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Surface critical exponents for a three-dimensional modified spherical model

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Abstract. A modified three-dimensional mean spherical model with a L-layer film geometry under Neumann–Neumann boundary conditions is considered. Two spherical fields are present in the model: a surface one fixes the mean square value of the spins at the boundaries at some $\rho > 0$, and a bulk one imposes the standard spherical constraint (the mean square value of the spins in the bulk equals 1). The surface susceptibility $\chi_{1,1}$ has been evaluated exactly. For $\rho = 1$ we find that $\chi_{1,1}$ is finite at the bulk critical temperature T_c, in contrast to the recently derived value of $\gamma_{1,1} = 1$ in the case of just one global spherical constraint. The result $\gamma_{1,1} = 1$ is only recovered if $\rho = \rho_c = 2 - (12K_c)^{-1}$, where K_c is the dimensionless critical coupling. When $\rho > \rho_c$, $\chi_{1,1}$ diverges exponentially as $T \to T_c^+$. An effective Hamiltonian is also proposed which leads to an exactly solvable model with $\gamma_{1,1} = 2$, the value for the $n \to \infty$ limit of the corresponding O(n) model.

1. Introduction

Recently [1] (hereafter referred to as I) the finite-size scaling behaviour of a three-dimensional system with a film geometry $L \times \infty^2$ was investigated within the mean spherical model with Neumann–Neumann and Neumann–Dirichlet boundary conditions and surface fields h_1 and h_L acting at the boundaries. The obtained results imply the well 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 (for a general review on surface critical phenomena see, for example [2–4], and for finite-size scaling [2, 5–7]). The conjecture has been made that the latter critical exponent corresponds to the special (surface-bulk) phase transition within the model. The last is in consistence with the general expectation for the finite-size scaling form of the free energy for this type of phase transitions if one assumes that the crossover exponent $\Phi = 0$, as it is for three-dimensional O(n) models [2]. It has also been derived that the critical exponent of the local surface susceptibility $\chi_{1,1}$ is $\gamma_{1,1}^{\rm sb} = 1$. The same result is known to hold for the spherical model with enhanced surface couplings under Dirichlet–Dirichlet boundary conditions [8]. Unfortunately, in the latter case the model quite unphysically predicts that the surface orders for a sufficiently large enhancement at some temperature above the bulk critical one even for $d = 3$. This is no more the case in the model improved by introducing a second spherical constraint on the spins at the boundaries [9], since the only critical point that remains for $d \leqslant 3$ is the bulk one. Then for $d = 3$ the exponent $\gamma_{1,1}^{\rm o} = -1$ corresponds to an ordinary phase transition [2, 10]. In I the case of equal bulk and surface couplings was considered and the question of if and how the surface behaviour of the system with Neumann–Neumann boundary conditions will change under additional spherical constraints on the spins at and near the surfaces was left open. One of the aims of this paper is to contribute to clarifying that point. To this end we consider the critical behaviour of the local surface susceptibility

$$\chi_{1,1}(T;\rho) = \lim_{L\to\infty}[-L\partial^2 f_L(T,h_1,h_L;\rho)/\partial h_1^2]_{|h_1=h_L=0} \tag{1.1}$$

