a generalization of) the Poisson summation formula, namely

$$\sum_a^b f(n) = \sum_{l=-\infty}^{\infty}\int_a^b \mathrm{e}^{2\pi \mathrm{i}ln} f(n)\,\mathrm{d}n + \frac{1}{2}f(a) + \frac{1}{2}f(b) \tag{3.5}$$

to get the identity

$$Q_L^{(p)}(z) = \sum_{n=0}^{L-1}\exp\left[z\cos\frac{2\pi}{L}n\right] = L\sum_{l=-\infty}^{\infty} I_{Ll}(z), \tag{3.6}$$

where $I_\nu(x)$ stands for the modified Bessel function of the first kind (Abramowitz and Stegun 1972).

Substituting (3.6) into (3.3) we obtain

$$\mathcal{S}_{d,L}^{(p)}(\phi) = L\sum_{l=-\infty}^{\infty}\int_0^{\infty}\mathrm{d}z\,\mathrm{e}^{-z\phi}[\mathrm{e}^{-2z}I_0(2z)]^{d-1}\,\mathrm{e}^{-2z}I_{Ll}(2z)$$
$$= LW_d(\phi) + 2L\sum_{l=1}^{\infty}\int_0^{\infty}\mathrm{d}z\,\mathrm{e}^{-z\phi}[\mathrm{e}^{-2z}I_0(2z)]^{d-1}\,\mathrm{e}^{-2z}I_{Ll}(2z), \tag{3.7}$$

where we have used the integral representation

$$W_d(\phi) = \int_0^{\infty}\mathrm{d}z\,\mathrm{e}^{-z\phi}[\mathrm{e}^{-2z}I_0(2z)]^d \tag{3.8}$$

and the relation $I_{-2p}(x) = I_{2p}(x)$ (Abramowitz and Stegun 1972).

For large L, using the asymptotic expansion (Singh and Pathria 1985a)

$$I_\nu(x) = \frac{\mathrm{e}^{x-\nu^2/2x}}{\sqrt{2\pi x}}\left[1+\frac{1}{8x}+\frac{9-32\nu^2}{2!(8x)^2}+\cdots\right], \tag{3.9}$$

after some straightforward steps, keeping only leading terms in L^{-1}, we get

$$\mathcal{S}_{d,L}^{(p)}(\phi) = LW_d(\phi) + L\frac{4}{(4\pi)^{\frac{d}{2}}}\phi^{\frac{d}{2}-1}\sum_{l=1}^{\infty}\frac{K_{\frac{d}{2}-1}\left(lL\sqrt{\phi}\right)}{\left(\frac{1}{2}lL\sqrt{\phi}\right)^{\frac{d}{2}-1}}, \tag{3.10}$$

where $K_\nu(x)$ is the modified Bessel function of the second kind (Abramowitz and Stegun 1972).

Collecting the above results the equation for the spherical field reads

$$K = W_d(\phi) + \frac{4}{(4\pi)^{\frac{d}{2}}}\phi^{\frac{d}{2}-1}\sum_{l=1}^{\infty}\frac{K_{\frac{d}{2}-1}(lL\sqrt{\phi})}{\left(\frac{1}{2}lL\sqrt{\phi}\right)^{\frac{d}{2}-1}}. \tag{3.11}$$

The finite-size behaviour of this equation has been studied in great detail by Chamati *et al* (1998) for arbitrary d for different geometries including questions like dimensional crossover, finite-size shift of the bulk critical temperature, etc. In particular it was found that the finite-size shift obeys the predictions of the finite-size scaling. For $2 < d < 4$, using the asymptotic behaviour

$$W_d(z) = W_d(0) + \frac{1}{(4\pi)^{d/2}}\Gamma\left[\frac{2-d}{2}\right]z^{(d-2)/2} + O(z^{(d-1)/2}), \tag{3.12}$$

equation (3.11) takes the scaling form

$$\varkappa = \frac{y^{d-2}}{(4\pi)^{d/2}}\left[\left|\Gamma\left[\frac{2-d}{2}\right]\right| - 4\sum_{l=1}^{\infty}\frac{K_{\frac{d}{2}-1}(ly)}{\left(\frac{1}{2}ly\right)^{\frac{d}{2}-1}}\right], \tag{3.13}$$

where we have introduced the scaling variable $y = L\sqrt{\phi}$ and $\varkappa = L^{1/\nu}(K_{c,d} - K)$ with $\nu = (d-2)^{-1}$—the critical exponent measuring the divergence of the correlation length. Consequently we have a solution of the form $\xi_L = \phi^{-1/2} = Lf_p(\varkappa)$, where $f_{(p)}$ is a universal scaling function. For arbitrary d the nature of the scaling function $f_{(p)}(\varkappa)$ can be determined only numerically (see e.g. Chamati *et al* (1998)). For the particular case $d = 3$, equation (3.13) takes a simple form

$$2\pi\varkappa = \ln 2\sinh\frac{y}{2}. \tag{3.14}$$

The solution of this equation leads to the universal scaling function

$$y = g_{(p)}(\varkappa) = 2\,\mathrm{arcsinh}\left(\tfrac{1}{2}\,\mathrm{e}^{2\pi\varkappa}\right) \tag{3.15}$$

At the critical point, $\varkappa = 0$, we obtain the critical amplitude of the finite-size correlation length ξ_L:

$$y_0 = g_{(p)}(0) = 2\ln\frac{1+\sqrt{5}}{2}. \tag{3.16}$$

The finite-size contributions to the free energy for any d can be accounted for by using the integral representation (3.2*b*). The aim here is to transform the sum

$$\begin{aligned}\mathcal{P}^{(p)}_{d,L}(\phi) &= \sum_{n=0}^{L-1} U_{d-1}\left[\phi + 2\left(1 - \cos\frac{2\pi}{L}n\right)\right]\\ &= \sum_{n=0}^{L-1}\int_0^{2\pi}\frac{\mathrm{d}\theta_1}{2\pi}\cdots\int_0^{2\pi}\frac{\mathrm{d}\theta_{d-1}}{2\pi}\ln\left[\phi + 2\left(1-\cos\frac{2\pi}{L}n\right) + 2\sum_{i=1}^{d-1}(1-\cos\theta_i)\right]\end{aligned} \tag{3.17}$$

into a more tractable form suitable for analytic treatment. After some straightforward algebra along the lines explained above, including the use of the identity (3.6), we arrive at

$$\mathcal{P}^{(p)}_{d,L}(\phi) = LU_d(\phi) - L\frac{4}{(4\pi)^{\frac{d}{2}}}\phi^{\frac{d}{2}}\sum_{l=1}^{\infty}\frac{K_{\frac{d}{2}}(lL\sqrt{\phi})}{\left(\frac{1}{2}lL\sqrt{\phi}\right)^{\frac{d}{2}}}. \tag{3.18}$$

Using (3.18) for the large L asymptotic behaviour of the free energy density (3.1a) we get

$$\beta F_d^{(p)}(T, L; \phi) = \beta F_d(T; \phi) - \frac{2}{(4\pi)^{\frac{d}{2}}}\phi^{\frac{d}{2}} \sum_{l=1}^{\infty} \frac{K_{\frac{d}{2}}(lL\sqrt{\phi})}{\left(\frac{1}{2}lL\sqrt{\phi}\right)^{\frac{d}{2}}}, \tag{3.19}$$

where

$$F_d(T; \phi) = \lim_{L\to\infty} F_d^{(\tau)}(T, L; \phi) = \frac{1}{2\beta}[\ln K + U_d(\phi) - K\phi - 2K] \tag{3.20}$$

is the bulk free energy density.