in the case when the mean square value of the spins at the boundaries is fixed at some positive number ρ by an additional spherical constraint. The model defined in this way will be called the modified spherical model. In equation (1.1) and in the remainder, $f_L(T,h_1,h_L;\rho)$ denotes the free-energy density (per k_BT and per spin) of a three-dimensional hypercubic lattice system with a film geometry $L\times\infty^2$ at temperature T. Neumann–Neumann boundary conditions are imposed across the finite dimension of extent L. Surface fields h_1 and h_L are supposed to act at the surfaces bounding the system. Since we are interested in the case $h_1 = h_L$, only one additional constraint on the boundary spins is imposed. It turns out that the behaviour of $\chi_{1,1}$ in the vicinity of the bulk critical point T_c depends crucially on ρ . It will be shown that only if $\rho = \rho_c := 2 - (12K_c)^{-1} = 1.340\,53\ldots$ one obtains the previously found value $\gamma_{1,1} = \gamma_{1,1}^{\mathrm{sb}} = 1$. If $\rho < \rho_c$ then $\chi_{1,1}$ has the singularity characteristic of the spherical model with Dirichlet boundary conditions, i.e. $\gamma_{1,1} = \gamma_{1,1}^{\mathrm{o}} = -1$. When $\rho > \rho_c$, $\chi_{1,1}$ diverges exponentially as $T \to T_c^+$, which reminds us of the behaviour of a two-dimensional O(n), $n > 2$, model close to $T = 0$. The calculation of the mean square value ρ_s of the spins at a Neumann boundary in the standard spherical model elucidates the appearance of the critical value of $\rho = \rho_c$: it turns out that $\rho_c = \rho_s$. Moreover, we note that the second spherical field, to be denoted by v (see equation (2.1) below), can be considered as a free parameter. It will be shown that by changing it one interpolates continuously from Neumann, via mixed, to Dirichlet boundary conditions. Following I, under Neumann boundary conditions we mean here the case when the interaction of the finite system with the ‘environment’ is modelled by letting the spins surrounding the system take the same values as their nearest neighbour inside the system. Under Dirichlet boundary conditions this interaction is modelled by fixing the spin configuration outside the system to zero value. (For a precise mathematical definition of the boundary conditions see I.) The mixed boundary conditions then correspond to the situation when the spins surrounding the system are set to take values proportional (but not equal) to those of their nearest neighbour inside the system. Obviously, the above terminology is justified by analogy with the continuum limit. Note that for any v, just due to the symmetry which arises from the identical boundary conditions and fields ($h_1 = h_L$) at the opposite surfaces, the system models by itself an analogue of a Neumann boundary at the middle layers. Therefore, if one considers the local surface succeptibility $\chi_{l,l}$ for the lth layer, one would expect to obtain the critical exponent for the Neumann boundary, $\gamma_{l,l} = 1$, for l around the middle of the system. The last is obviously true even if the system is with otherwise Dirichlet boundary conditions. Finally, it will be shown that if v is a given function of the temperature, one obtains $\gamma_{1,1}^{\mathrm{sb}} = 2$, which is the corresponding value for the O(n) model in the limit $n \to \infty$.

As is well known, the infinite translational-invariant spherical model is equivalent to the $n \to \infty$ limit of a similar system of n -component vectors [11, 12]. However, the spherical model with surfaces (or, more generally, without translation-invariant symmetry) is in fact *not* such a limit [13] (for the results available for the spherical model see, for example [2, 5–7] and references therein). In other words, the spherical model under nonperiodic boundary conditions is not in the same surface universality class as the corresponding O(n) model in the limit $n \to \infty$, in contrast to the bulk universality classes. The last becomes apparent when one investigates surface phase transitions for an O(n) model in the limit $n \to \infty$. In that case one obtains [2] $\Delta_1 = 1/(d-2)$ (i.e. $\Delta_1 = 1$ for $d = 3$) for ordinary and $\Delta_1 = 2/(d-2)$ (i.e. $\Delta_1 = 2$ for $d = 3$) for special phase transitions. It is believed that the corresponding equivalence will be recovered if one imposes spherical constraints in a way which ensures that the mean square value of each spin of the system is the same [13] (unfortunately such a model is rather untractable). One of the aims of this paper is to see if, and up to what extent, the behaviour of the system with two spherical fields will be closer to the O(n) model in the limit $n \to \infty$, in comparison with the standard mean spherical model (with only one spherical field).

This paper is organized as follows. In section 2 we describe the model and present convenient starting expressions for the mean spherical constraints, the free-energy density and the local surface susceptibility. Our main results on the behaviour of $\chi_{1,1}$ and $\chi_{l,l}$ as a function on T and ρ are given in section 3. The paper closes with a short discussion given in section 4.

2. The model

We explicitly consider 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 domain $\Lambda \subset \mathbb{Z}^3$, $\Lambda = L_1 \times L_2 \times L_3$, containing $|\Lambda|$ sites, is given by

$$\beta\mathcal{H}_\Lambda^{(\tau)}(\sigma_\Lambda|K, h_\Lambda; s) = -K\sigma_\Lambda^\dagger \cdot Q_\Lambda^{(\tau)} \cdot \sigma_\Lambda + s\sigma_\Lambda^\dagger \cdot \sigma_\Lambda + v\sigma_s^\dagger \cdot \sigma_s - h_\Lambda^\dagger \cdot \sigma_\Lambda. \tag{2.1}$$

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

$$Q_\Lambda^{(\tau)} = (\Delta_1^{(\tau_1)} + 2E_1) \times (\Delta_2^{(\tau_2)} + 2E_2) \times (\Delta_3^{(\tau_3)} + 2E_3) \tag{2.2}$$

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. In equation (2.1) $\beta = 1/k_B T$ is the inverse temperature; $K = \beta J$ is the dimensionless coupling constant; $h_\Lambda = \{h(\boldsymbol{r}), \boldsymbol{r} \in \Lambda\}$, with $h(\boldsymbol{r}) \in \mathbb{R}$, which is an external magnetic field; and s and v are the spherical fields which are to be determined from the mean spherical constraints (see below); $\sigma_s = \{\sigma(\boldsymbol{r}), \boldsymbol{r} \in S\}$, $S = \{(r_1, r_2, 1) \cup (r_1, r_2, L_3)\}$, $r_1 = 1, \ldots, L_1$, $r_2 = 1, \ldots, L_2$.

The free-energy density of the modified mean spherical model in a finite region Λ is given by the Legendre transformation

$$\beta f_\Lambda^{(\tau)}(K, h_\Lambda; \rho) := \sup_{s,v}\{-|\Lambda|^{-1} \ln Z_\Lambda^{(\tau)}(K, h_\Lambda; s, v) - s - \rho v|S|/|\Lambda|\} \tag{2.3}$$

where $|S|$ is the total number of spins at the boundaries S and

$$Z_\Lambda^{(\tau)}(K, h_\Lambda; s, v) = \int_{\mathbb{R}^{|\Lambda|}} \exp[-\beta\mathcal{H}_\Lambda^{(\tau)}(\sigma_\Lambda|K, h_\Lambda; s, v)] \prod_{\boldsymbol{r}\in\Lambda} \mathrm{d}\sigma(\boldsymbol{r}) \tag{2.4}$$

is the partition function. The supremum is attained at the solutions of the mean spherical constraints

$$\langle\sigma_\Lambda^\dagger \cdot \sigma_\Lambda\rangle = |\Lambda| \tag{2.5}$$

and

$$\langle\sigma_s^\dagger \cdot \sigma_s\rangle = \rho|S| \tag{2.6}$$

where $\langle\cdots\rangle$ denotes expectation value with respect to the Hamiltonian $\beta\mathcal{H}_\Lambda^{(\tau)}(\sigma_\Lambda|K, h_\Lambda; s)$. Let us denote by $-2 + 2\cos\varphi_{L_i}^{\tau_i}(k_i)$, $k_i = 1, \ldots, L_i$, $i = 1, 2, 3$, the eigenvalues of the matrix $\Delta_i^{(\tau_i)}$. Let us further suppose, say, periodic boundary conditions across L_1 and L_2

and Neumann–Neumann boundary conditions across L_3. Then, by direct evaluation of the integrals in the partition function (2.4), after taking the limit $L_1, L_2 \to \infty$ at a fixed $L_3 = L$, one obtains for the free energy

$$\beta f_L^{(n)}(K, h_1, h_L; \rho) = \frac{1}{2}\log\frac{K}{\pi} - 6K + \sup_{\phi,\omega}\left\{\frac{1}{L}\frac{1}{8\pi^2}\int_0^{2\pi}\mathrm{d}\theta_1\int_0^{2\pi}\mathrm{d}\theta_2\sum_{k=1}^{L}\log[\phi + 2\sum_{i=1}^{2}(1-\cos\theta_i) + 2[1-\cos\varphi_L^n(k;\omega)] - \frac{1}{4KL}\sum_{k=1}^{L}\frac{\left|h_L^{(n)}(k;\omega)\right|^2}{\phi + 2[1-\cos\varphi_L^n(k;\omega)]} - K\left(\phi + \frac{2}{L}\rho\omega\right)\right\}. \tag{2.7}$$

Here $-2 + 2\cos\varphi_L^n(k;\omega)$, $k = 1, \ldots, L$ are the eigenvalues of the matrix

$$\Delta_L^{(n)}(\omega) = \Delta_L^{(n)} - \omega(\delta_{1,1} + \delta_{L,L}) \tag{2.8}$$

and

$$h_L^{(n)}(k;\omega) = h_1 u_L^n(1, k;\omega) + h_L u_L^n(L, k;\omega) \tag{2.9}$$

where $\{u_L^n(r, k;\omega), r = 1, \ldots, L\}$, $k = 1, \ldots, L$ are its eigenvectors; the superscript n stays there for Neumann–Neumann boundary conditions. In equations (2.7)–(2.9) the following definitions have been used

$$\phi = s/K - 6 \tag{2.10}$$

$$\omega = v/K. \tag{2.11}$$

From the requirement for the existence of the partition function one has the constraint

$$\phi + 2\min_{k=1,\ldots,L}[1-\cos\varphi_L^n(k;\omega)] > 0. \tag{2.12}$$

The eigenvalues and the eigenvectors of the matrix $\Delta_L^{(n)}(\omega)$ can be obtained in a way similar to the one used in [9, 14]. The results are:

(i) for given L and ω, when $|1-\omega| \neq 1$, the numbers $\varphi_L^n(k;\omega)$, $k = 1, \ldots, L$ are the L roots of the equations

$$1 - \omega = \frac{\sin[\frac{1}{2}(L+1)\varphi]}{\sin[\frac{1}{2}(L-1)\varphi]} \tag{2.13}$$

and

$$1 - \omega = \frac{\cos[\frac{1}{2}(L+1)\varphi]}{\cos[\frac{1}{2}(L-1)\varphi]} \tag{2.14}$$

with $0 < \mathrm{Re}(\varphi) < \pi$ and $\mathrm{Im}(\varphi) > 0$. For concreteness and simplification of the notations below, without loss of generality in the final results, we assume L to be an odd integer. Then, it is easy to see that equation (2.13) possesses $(L-1)/2$ solutions of the specified type, whereas equation (2.14) gives the remaining $(L+1)/2$ solutions. From (2.13) and (2.14) one obtains that (for fixed L and k)

$$\frac{\mathrm{d}\varphi}{\mathrm{d}\omega} = \frac{1}{L}\frac{2\sin\varphi}{(1-\omega)^2 - 2(1-\omega)\cos\varphi + 1 + L^{-1}[1-(1-\omega)^2]}. \tag{2.15}$$

Further, if $|1-\omega| < 1$ all the L roots are real. In that case there is only one root of equation (2.13) per interval $(2\pi k/(L-1), 2\pi(k+1)/(L-1))$, $k = 0, \ldots, (L-3)/2$.

Similarly, equation (2.14) only has one root per interval $(\pi(2k-1)/(L-1), \pi(2k+1)/(L-1))$, $k=1,\ldots,(L-3)/2$, and one root in each of the intervals $(0,\pi/(L-1))$ and $(\pi-\pi/(L-1),\pi)$. Let us now consider the case $|1-\omega|>1$. Then, if $\omega<0$, one again only has one root of equation (2.13) per interval $(2\pi k/(L-1), 2\pi(k+1)/(L-1))$, $k=1,\ldots,(L-3)/2$, and, similarly, one root of equation (2.14) per interval $(\pi(2k-1)/(L-1), \pi(2k+1)/(L-1))$, $k=1,\ldots,(L-3)/2$, and one root in $(\pi-\pi/(L-1),\pi)$, i.e. altogether $L-2$ real roots in the interval $(0,\pi)$. The two remaining roots are given by

$$\varphi_0 = \mathrm{i}\log(1-\omega) \pm \mathrm{O}((1-\omega)^{-(L-1)}). \tag{2.16}$$

(Strictly speaking the roots are only degenerate up to exponentially small corrections.) In the case $\omega>2$ one again has $L-2$ real roots in the interval $(0,\pi)$ and the remaining two roots are then given by $\varphi_0 = \pi + \mathrm{i}\log(\omega-1) \pm \mathrm{O}((\omega-1)^{-(L-1)})$.

(ii) The components of the eigenvectors $\{u^n_{_L}(r,k;\omega), r=1,\ldots,L\}$, $k=1,\ldots,L$ of the matrix $\Delta^{(n)}_L(\omega)$ are given by the expression ($|1-\omega|\neq 1$)

$$u^n_{_L}(r,k;\omega) = \sqrt{\frac{2}{L}}\,\frac{\sin[r\varphi^n_L(k;\omega)] - (1-\omega)\sin[(r-1)\varphi^n_L(k;\omega)]}{\{(1-\omega)^2 - 2(1-\omega)\cos\varphi^n_L(k;\omega) + 1 + L^{-1}[1-(1-\omega)^2]\}^{1/2}}. \tag{2.17}$$

(iii) For completeness we also give the results for the well known case $|1-\omega|=1$ (see, e.g, I, [14]). Then $\varphi^n_L(k;0) = \pi(k-1)/L$, $\varphi^n_L(k;2) = \pi k/L$, $k=1,\ldots,L$, and the components of the eigenvectors are $u^n_{_L}(r,k;0) = \sqrt{(2-\delta_{k,1})/L}\cos[(r-1/2)\varphi^n_L(k;0)]$ and $u^n_{_L}(r,k;2) = \sqrt{2/L}\sin[(r-\frac{1}{2})\varphi^n_L(k;2)]$, respectively.