For $2 < d < 4$, in the vicinity of the bulk critical point, we have the expansion

$$U_d(z) = U_d(0) + K_{c,d}z + \frac{1}{(4\pi)^{d/2}}\frac{2}{d}\Gamma\left[\frac{2-d}{2}\right]z^{d/2} + O(z^{(d+1)/2}). \tag{3.21}$$

Then the singular part of the free energy density (3.19) takes the scaling form

$$\beta f_{s,d}^{(p)}(y, \varkappa) = \frac{1}{2}L^{-d}\left[\varkappa y^2 + \frac{2y^d}{(4\pi)^{d/2}}\left(\frac{1}{d}\Gamma\left[\frac{2-d}{2}\right] - 2\sum_{l=1}^{\infty}\frac{K_{\frac{d}{2}}(ly)}{\left(\frac{1}{2}ly\right)^{\frac{d}{2}}}\right)\right], \tag{3.22}$$

where y is the solution of (3.13). Thus, the scaling behaviour of the free energy density is consistent with the finite-size scaling hypothesis (1.1). The Casimir amplitude for $d = 3$ i.e. the critical amplitude of the singular part of the free energy density can be computed analytically, having in mind the solution (3.16), with the aid of polylogarithmic identities (Sachdev 1993). The result is (Sachdev (1993), Danchev (1998)):

$$\Delta^{(p)} = -\frac{2\zeta(3)}{5\pi} = -0.153\,051\ldots. \tag{3.23}$$

This value is compatible with estimations obtained for more realistic $O(n)$ models using different approaches. For more details we refer the reader to Grüneberg and Diehl (2008).

As one would expect from previous studies on the mean spherical model, the results obtained for periodic boundary conditions are in conformity with the finite-size scaling hypothesis. In the following we will extend the method described here to the other boundary conditions. The generalization is somehow straightforward, however we will see the appearance of some subtleties that need careful consideration.

4. Antiperiodic boundary conditions

The explicit expressions for the free energy density (2.6) and the equation for the spherical field (2.8) for arbitrary dimension read

$$\beta F_d^{(a)}(T, L; \phi) = \frac{1}{2}\ln K + \frac{1}{2L}\sum_{n=0}^{L-1} U_{d-1}\left[\phi + \omega_0^{(a)} - \omega_n^{(a)}\right] - \frac{1}{2}K\left(\phi + \omega_0^{(a)}\right) - K, \tag{4.1a}$$

and

$$K = \frac{1}{L}\sum_{n=0}^{L-1} W_{d-1}\left[\phi + \omega_0^{(a)} - \omega_n^{(a)}\right]. \tag{4.1b}$$

respectively. Here the lowest eigenmode $\omega_0^{(a)} \neq 0$, in contrast to the case of periodic boundary conditions.

Unlike the analysis of Singh and Pathria (1985b) we shall not omit $\omega_0^{(\tau)} = -2 + 2\cos\frac{\pi}{L}$ from our equations, rather we will use the combination $\sigma^{(a)} = \phi + \omega_0^{(a)}$ as a variable in our consideration of the sums entering (4.1a) and (4.1b). We will see that this is crucial to our further treatment. Indeed, in our notations, ϕ is expected to define the correlation length and no other definition for this quantity is necessary as it has been suggested in Allen and Pathria (1993), where the behaviour of the order parameter correlation function for the finite mean-spherical model with antiperiodic boundary conditions has been investigated in detail.

The analysis of section 3 for periodic boundary conditions can be applied to the sums

$$\mathcal{S}_{d,L}^{(a)}[\sigma^{(a)}] = \sum_{n=0}^{L-1} W_{d-1}\left[\sigma^{(a)} - \omega_n^{(a)}\right] \tag{4.2a}$$

$$\mathcal{P}_{d,L}^{(a)}[\sigma^{(a)}] = \sum_{n=0}^{L-1} U_{d-1}\left[\sigma^{(a)} - \omega_n^{(a)}\right] \tag{4.2b}$$

appearing on the left-hand side of (4.1a) and (4.1b), respectively. Now instead of the identity (3.6) we use (Singh and Pathria (1985b))

$$Q_L^{(a)}(z) = \sum_{n=0}^{L-1} \exp\left[z\cos\frac{2\pi}{L}\left(n+\frac{1}{2}\right)\right] = L\sum_{l=-\infty}^{\infty}\cos(\pi l) I_{Ll}(z), \tag{4.3}$$

to end up with the final expressions

$$\beta F_d^{(a)}(T,L;\phi) = \beta F_d\big(T;\phi+\omega_0^{(a)}\big) - \frac{2}{(4\pi)^{d/2}}(\phi+\omega^{(a)})^{\frac{d}{2}}\sum_{l=1}^{\infty}(-1)^l\frac{K_{\frac{d}{2}}\big(lL\sqrt{\phi+\omega_0^{(a)}}\big)}{\big(\frac{1}{2}lL\sqrt{\phi+\omega_0^{(a)}}\big)^{\frac{d}{2}}} \tag{4.4a}$$

and

$$K = W_d\big(\phi+\omega_0^{(a)}\big) + \frac{4}{(4\pi)^{d/2}}(\phi+\omega^{(a)})^{\frac{d}{2}-1}\sum_{l=1}^{\infty}(-1)^l\frac{K_{\frac{d}{2}-1}\big(lL\sqrt{\phi+\omega_0^{(a)}}\big)}{\big(\frac{1}{2}lL\sqrt{\phi+\omega_0^{(a)}}\big)^{\frac{d}{2}-1}}. \tag{4.4b}$$

For $2 < d < 4$, making use of the asymptotic expansion (3.12), for large L and in the vicinity of the bulk critical point, with $\phi + \omega_0^{(a)} < 1$, we have the scaling behaviour

$$\varkappa = \frac{(y^2-\pi^2)^{\frac{d-2}{2}}}{(4\pi)^{d/2}}\left[\left|\Gamma\left[\frac{2-d}{2}\right]\right| - 4\sum_{l=1}^{\infty}(-1)^l\frac{K_{\frac{d}{2}-1}(l\sqrt{y^2-\pi^2})}{\big(\frac{1}{2}l\sqrt{y^2-\pi^2}\big)^{\frac{d}{2}-1}}\right], \tag{4.5}$$

where we have used $\omega_0^{(a)} \approx -\frac{\pi^2}{L^2}$. Following the analysis of Allen and Pathria (1993) it is easy to show that $\sqrt{\phi}$ coincides with the inverse of the finite-size correlation length ξ_L. In this case, the solution of (4.5) may be written as $\xi_L = Lf_{(a)}(\varkappa)$, where $f_{(a)}$ is a universal scaling function.

The critical temperature of the film corresponds to $y = \pi$ i.e. $\phi = \left(\frac{\pi}{L}\right)^2$, which is the asymptotic of the lowest mode $\omega_0^{(a)}$ for large L. Setting $y = \pi$ in equation (4.5), we find that the critical point of the film is shifted from the bulk one by a quantity proportional to $L^{-1/\nu}$ in agreement with the finite-size scaling predictions.

For arbitrary dimension d, equation (4.5) can be solved only numerically. Here we will specialize to the three-dimensional system, which allows analytic treatment. For $d = 3$, equation (4.5) transforms into

$$2\pi\varkappa = \ln 2\cosh\tfrac{1}{2}\sqrt{y^2-\pi^2}, \tag{4.6}$$

whose positive solution reads

$$y = g_{(a)}(\varkappa), \tag{4.7}$$

with the universal scaling function

$$g_{(a)}(\varkappa) = \left(\pi^2 + 4\left[\operatorname{arccosh}\left(\frac{1}{2}\,\mathrm{e}^{2\pi\varkappa}\right)\right]^2\right)^{1/2}. \tag{4.8}$$

At the bulk critical point, i.e. $\varkappa = 0$, we obtain

$$y_0 = g_{(a)}(0) = \tfrac{\sqrt{5}}{3}\pi. \tag{4.9}$$

This is the critical amplitude of the finite-size correlation length ξ_L. This result has been obtained also by Allen and Pathria (1993) using a different definition for the correlation length imposed by the choice of a different initial equation for the spherical field.

Using the asymptotic behaviour (3.21), valid for $2 < d < 4$, and the fact that y is the solution of equation (4.5), we may write the singular part of the free energy density (4.1*a*) in a scaling form as

$$f_{s,d}^{(a)}(y,\varkappa)L^d = \frac{1}{2}\varkappa(y^2-\pi^2) + \frac{(y^2-\pi^2)^{\frac{d}{2}}}{(4\pi)^{d/2}} \times\left(\frac{1}{d}\Gamma\left[\frac{2-d}{2}\right] - 2\sum_{l=1}^{\infty}(-1)^l\frac{K_{\frac{d}{2}}(l\sqrt{y^2-\pi^2})}{\left(\frac{1}{2}l\sqrt{y^2-\pi^2}\right)^{\frac{d}{2}}}\right). \tag{4.10}$$

In accordance with the finite-size scaling hypothesis (1.1). For the important case $d = 3$, its critical amplitude at the bulk critical temperature and consequently the corresponding Casimir amplitude for antiperiodic boundary conditions is[4]

$$\Delta^{(a)} = 0.274\,543\ldots. \tag{4.11}$$

Note that the Casimir amplitude here is positive in contrast to the case of periodic boundary conditions, see e.g. (3.23), but approximately twice higher in magnitude. This result is compatible with that of Krech and Dietrich (1992) obtained using renormalization group.

Before closing this section let us mention that the expressions for periodic boundary conditions and those corresponding to antiperiodic boundary conditions may be written in unified general forms with a parameter characteristic of twisted boundary conditions. In the remainder of the paper we will use these methods to analyse the finite-size effects of the mean spherical model with a film geometry subject to more realistic boundary conditions.

5. Dirichlet boundary conditions

5.1. Equation for the spherical field

Here we will evaluate the finite-size contributions of the sum appearing in (2.8) in the case of Dirichlet boundary conditions for arbitrary d. We start with

$$\mathcal{S}_{d,L}^{(D)}(\phi) = \sum_{n=1}^{L} W_{d-1}\left[\phi + 2\cos\frac{\pi}{L+1} - 2\cos\frac{\pi n}{L+1}\right], \tag{5.1}$$

[4] This result was obtained independently by Dantchev and Grüneberg (2008).

which upon extending the sum to $n = 2L + 1$ may be written

$$\mathcal{S}_{d,L}^{(D)}(\phi) = \frac{1}{2}\sum_{n=0}^{2L+1} W_{d-1}\left[\phi + 2\cos\frac{\pi}{L+1} - 2\cos\frac{\pi n}{L+1}\right] \\ -\frac{1}{2}W_{d-1}\left[\phi + 2\cos\frac{\pi}{L+1} + 2\right] - \frac{1}{2}W_{d-1}\left[\phi + 2\cos\frac{\pi}{L+1} - 2\right]. \tag{5.2}$$

The last two terms correspond to $n = L+1$ and $n = 0$, respectively. Comparing with (3.3) we find that the sum on the right-hand side is exactly $\mathcal{S}_{d,2L+2}^{(p)}\big(\phi + \omega_0^{(D)}\big)$ corresponding to periodic boundary conditions with a film of thickness $2L + 2$. This suggests that the analysis of the sum appearing in (5.2) can be performed following the method outlined in section 3 (see e.g. (3.10)).

The equation for the spherical field follows from (2.8), (5.2) and (3.10). This is (to the leading order in L^{-1})

$$K = W_d\left(\phi - \frac{\pi^2}{L^2}\right) + \frac{1}{L}\left[W_d\left(\phi - \frac{\pi^2}{L^2}\right) - \frac{1}{2}W_{d-1}\left(\phi - \frac{\pi^2}{L^2} + 4\right) - \frac{1}{2}W_{d-1}\left(\phi - \frac{\pi^2}{L^2}\right)\right] \\ + \frac{4}{(4\pi)^{d/2}}\left(\phi - \frac{\pi^2}{L^2}\right)^{\frac{d}{2}-1}\sum_{l=1}^{\infty}\frac{K_{\frac{d}{2}-1}\big(2lL\sqrt{\phi - \frac{\pi^2}{L^2}}\big)}{\big(lL\sqrt{\phi - \frac{\pi^2}{L^2}}\big)^{\frac{d}{2}-1}}, \tag{5.3}$$

where we have used the large asymptotic behaviour $\omega_0^{(D)} \approx -\frac{\pi^2}{L^2}$. Equation (5.3) is the general form of the equation for the spherical field for arbitrary dimension d. Note that the right-hand side is composed of a bulk term, a size-dependent surface term

$$W_d\left(\phi - \frac{\pi^2}{L^2}\right) - \frac{1}{2}W_{d-1}\left(\phi - \frac{\pi^2}{L^2} + 4\right) - \frac{1}{2}W_{d-1}\left(\phi - \frac{\pi^2}{L^2}\right) \tag{5.4}$$

and finite-size corrections. Here, all the quantities are function of the combination $\phi - \frac{\pi^2}{L^2}$. Thus, the critical properties of the mean spherical model of finite thickness under Dirichlet boundary conditions should be investigated using $\phi - \frac{\pi^2}{L^2}$ as a small parameter keeping in mind that $\phi \ll 1$ and $L \gg 1$.