Finally, we remind ourselves that we are mainly interested in the behaviour of the local surface susceptibility for which we obtain from equations (1.1) and (2.7)

$$\chi_{1,1}(T;\rho) = \frac{1}{2K}\lim_{L\to\infty}\sum_{k=1}^{L}\frac{|u^n_L(1,k;\omega)|^2}{\phi + 2[1-\cos\varphi^n_L(k;\omega)]}. \tag{2.18}$$

If, instead of the local susceptibility at the surface of the system, one is interested in the local susceptibility of the lth layer, $\chi_{l,l}(T;\rho)$, the corresponding result reads

$$\chi_{l,l}(T;\rho) = \frac{1}{2K}\lim_{L\to\infty}\sum_{k=1}^{L}\frac{|u^n_L(l,k;\omega)|^2}{\phi + 2[1-\cos\varphi^n_L(k;\omega)]}. \tag{2.19}$$

The above expression can be obtained in a way analogous to the derivation of $\chi_{1,1}$ by imposing a local magnetic field h_l on the spins in the lth layer.

To determine the behaviour of the spherical fields ϕ and ω one has to analyse equations (2.5) and (2.6). From (2.3), (2.7), (2.10), (2.11) and (2.15) one explicitly obtains the set of equations

$$2K = \frac{1}{4\pi^2}\int_0^{2\pi}\mathrm{d}\theta_1\int_0^{2\pi}\mathrm{d}\theta_2\,\frac{1}{L}\sum_{k=1}^{L}\left\{\phi + 2\sum_{i=1}^{2}(1-\cos\theta_i) + 2[1-\cos\varphi^n_L(k;\omega)]\right\}^{-1} \tag{2.20}$$

and

$$\begin{aligned}2K\rho = {} & \frac{1}{4\pi^2}\int_0^{2\pi}\mathrm{d}\theta_1\int_0^{2\pi}\mathrm{d}\theta_2\,\frac{1}{L}\sum_{k=1}^{L}2\sin^2\varphi^n_L(k;\omega)\\ & \times\left\{\phi + 2\sum_{i=1}^{2}(1-\cos\theta_i) + 2[1-\cos\varphi^n_L(k;\omega)]\right\}^{-1}\\ & \times\{(1-\omega)^2 - 2(1-\omega)\cos\varphi^n_L(k;\omega) + 1 + L^{-1}[1-(1-\omega)^2]\}^{-1}.\end{aligned} \tag{2.21}$$

These equations determine the point at which the finite-size free energy density (2.7), which is an analytical and strictly concave function of ϕ and ω in the domain given by inequality (2.12), reaches its global maximum. Clearly, in the thermodynamic limit the free-energy density is independant of the surface spherical field ω. As is well known, for all $K \geqslant K_c$ its supremum sticks to the endpoint $\phi_0 = 0$ of the allowed interval $\phi_0 > 0$, where the bulk free-energy density is finite. When $K < K_c$, the supremum is attained at a point $\phi_0 = \phi_0(K) > 0$, which satisfies the limit form of equation (2.20) [17],

$$2K = W_3(\phi_0) \tag{2.22}$$

where

$$W_d(\phi) = \frac{1}{\pi^d}\int_0^\pi \mathrm{d}\theta_1 \cdots \int_0^\pi \mathrm{d}\theta_d \left[\phi + 2\sum_{i=1}^{d}(1-\cos\theta_i)\right]^{-1} \tag{2.23}$$

is the d-dimensional Watson integral, $W_d(0) = 2K_c$. In general, the solutions ϕ and ω of equations (2.20) and (2.21) can be written in the form $\phi = \phi_0 + \Delta\phi$, $\omega = \omega_0 + \Delta\omega$, where $\Delta\phi$ and $\Delta\omega$ tend to zero when $L \to \infty$, and ϕ_0 and ω_0 are solutions of the corresponding equations where the limit $L \to \infty$ is taken.

Equations (2.16)–(2.23) provide the basis for our further analysis. Before passing to it we note that, instead of considering ω as a variable that has to be determined from equations (2.20) and (2.21), one can consider it as an additional free parameter. Then, from equation (2.8) it is clear that $\omega = 0$ yields the standard spherical model with Neumann–Neumann boundary conditions, whereas $\omega = 1$ yields the same model under Dirichlet–Dirichlet boundary conditions. When $0 < \omega < 1$ we have mixed (or 'intermediate' [15]) boundary conditions which interpolate between the above two extreme cases. Therefore, in this way one should reproduce the previously known results for the properties of the local susceptibilities. In addition, as we shall later see, by choosing ω to be a given function of the temperature, one can define an effective spherical model with $\gamma_{1,1} = 2$, which corresponds to the critical exponent for the surface-bulk phase transition within the $\mathrm{O}(n)$ model in the limit $n \to \infty$.