The scaling behaviour of (5.3) depends strongly upon d, indeed the asymptotic expansion of $W_{d-1}(z)$ for small argument takes different expressions for different values of d. We first start with the important three-dimensional case that has been extensively studied in the literature. Later we will extend our analysis to the interval $3 < d < 4$. This constraint for d ensures the validity of the asymptotic expansion (3.12) for $W_d(z)$ and $W_{d-1}(z)$ at the same time.

For $d = 3$, using (3.12) with $d = 3$ and

$$W_2(z) = \frac{1}{4\pi}(5\ln 2 - \ln z) + O(z\ln z), \tag{5.5}$$

from (5.3) we have

$$K - K_{c,3} = \frac{1}{L}\left[K_{c,3} - \frac{1}{2}W_2(4) - \frac{5\ln 2}{8\pi}\right] - \frac{1}{4\pi L}\ln L - \frac{1}{4\pi L}\ln\frac{\sinh 2\sqrt{L^2\phi - \pi^2}}{\sqrt{L^2\phi - \pi^2}}, \tag{5.6}$$

which, apart from an unimportant numerical factor that enters in the definition of K, coincides with equation (4.69) of Barber and Fisher (1973) obtained at $d = 3$ via a different method. Consequently our result disagrees with that of Chen and Dohm (2003), where it has been argued that equation (4.69) of Barber and Fisher (1973) was incorrect far from $K_{c,3}$.[5] At the bulk

[5] The origin of this discrepancy is discussed in Chen and Dohm (2003).

critical point, solving (5.6), with the assumption $L\sqrt{\phi} \ll 1$, we find $\phi \sim L^{-3}$ in agreement with Chen and Dohm (2003), Dantchev and Brankov (2003). It is worth mentioning that (5.6) cannot be put in a scaling form because of the logarithmic dependence on L. However, if one considers a shifted critical point that absorbs the term proportional to $\ln L$ and the surface contributions according to Barber and Fisher (1973)

$$K_{s,3}^{(D)} = K_{c,3} + \frac{1}{L}\left[K_{c,3} - \frac{1}{2}W_2(4) - \frac{7\ln 2}{8\pi}\right] - \frac{1}{4\pi L}\ln L, \tag{5.7}$$

it is possible to recover the scaling behaviour. Note that expression (5.7) does not conform with the predictions of the theory of finite-size scaling for the finite-size shift of the critical temperature, since there is a term containing $\ln L$.

In the case $3 < d < 4$, using the asymptotic expansion (3.12), the equation for the spherical field (5.3) may be written as

$$\begin{aligned} -\varkappa = {} & L^{d-3}\left[W_d(0) - \frac{1}{2}W_{d-1}(0) - \frac{1}{2}W_{d-1}(4)\right] \\ & + \frac{1}{(4\pi)^{d/2}}(y^2-\pi^2)^{\frac{d}{2}-1}\left[\Gamma\left(\frac{2-d}{2}\right) - \sqrt{\pi}\Gamma\left(\frac{3-d}{2}\right)(y^2-\pi^2)^{-\frac{1}{2}}\right] \\ & + \frac{1}{(4\pi)^{d/2}}(y^2-\pi^2)^{\frac{d}{2}-1}\sum_{l=1}^{\infty}\frac{K_{\frac{d}{2}-1}(2l\sqrt{y^2-\pi^2})}{(l\sqrt{y^2-\pi^2})^{\frac{d}{2}-1}}, \end{aligned} \tag{5.8}$$

where we have introduced the usual notations $\varkappa = L^{1/\nu}(K_{c,d} - K)$ and $y = L\sqrt{\phi}$. The first term on the right-hand side shows that the standard finite-size scaling hypothesis breaks down in the vicinity of the bulk critical temperature. It is likely that the introduction of a scaling function depending on $\varkappa$ and an additional variable to take care of the term proportional to L^{d-3} aiming at the modification of the finite-size scaling would cure this deficiency.

From equation (5.3) it is easy to see that leading large L behaviour of the finite-size shift from the bulk critical temperature to the one where the film is expected to have a singular behaviour is L^{-1}. This result, valid for any dimension, shows that the finite-size scaling hypothesis is violated as it has been pointed out by Brézin (1983).

5.2. *Free energy density*

Let us now turn to the evaluation of the free energy density (2.6). We need the asymptotic behaviour of the sum

$$\mathcal{P}_{d,L}^{(D)}(\phi) = \sum_{n=1}^{L} U_{d-1}\left[\phi + 2\cos\frac{\pi}{L+1} - 2\cos\frac{\pi n}{L+1}\right], \tag{5.9}$$

entering expression (2.6) of the free energy. Here again we extend the sum to $n = 2L + 1$, to get

$$\begin{aligned} \mathcal{P}_{d,L}^{(D)}(\phi) = {} & \frac{1}{2}\sum_{n=0}^{2L+1} U_{d-1}\left[\phi + 2\cos\frac{\pi}{L+1} - 2\cos\frac{\pi n}{L+1}\right] \\ & - \frac{1}{2}U_{d-1}\left[\phi + 2\cos\frac{\pi}{L+1} + 2\right] - \frac{1}{2}U_{d-1}\left[\phi + 2\cos\frac{\pi}{L+1} - 2\right]. \end{aligned} \tag{5.10}$$

The sum on the right-hand side of (5.10) corresponds to $P^{(p)}_{d,2L+2}\big(\phi + \omega_0^{(D)}\big)$ from (3.17). Then from (3.18) and (5.10) we get the free energy density

$$\beta F_d^{(D)}(T, L; \phi) = \beta F_d\left(T; \phi - \frac{\pi^2}{L^2}\right) + \frac{1}{L}\beta F^{(D)}_{d,\mathrm{surf.}}\left(T; \phi - \frac{\pi^2}{L^2}\right) - \frac{2}{(4\pi)^{\frac{d}{2}}}\left(\phi - \frac{\pi^2}{L^2}\right)^{\frac{d}{2}} \sum_{l=1}^{\infty} \frac{K_{\frac{d}{2}}\left(2lL\sqrt{\phi - \frac{\pi^2}{L^2}}\right)}{\left(lL\sqrt{\phi - \frac{\pi^2}{L^2}}\right)^{\frac{d}{2}}}, \tag{5.11}$$

where

$$\beta F^{(D)}_{d,\mathrm{surf.}}(T; \sigma) = \tfrac{1}{2}\big[U_d(\sigma) - \tfrac{1}{2}U_{d-1}(\sigma + 4) - \tfrac{1}{2}U_{d-1}(\sigma)\big]$$

accounts for size-dependent contributions stemming from the surfaces. In the following we will discuss the finite-size behaviour of the free energy and its dependence on the dimensionality d. Again we discuss separately the cases $d = 3$ and $3 < d < 4$ imposed by the validity of the expansion (3.21) for $U_d(z)$ and $U_{d-1}(z)$, simultaneously.

For $d = 3$, we use the expansions (3.21) and

$$U_2(z) = U_2(0) - \frac{1}{4\pi} z \ln z + \frac{1}{4\pi}(1 + 5\ln 2)z + O(z^2 \ln z) \tag{5.12}$$

to obtain the singular part of the free energy density

$$\beta f^{(D)}_{s,3} L^3 = \frac{1}{2}\varkappa(y^2 - \pi^2) - \frac{1}{12\pi}(y^2 - \pi^2)^{\frac{3}{2}} + \frac{1}{2}\left[K_{c,3} - \frac{1}{2}W_2(4) - \frac{1 + 5\ln 2}{8\pi}\right](y^2 - \pi^2) + \frac{1}{16\pi}(y^2 - \pi^2)\ln(y^2 - \pi^2) - \frac{1}{8\pi}(y^2 - \pi^2)\ln L - \frac{1}{8\pi}\sqrt{y^2 - \pi^2}\,\mathrm{Li}_2\big(\exp\big[-2\sqrt{y^2 - \pi^2}\big]\big) - \frac{1}{16\pi}\mathrm{Li}_3\big(\exp\big[-2\sqrt{y^2 - \pi^2}\big]\big). \tag{5.13}$$

At the shifted critical point $K^{(D)}_{s,3}$ (see (5.7)), $f^{(D)}_{s,3}$ takes a scaling form, as it has been pointed out in Barber (1974). Note that at the bulk critical temperature $f^{(D)}_{s,3}$ is proportional to $L^{-3}\ln L$ implying that the finite size-scaling hypothesis (1.1) breaks down for the mean spherical model with Dirichlet boundary conditions at $d = 3$, while in more realistic models the finite-size scaling is valid and the critical Casimir amplitude can be estimated (Krech and Dietrich 1992).

Another expression for the scaling behaviour of the singular part of free energy density was obtained by Barber (1974). In our notations it reads

$$\beta f^{B}_{s,3} L^3 = \frac{1}{2}\varkappa y^2 - \frac{y^2}{8\pi}\ln L + \frac{y^2}{2}\left[K_{c,3} - \frac{1}{2}W_2(4) - \frac{7\ln 2}{8\pi}\right] + Q_0(y), \tag{5.14}$$

where

$$Q_0(x) = \frac{\pi}{8}\left[R(-1) - R\left(\frac{x^2}{\pi^2} - 1\right)\right] \tag{5.15}$$

with

$$R(z) = \int_0^z \ln\frac{\sinh \pi\sqrt{w}}{\pi\sqrt{w}}\,\mathrm{d}w.$$

By comparing (5.13) and (5.14) we see that the first three terms on the right-hand side of (5.14) have their counterparts in (5.13) obtained through the replacement $y^2 \to y^2 - \pi^2$. It seems that the terms linear in π^2 and the term proportional to $L^{-3}\ln L$ were neglected in (5.14). It remains to see what is the situation for the rest of the terms. Unfortunately no direct

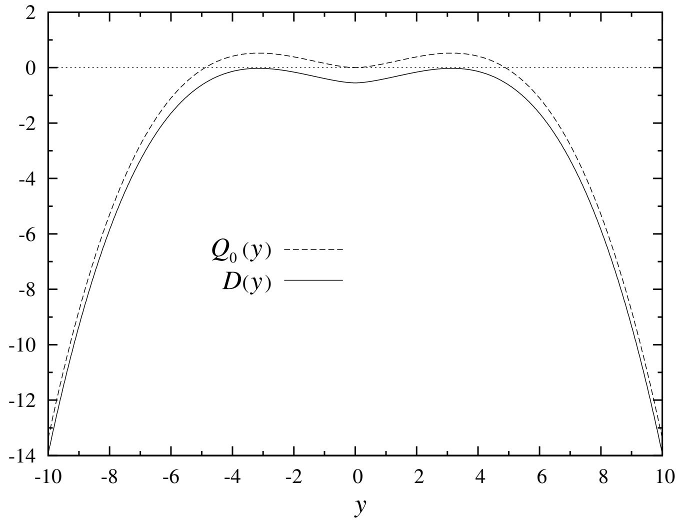

Figure 1. Behaviours of the functions $Q_0(y)$ (5.14) and $D(y)$ (5.16) against y.

analytic comparison can be made, despite the fact that the integral representation (5.15) can be expressed in terms of polylogarithms. To achieve the comparison recourse must be sought in numerical methods, so we plot the function $Q_0(y)$ and

$$D(y) = \frac{1}{16\pi}(2\ln 2 - 1)(y^2 - \pi^2) - \frac{1}{12\pi}(y^2 - \pi^2)^{\frac{3}{2}} + \frac{1}{16\pi}(y^2 - \pi^2)\ln(y^2 - \pi^2)$$
$$- \frac{1}{8\pi}\sqrt{y^2 - \pi^2}\,\mathrm{Li}_2(\exp[-2\sqrt{y^2 - \pi^2}]) - \frac{1}{16\pi}\,\mathrm{Li}_3(\exp[-2\sqrt{y^2 - \pi^2}]) \tag{5.16}$$

from (5.13) which contains terms that are not present in (5.14) and those that were apparently neglected. The result is shown in figure 1.[6] We see clearly that both functions have similar behaviours and are shifted one from the other by a constant. This has been checked by computing the derivatives of both functions which gives us the same result. The difference between the two functions is estimated to be

$$Q_0(y) - D(y) = \frac{\pi}{16}\left[-1 + \ln(4\pi^2) + \frac{1}{\pi^2}\zeta(3)\right]. \tag{5.17}$$

Thus, the scaling functions (5.13) and (5.14) are equal up to an irrelevant constant that does not become singular at the bulk critical point.

For $3 < d < 4$, using the asymptotic expansion (3.21), the scaling form of the singular part of the free energy density (5.11) reads

$$2f_{s,d}^{(D)}L^d = \varkappa(y^2 - \pi^2) + L^{d-3}\left[W_d(0) - \frac{1}{2}W_{d-1}(0) - \frac{1}{2}W_{d-1}(4)\right](y^2 - \pi^2)$$
$$+ \frac{2}{(4\pi)^{\frac{d}{2}}}(y^2 - \pi^2)^{\frac{d}{2}}\left[\frac{1}{d}\Gamma\left(\frac{2-d}{2}\right) - \frac{\sqrt{\pi}}{d-1}\Gamma\left(\frac{3-d}{2}\right)\frac{1}{\sqrt{y^2 - \pi^2}}\right]$$

[6] The numerical evaluation of the named expressions was performed with the aid of WOLFRAM MATHEMATICA 6.

$$- \frac{2}{(4\pi)^{\frac{d}{2}}} (y^2 - \pi^2)^{\frac{d}{2}} \sum_{l=1}^{\infty} \frac{K_{\frac{d}{2}}(2l\sqrt{y - \pi^2})}{(l\sqrt{y^2 - \pi^2})^{\frac{d}{2}}}. \tag{5.18}$$

Just like the equation for the spherical field we find that the surface contributions to the singular part of the free energy violates the standard finite-size scaling hypothesis (1.1). A reformulation of the scaling behaviour would require the introduction of a function with two arguments: the scaling variable $\varkappa$ and a scaling variable that incorporates the size-dependent term L^{d-3}.