3. Critical behaviour of the local susceptibilities

Here we study the critical behaviour of the local susceptibilities $\chi_{1,1}$ and $\chi_{l,l}$ for l close to the middle of the system.

From equations (2.18) and (2.17) we obtain for the surface susceptibility

$$\chi_{1,1}(T;\rho) = \frac{1}{K}\lim_{L\to\infty}\frac{1}{L}\sum_{k=1}^{L}\frac{\sin^2\varphi_L^n(k;\omega)}{\phi + 2[1-\cos\varphi_L^n(k;\omega)]}$$
$$\times[1 - 2(1-\omega)\cos\varphi_L^n(k;\omega) + (1-\omega)^2 + [1-(1-\omega)^2]/L]^{-1} \tag{3.1}$$

where the limit $L \to \infty$ in (3.1) is to be taken over the finite-size solutions ω and ϕ of equations (2.20) and (2.21). If $|1-\omega| < 1$, from the properties of $\varphi_L^n(k;\omega)$, $k = 1, \ldots, L$, described in section 2, it follows that as $L \to \infty$ the sum in equation (3.1) tends to the corresponding well defined integral

$$\chi_{1,1}(T;\rho) = \frac{1}{K}\frac{1}{\pi}\int_0^\pi \frac{\sin^2\varphi}{[\phi_0 + 2(1-\cos\varphi)][1 - 2(1-\omega_0)\cos\varphi + (1-\omega_0)^2]}\,\mathrm{d}\varphi. \tag{3.2}$$

The integral can be taken exactly [16] with the result

$$\chi_{1,1}(T;\rho) = \frac{1}{K}\frac{1}{\sqrt{\phi_0(4+\phi_0)} + \phi_0 + 2\omega_0}. \tag{3.3}$$

When $|1-\omega| > 1$ one has to take into account the contribution of the two complex roots which turns out to be of the same order as the contribution of all other roots. The contribution of the latter $L-2$ roots is again given by the integral on the right-hand side of equation (3.2). Performing the calculations one obtains the same analytical expression for $\chi_{1,1}(T;\rho)$ as the one given by equation (3.3).

The surface spherical field ω_0 satisfies the corresponding limit form of the spherical constraint (2.21) at fixed $\phi_0 = 0$ for $K \geqslant K_c$, and $\phi_0 = \phi_0(K)$ for $K < K_c$. The right-hand side of this equation can be treated in a way similar to that for (3.1). When $|1-\omega| < 1$, due to the properties of the roots $\varphi_L^n(k;\omega)$, $k = 1, \ldots, L$, the sum in (2.21) converges as $L \to \infty$ to the corresponding well defined integral, which can be taken exactly. Performing this procedure, one finally obtains

$$2K\rho = G_3(\phi_0, \omega_0) \tag{3.4}$$

where

$$G_d(\phi,\omega) = \frac{2}{\pi^d}\int_0^\pi \mathrm{d}\theta_1 \cdots \int_0^\pi \mathrm{d}\theta_{d-1} \left\{ \phi + 2\omega + 2\sum_{i=1}^{d-1}(1-\cos\theta_i) + \left[\phi + 2\sum_{i=1}^{d-1}(1-\cos\theta_i)\right]^{1/2}\left[\phi + 4 + 2\sum_{i=1}^{d-1}(1-\cos\theta_i)\right]^{1/2}\right\}^{-1}. \tag{3.5}$$

When $|1-\omega| > 1$, one has to treat the contribution from the two complex roots separately. The contribution from the $L-2$ real roots again leads to a well defined integral that can be taken exactly. As for $\chi_{1,1}(T;\rho)$, the final result is given by the same analytical expression as in the case $|1-\omega| < 1$, i.e. equation (3.4) is actually valid for all ω_0 (the restrictions on ω_0 and ϕ_0 stemming from the constraint (2.12) are stated below).

Let us denote by $G_3^+(\phi,\omega)$ the branch of the function $G_3(\phi,\omega)$ defined for $\omega \geqslant 0$ and by $G_3^-(\phi,\omega)$ the one for $\omega < 0$. Then, by means of identical transformations it is easy to show that

$$G_3^-(\phi,\omega) = (1-\omega)^{-2} G_3^+\left(\phi, \frac{|\omega|}{1-\omega}\right) - \frac{\omega(2-\omega)}{(1-\omega)^2} W_2\left(\phi - \frac{\omega^2}{1-\omega}\right) \tag{3.6}$$

and

$$G_3^+(\phi,\omega) = (1-\omega)^{-1}[2W_3(\phi) - \tfrac{1}{6} + \tfrac{1}{6}\phi W_3(\phi)] - \frac{\omega}{(1-\omega)(2-\omega)}\frac{2}{\pi^2}\int_0^\pi \mathrm{d}\theta_1 \int_0^\pi \mathrm{d}\theta_2 \left\{ \phi + 2\sum_{i=1}^{2}(1-\cos\theta_i) + \frac{\omega}{2-\omega}\left[\phi + 2\sum_{i=1}^{2}(1-\cos\theta_i)\right]^{1/2}\left[\phi + 4 + 2\sum_{i=1}^{2}(1-\cos\theta_i)\right]^{1/2}\right\}^{-1}. \tag{3.7}$$

Finally, in the limit $L \to \infty$, constraint (2.12) for the existence of the partition function yields the allowed domain of values of the spherical fields,

$$\phi_0 \geqslant \begin{cases} 0 & \text{if } \omega_0 \geqslant 0 \\ \omega_0^2/\ (1-\omega_0) & \text{if } \omega_0 \leqslant 0. \end{cases} \tag{3.8}$$

From equation (3.3) it follows that the above inequalities imply $\chi_{1,1}(T;\rho) \geqslant 0$, as it should be expected on general physical grounds.

As it is evident from equation (3.5), $G_3(\phi,\omega)$ is a monotonically decreasing function of ω which tends to zero from above as $\omega \to +\infty$. Due to inequalities (3.8), at $\phi = 0$ we have to consider it on the half-line $\omega \geqslant 0$, where it is bounded from above by its value at $\omega = 0$, see equation (3.7),

$$G_3(0,0) = 4K_c - \tfrac{1}{6} := 2K_c\rho_c. \tag{3.9}$$

On the other hand, if $\phi > 0$, the definition domain of $G_3(\phi,\omega)$ is restricted by (3.8) to the half-line $\omega \geqslant \omega_1(\phi)$, where

$$\omega_1(\phi) = -(\phi + \phi^2/4)^{1/2} - \phi/2. \tag{3.10}$$

From representation (3.6) and the known expansion of $W_2(x)$ as $x \downarrow 0$,

$$W_2(x) = (4\pi)^{-1}\ln x^{-1} + \mathrm{O}(1) \tag{3.11}$$

it follows that $G_3(\phi,\omega)$ diverges logarithmically to $+\infty$ as $\omega \downarrow \omega_1(\phi)$.

Before passing to the analysis of the above equations, in order to determine the behaviour of $\chi_{1,1}(T;\rho)$, let us first consider the simpler case of ω as a free parameter. Then, for Neumann–Neumann boundary conditions one has (see equations (2.2) and (2.8)) $\omega = 0$, whereas one has $\omega = 1$ for Dirichlet–Dirichlet boundary conditions. Thus, from (3.3) and the well known behaviour of ϕ_0 in the vicinity of the bulk critical temperature $\phi_0 \simeq [8\pi(K_c - K)]^2$ [17], one immediately obtains all previously known results for the critical behaviour of the local surface susceptibility [1, 10]:

(a) Neumann–Neumann boundary conditions ($\omega = 0$; the result given below follows directly from equation (3.5) in [1] for $h_1 = h_L$)

$$\chi_{1,1}(T) = (2K)^{-1}\{\phi_0/2 + [\phi_0(1+\phi_0/4)]^{1/2}\}^{-1} \tag{3.12}$$

i.e. $\gamma_{1,1} = 1$.

(b) Dirichlet–Dirichlet boundary conditions ($\omega = 1$; see equation (61) in [10])

$$\chi_{1,1}(T) = (2K)^{-1}\{1 + \phi_0/2 + [\phi_0(1+\phi_0/4)]^{1/2}\}^{-1} \tag{3.13}$$

i.e. $\gamma_{1,1} = -1$.

For $\omega \neq 0, 1$ one has the case of the so-called intermediate [15] boundary conditions. As it is clear from (3.3), $\chi_{1,1}$ diverges in the vicinity of $T = T_c$ if and only if $\omega = 0$, i.e. under Neumann–Neumann boundary conditions.