6. Neumann boundary conditions

6.1. Equation for the spherical field

To investigate the finite-size effects in the mean spherical model of finite thickness subject to Neumann boundary conditions, through equation (2.8), we need to estimate the large asymptotic behaviour of the sum

$$\begin{aligned} \mathcal{S}_{d,L}^{(N)}(\phi) &= \sum_{n=1}^{L} W_{d-1}\left[\phi + 2 - 2\cos\frac{\pi(n-1)}{L}\right] \\ &= \frac{1}{2}\sum_{n=0}^{2L-1} W_{d-1}\left[\phi + 2 - 2\cos\frac{\pi n}{L}\right] - \frac{1}{2}W_{d-1}\left[\phi + 4\right] + \frac{1}{2}W_{d-1}\left[\phi\right]. \end{aligned} \tag{6.1}$$

The sum in the last line is exactly $\mathcal{S}_{d,2L}^{(N)}(\phi)$ (see (3.3)). Consequently, from (6.1) and (3.10), the equation for the spherical field is given by

$$K = W_d(\phi) - \frac{1}{2L}\left[W_{d-1}(\phi + 4) - W_{d-1}(\phi)\right] + \frac{4}{(4\pi)^{d/2}}\phi^{\frac{d}{2}-1}\sum_{l=1}^{\infty}\frac{K_{\frac{d}{2}-1}(2lL\sqrt{\phi})}{(lL\sqrt{\phi})^{\frac{d}{2}-1}}, \tag{6.2}$$

to the leading order in L^{-1}.

In addition to the restriction on d imposed by the fact that $d = 2$ is the lower critical dimension and $d = 4$ is the upper one, which is contained in $W_d(z)$ there is another one originating from $W_{d-1}(z)$ that restricts the validity of the asymptotic behaviour (3.12) to the interval $3 < d < 4$. For that reason we will investigate in some details only the cases $d = 3$ and $3 < d < 4$. The remaining part of the interval i.e. $2 < d < 3$ requires special treatment.

At $d = 3$, equation (6.2) takes the simple form

$$K - K_{c,3} = -\frac{1}{2L}\left[W_2(4) - \frac{5}{4\pi}\ln 2\right] + \frac{1}{4\pi L}\ln L - \frac{1}{4\pi L}\ln[2L\sqrt{\phi}\sinh(L\sqrt{\phi})]. \tag{6.3}$$

This equation was derived in Dantchev and Brankov (2003) using a method based on Barber and Fisher (1973). At the bulk critical temperature $K_{c,3}$ the spherical field behaves as $\phi \sim L^{-1}$ to the leading order assuming $L\sqrt{\phi} \ll 1$. In the limit $L\sqrt{\phi} \gg 1$ one would expect a logarithmic behaviour as pointed out by Dantchev and Brankov (2003). At the shifted critical temperature, defined through (Dantchev and Brankov 2003)

$$K_{s,3}^{(N)} = K_{c,3} - \frac{1}{2L}\left[W_2(4) - \frac{3}{4\pi}\ln 2\right] + \frac{1}{4\pi L}\ln L, \tag{6.4}$$

equation (6.3) may be written in a scaling form. An inspection of expression (6.4) shows that the predictions of the theory of finite-size scaling for the shifted critical temperature is not fulfilled due to the presence of the term proportional to $\ln L$.

For $3 < d < 4$ the scaling form of the equation for the spherical field (6.2) is given by

$$\varkappa = \frac{1}{2}L^{d-3}\left[W_{d-1}(4) - W_{d-1}(0)\right] - \frac{1}{(4\pi)^{d/2}}\left[\Gamma\left(\frac{2-d}{2}\right) - \frac{\sqrt{\pi}}{y}\Gamma\left(\frac{3-d}{2}\right)\right]y^{d-2} - \frac{4}{(4\pi)^{d/2}}y^{d-2}\sum_{l=1}^{\infty}\frac{K_{\frac{d}{2}-1}(2ly)}{(ly)^{\frac{d}{2}-1}}. \tag{6.5}$$

Here again we used the notations $\varkappa = L^{-1/\nu}(K_{c,d} - K)$ and $y = L\sqrt{\phi}$. As above for the case of Dirichlet boundary conditions the standard finite-size scaling hypothesis is violated here as well and would need a reformulation in order to take into account the term proportional to L^{d-3}. Furthermore, equation (6.5) shows that the leading asymptotic behaviour of the finite-size shift of the critical temperature is L^{-1}, which is not consistent with the predictions of the theory of finite-size scaling.

6.2. Free energy density

The free energy density (2.6) in the case of Neumann boundary conditions is obtained by analysing the sum

$$\begin{aligned}\mathcal{P}^{(N)}_{d,L}(\phi) &= \sum_{n=1}^{L} U_{d-1}\left[\phi + 2 - 2\cos\frac{\pi(n-1)}{L}\right]\\ &= \frac{1}{2}\sum_{n=0}^{2L-1} U_{d-1}\left[\phi + 2 - 2\cos\frac{\pi n}{L}\right] - \frac{1}{2}U_{d-1}\left[\phi+4\right] + \frac{1}{2}U_{d-1}[\phi]\end{aligned} \tag{6.6}$$

which contains the term $\mathcal{P}^{(p)}_{d,2L}(\phi)$, equivalent to (3.17). Using (6.6) and (3.18) we obtain explicitly

$$\beta F^{(N)}_{d}(T, L; \phi) = \beta F_d(T; \phi) + \frac{1}{L}\beta F^{(N)}_{d,\mathrm{surf.}}(\phi) - \frac{2}{(4\pi)^{\frac{d}{2}}}\phi^{\frac{d}{2}}\sum_{l=1}^{\infty}\frac{K_{\frac{d}{2}}(2lL\sqrt{\phi})}{(lL\sqrt{\phi})^{\frac{d}{2}}}, \tag{6.7}$$

where

$$\beta F^{(N)}_{d,\mathrm{surf.}}(\phi) = \tfrac{1}{4}U_{d-1}[\phi] - \tfrac{1}{4}U_{d-1}[\phi+4] \tag{6.8}$$

is the surfaces contribution.

Again we are faced with a situation where we have to restrict the validity of our expressions due the expansion (3.21), which should hold for $U_d(z)$ and $U_{d-1}(z)$ simultaneously. Here we consider the cases $d = 3$ and $3 < d < 4$ separately.

At $d = 3$, using (3.21) and (5.12) the singular part of the free energy density (6.6) reads

$$\beta f^{(N)}_{d,3}L^3 = \frac{1}{2}\varkappa y^2 - \frac{1}{12\pi}y^3 - \frac{1}{4}\left[W_2(4) - \frac{1+5\ln 2}{4\pi}\right]y^2 - \frac{1}{8\pi}y^2\ln y + \frac{1}{8\pi}y^2\ln L - \frac{1}{8\pi}y\,\mathrm{Li}_2(\mathrm{e}^{-2y}) - \frac{1}{16\pi}y\,\mathrm{Li}_3(\mathrm{e}^{-2y}). \tag{6.9}$$

Here again we have a logarithmic dependence on L and surface contributions leading to the violation of the finite-size scaling hypothesis (1.1). This makes the spherical model unsuitable for the evaluation of the Casimir amplitude for $O(n)$ systems with Neumann boundary conditions. The value of this quantity is known from renormalization group (Grüneberg and Diehl 2008).

For $3 < d < 4$, the singular part of the free energy reads

$$\beta f_{s,d}^{(N)} L^d = \frac{1}{2}\varkappa y^2 + \frac{1}{4}L^{d-3}\left[W_{d-1}(0) - W_{d-1}(4)\right] y^2 + \frac{1}{2(4\pi)^{d/2}} \times \left[\frac{1}{d}\Gamma\left(\frac{2-d}{2}\right) + \frac{\sqrt{\pi}}{d-1}\Gamma\left(\frac{3-d}{2}\right)\right] - \frac{2}{(4\pi)^{d/2}} y^d \sum_{l=1}^{\infty} \frac{K_{\frac{d}{2}}(2ly)}{(ly)^{\frac{d}{2}}}. \qquad (6.10)$$

This suggests that standard finite-size scaling hypothesis (1.1) is not valid for the mean spherical model confined to a film geometry with Neumann boundary conditions. Similar to the case of Dirichlet boundary conditions a modified finite-size scaling hypothesis is necessary to get the appropriate scaling behaviour.

7. Neumann–Dirichlet boundary conditions

7.1. Equation for the spherical field

To extract the finite-size effects from (2.8) in the case of mixed boundary conditions i.e. Neumann and Dirichlet on the bounding surfaces, the sum to be considered is

$$\begin{aligned} \mathcal{S}_{d,L}^{(DN)}(\phi) &= \sum_{n=1}^{L} W_{d-1}\left[\phi + 2\cos\frac{\pi}{2L+1} - 2\cos\frac{2\pi\left(n-\frac{1}{2}\right)}{2L+1}\right] \\ &= \frac{1}{2}\sum_{n=0}^{2L} W_{d-1}\left[\phi + 2\cos\frac{\pi}{2L+1} - 2\cos\frac{2\pi\left(n+\frac{1}{2}\right)}{2L+1}\right] \\ &\quad - \frac{1}{2}W_{d-1}\left[\phi + 2\cos\frac{\pi}{2L+1} + 2\right]. \end{aligned} \qquad (7.1)$$

By inspection of the sum in the second line we see that the analysis of this case is tightly related to that of antiperiodic boundary conditions. In other words this sum is exactly $S_{d,2L+1}^{(a)}\left(\phi + \omega_0^{(ND)}\right)$ with $S_{d,2L+1}^{(a)}(\sigma)$ defined in (4.2*a*) meaning that in this case the finite-size corrections correspond to a film of thickness $2L + 1$ subject to antiperiodic boundary conditions. Then, along lines similar to the analysis of section 4, for the equation for the spherical field we get, for arbitrary d,

$$K = W_d\left(\phi - \frac{\pi^2}{4L^2}\right) + \frac{1}{2L}\left[W_d\left(\phi - \frac{\pi^2}{4L^2}\right) - W_{d-1}\left(\phi - \frac{\pi^2}{4L^2} + 4\right)\right] + \frac{4}{(4\pi)^{d/2}}\left(\phi - \frac{\pi^2}{4L^2}\right)^{\frac{d}{2}-1} \sum_{k=1}^{\infty}(-1)^l \frac{K_{\frac{d}{2}-1}\left(2lL\sqrt{\phi - \frac{\pi^2}{4L^2}}\right)}{\left(lL\sqrt{\phi - \frac{\pi^2}{4L^2}}\right)^{\frac{d}{2}-1}} \qquad (7.2)$$

to the leading order in L^{-1}. As before we will restrict ourselves between the lower and the upper critical dimensions. For $2 < d < 4$, using (3.12), we have

$$\varkappa = \frac{\left(y^2 - \frac{\pi^2}{4}\right)^{\frac{d-2}{2}}}{(4\pi)^{d/2}}\left[\left|\Gamma\left[\frac{2-d}{2}\right]\right| - 4\sum_{l=1}^{\infty}(-1)^l \frac{K_{\frac{d}{2}-1}\left(2l\sqrt{y^2 - \frac{\pi^2}{4}}\right)}{\left(l\sqrt{y^2 - \frac{\pi^2}{4}}\right)^{\frac{d}{2}-1}}\right] - \frac{1}{2}L^{d-3}\left[K_{c,d} - W_{d-1}(4)\right]. \qquad (7.3)$$

With $y = L\sqrt{\phi}$ and $\varkappa = L^{1/\nu}(K_{c,d} - K)$. The solution of this equation depends *explicitly* on the size L which leads us to the conclusion that the standard finite-size scaling is violated here as well. To resolve this issue one would need a modified finite-size scaling assumption. This remains valid also for the corresponding finite-size shift of the critical temperature whose leading asymptotic behaviour is L^{-1}, rather than the predicted $L^{-1/\nu}$. Remark however that for $d = 3$ the term L^{d-3} vanishes and the finite-size scaling is expected to hold. Indeed, at $d = 3$, (7.3) turns into the simple form

$$4\pi\varkappa = \ln 2\cosh\sqrt{y^2 - \frac{\pi^2}{4}} - 2\pi[K_{c,3} - W_2(4)], \tag{7.4}$$

This equation is identical to equation (4.31) of Dantchev and Brankov (2003) obtained by a method adapted after Barber and Fisher (1973). The positive solution of (7.3) may be written in the scaling form

$$y = g_{(ND)}(\varkappa), \tag{7.5}$$

where the universal scaling function is given by

$$g_{(ND)}(\varkappa) = \left[\frac{\pi^2}{4} + \left(\operatorname{arccosh}\left[\frac{1}{2}\exp\left(4\pi\varkappa + 2\pi\left[K_{c,3} - W_2(4)\right]\right)\right]\right)^2\right]^{1/2}. \tag{7.6}$$

At the bulk critical temperature, $\varkappa = 0$, we find the critical amplitude

$$y_0 = g_{(ND)}(0) = 1.456\,84\ldots. \tag{7.7}$$

7.2. Free energy density

The free energy density from equation (2.6) in the case of Neumann–Dirichlet is obtained as a result of the analysis of the sum

$$\begin{aligned}\mathcal{P}_{d,L}^{(DN)}(\phi) &= \sum_{n=1}^{L} U_{d-1}\left[\phi + 2\cos\frac{\pi}{2L+1} - 2\cos\frac{2\pi\left(n-\frac{1}{2}\right)}{2L+1}\right] \\ &= \frac{1}{2}\sum_{n=0}^{2L} U_{d-1}\left[\phi + 2\cos\frac{\pi}{2L+1} - 2\cos\frac{2\pi\left(n+\frac{1}{2}\right)}{2L+1}\right] \\ &\quad - \frac{1}{2}U_{d-1}\left[\phi + 2\cos\frac{\pi}{2L+1} + 2\right].\end{aligned} \tag{7.8}$$

So apart from a surface term (the last term) the asymptotic form of the free energy has a similar expression to (4.4*a*) in the case of the antiperiodic boundary conditions with the replacements $\omega_0^{(a)} \to \omega_0^{(ND)}$ and $L \to 2L$ i.e.

$$\begin{aligned}\beta F_d^{(ND)}(T, L; \phi) &= \beta F_d\left(T; \phi + \omega_0^{(ND)}\right) + \frac{1}{L}\beta F_{d,\text{surf.}}^{(ND)}\left(\phi + \omega_0^{(ND)}\right) \\ &\quad - \frac{2}{(4\pi)^{d/2}}\left(\phi + \omega^{(ND)}\right)^{\frac{d}{2}}\sum_{l=1}^{\infty}(-1)^l\frac{K_{\frac{d}{2}}\left(2lL\sqrt{\phi + \omega_0^{(ND)}}\right)}{\left(lL\sqrt{\phi + \omega_0^{(ND)}}\right)^{\frac{d}{2}}},\end{aligned} \tag{7.9}$$

with the surface contribution

$$F_{d,\text{surf.}}^{(ND)}(\sigma) = \tfrac{1}{4}[U_d(\sigma) - U_{d-1}(\sigma + 4)]. \tag{7.10}$$

For $2 < d < 4$, the singular part of the free energy density follows also from that for antiperiodic boundary conditions (4.10) and the corrections originating from the surfaces. In this case we get

$$\beta f_{s,d}^{(ND)}(y,\varkappa) = \frac{1}{2}L^{-d}\varkappa\left(y^2-\frac{\pi^2}{4}\right) + \frac{1}{4}L^{-3}[K_{c,d}-W_{d-1}(4)]\left(y^2-\frac{\pi^2}{4}\right) + L^{-d}\frac{\left(y^2-\frac{\pi^2}{4}\right)^{\frac{d}{2}}}{(4\pi)^{d/2}}\left(\frac{1}{d}\Gamma\left[\frac{2-d}{2}\right] - 2\sum_{l=1}^{\infty}(-1)^l\frac{K_{\frac{d}{2}}\left(2l\sqrt{y^2-\frac{\pi^2}{4}}\right)}{\left(l\sqrt{y^2-\frac{\pi^2}{4}}\right)^{\frac{d}{2}}}\right). \quad (7.11)$$

Here again there is a term proportional to L^{d-3} that violates the standard finite-size scaling hypothesis (1.1) in the vicinity of $K_{c,d}$ and its modification is necessary to get the correct scaling. At $d = 3$ there is no explicit dependence in L. In this case, the critical amplitude of the singular part of the free energy density is obtained from (7.11). Thus the Casimir amplitude for the three-dimensional mean spherical film subject to Neumann–Dirichlet boundary conditions is

$$\Delta^{(ND)} = 0.019\,22\ldots. \quad (7.12)$$

This exact result is in conformity with that of Krech and Dietrich (1992) obtained using renormalization group. Similar to the case of antiperiodic boundary conditions the Casimir amplitude is positive but smaller in magnitude indicating a weaker repulsing force between the surfaces bounding the system.

8. Discussion

We investigated the finite-size effects in the d-dimensional ferromagnetic mean spherical model of finite thickness L subject to different kinds of boundary conditions: periodic (p), antiperiodic (a), Dirichlet (D) and Neumann (N) on both surfaces bounding the model, and a combination of Neumann and Dirichlet on each surface (ND). We proposed a method for the computation of the finite-size corrections of the free energy for arbitrary dimension. Our analysis showed that for Dirichlet and Neumann boundary conditions the finite-size effects are essentially equivalent to the case of periodic boundary conditions for a film of thickness $2L$ and additional surface terms. Similarly, the case of Neumann–Dirichlet was found to be related to the case of antiperiodic boundary conditions with thickness $2L$.

The free energy density and the equation for the spherical field were computed for a film with arbitrary dimension d subject to the different boundary conditions. In the particular case $d = 3$, our general expressions for (D), (N) and (ND) reduce to those obtained by Barber and Fisher (1973) and Danchev *et al* (1997), Dantchev and Brankov (2003). It is found that the singular part of the free energy density has the standard finite-size scaling form for $2 < d < 4$ only in the cases (p) and (a) i.e. for those boundary conditions which do not break the translation invariance of the model. In these cases we estimated the critical amplitude of the singular part of the free energy and obtained the values: $\Delta^{(p)} = -2\zeta(3)/(5\pi) = -0.153\,051\ldots$ and $\Delta^{(a)} = 0.274\,543\ldots$ for (p) and (a), respectively. Interpreted in terms of the Casimir effect this imply that in the case (p) we have fluctuation-induced attraction between the surfaces bounding the model and a repulsion in the case (a).

For a film subject to (D) or (N) the critical point of the film is shifted from the bulk one by surface and finite-size terms, whose leading asymptotic behaviour is proportional to L^{-1}. This result disagrees with the scaling behaviour of the finite-size shift predicted by the theory of finite-size scaling. In the vicinity of the bulk critical point the standard finite-size scaling is not valid in general. At $d = 3$, the solution of the equation for the spherical field is proportional to L^{-3} for (D) and to L^{-1} for (N), while the singular part of the free energy exhibits a logarithmic dependence on L. For $3 < d < 4$, the standard finite-size scaling for the singular part of the free energy needs to be modified.

In the case (ND), the film has its own critical point shifted from the bulk one by surface terms, as well as finite-size effects. The finite-size shift of the critical temperature and the scaling form of the free energy do not conform with the theory of finite-size scaling. For $2 < d < 4$, the standard finite-size scaling has to be modified in the neighbourhood of the bulk critical temperature. A surprising fact is that the finite-size scaling hypothesis is again valid at $d = 3$. At T_c, the square root of the equation for the spherical field is equal to $1.456\,84\ldots L^{-1}$ and the Casimir amplitude is found to be $\Delta^{(ND)} = 0.019\,22\ldots$ i.e. a weaker than the case (a) fluctuation-induced repulsion.

It is well known that the mean spherical model is not able to capture the gross features of $O(n)$ models when it is subject to boundary conditions that break the translational invariance. To solve this problem remaining in the framework of the spherical model one would introduce additional spherical fields to ensure the proper behaviour of the surface spins (Singh *et al* 1975). Otherwise one can try recovering the equivalence between the spherical model and $O(n)$ spin models by imposing spherical constraints ensuring the same mean square value for all spins of the system (Knops 1973). In the case of a film geometry this is equivalent to having a spherical constraint on each layer of the system with a space-dependent spherical field along the finite direction (Hikami and Abe 1976, Bray and Moore 1977, Ohno and Okabe 1983) whose relaxed version reduces to the model under consideration. Even in this case an accurate study of the problems related to finite-size scaling remains rather untractable analytically (see e.g. Hikami and Abe 1976, Brézin 1983).

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