Let us now comment on the critical value ρ_c of the parameter ρ, defined in equation (3.9). By using a translation invariance argument, for the mean square length of the spins at the Newmann boundary of the standard spherical model with one global spherical field ϕ one obtains in zero magnetic field

$$\langle\sigma^2(r_1,r_2,1)\rangle = \frac{1}{2KL_1L_2} \times \sum_{k_1,k_2,k_3=1}^{L} \frac{|u_L^n(1,k_3;0)|^2}{\phi + 2\sum_{i=1}^{2}[1-\cos(2\pi k_i/L_i)] + 2[1-\cos(\pi(k_3-1)/L_3)]}. \tag{3.14}$$

In the limit of an infinite film geometry this equation yields ($L_3 = L$ is kept finite)

$$\lim_{L_1,L_2\to\infty}\langle\sigma^2(r_1,r_2,1)\rangle = \frac{1}{K}[W_3(\phi) - \tfrac{1}{12} + \phi W_3(\phi)/12 + W_2(\phi)/2L]. \tag{3.15}$$

Hence, at the critical point $K = K_c$ of the infinite system ($L = \infty$), by taking into account the bulk spherical constraint at $\phi_0 = 0$, namely $W_3(0) = 2K_c$, one obtains that the mean square length ρ_s of the spins at the Neumann boundary of the standard spherical model equals precisely the critical value ρ_c for the surface spins in the modified spherical model.

Finally, we note that by taking

$$\omega = -8\pi(K_c - K) \tag{3.16}$$

one obtains for the considered system with layer geometry and Neumann–Neumann boundary conditions $\gamma_{1,1} = 2$, which is the corresponding critical exponent for the O(n) models in the limit $n \to \infty$. In that case $\gamma'_{1,1}$ also exists, and $\gamma'_{1,1} = 1$. Obviously, such a choice of ω defines an effective Hamiltonian that leads to an exactly solvable model with the critical exponents stated above.

Now we pass to the analysis of the behaviour of $\chi_{1,1}(T;\rho)$ given by equation (3.3) where ω_0 is determined as a function of K and ρ from equation (3.4).

3.1. Critical behaviour of the local surface susceptibility

Here we confine our analysis to the surface critical regimes that emerge on approaching the bulk critical temperature from above, i.e. when $K = K_c + \Delta K$, where $\Delta K < 0$ and $|\Delta K| \to 0$. Then, as it is well known, the leading asymptotic form of the bulk spherical field follows from the asymptotic expansion

$$W_3(\phi) = 2K_c - (4\pi)^{-1}\phi^{1/2} + \mathrm{O}(\phi) \qquad \phi \downarrow 0 \tag{3.17}$$

and reads [10]

$$\phi = 64\pi^2|\Delta K|^2 \qquad \Delta K \uparrow 0. \tag{3.18}$$

From expression (3.3) it is clear that the local surface susceptibility may exhibit divergent behaviour in two different regimes: (a) when $\omega_0 \downarrow 0$, and (b) when $\omega_0 \downarrow \omega_1(\phi) \uparrow 0$. As it is clear from equation (3.4) and the above-mentioned properties of the function $G_3(\phi,\omega)$, the first regime may only occur when $K\rho \uparrow K_c\rho_c$, which, in view of our assumption $\Delta K \uparrow 0$, requires $\rho = \rho_c$. The second divergent regime of the local surface susceptibility takes place at any fixed $\rho > \rho_c$. Below we derive the leading-order asymptotic solutions for ω_0 in each of the two cases.

Case (a): $\rho = \rho_c$. To obtain an asymptotic expansion of $G_3(\phi,\omega)$ in both arguments $\phi \downarrow 0$ and $\omega \downarrow 0$, we notice that the integral on the right-hand side of equation (3.7) diverges at $\phi = \omega = 0$ and the divergence arises from the integration over the neighbourhood of the point $\theta_1 = \theta_2 = 0$. Therefore, its leading-order asymptotic behaviour is given by the small argument expansion of the trigonometric functions which yields

$$G_3^+(\phi,\omega) = 2K_c\rho_c - (2\pi)^{-1}\phi^{1/2} + (\omega/2\pi)\ln(\phi^{1/2}+\omega) + \mathrm{O}(\phi) + \mathrm{O}(\omega). \tag{3.19}$$

By setting $\rho = \rho_c$, we obtain that $\omega_0 \downarrow 0$ obeys the asymptotic equation ($\Delta K \uparrow 0$)

$$-(\omega_0/2\pi)\ln(8\pi|\Delta K| + \omega_0) = |\Delta K|/(6K_c). \tag{3.20}$$

The solution which tends to zero from above as $|\Delta K| \to 0$ is

$$\omega_0 \simeq -\frac{\pi|\Delta K|}{3K_c\ln(8\pi|\Delta K|)}. \tag{3.21}$$

Obviously, this critical regime leads to $\gamma_{1,1} = 1$.

Case (b): $\rho > \rho_c$. The asymptotic behaviour of $G_3(\phi,\omega)$ as $\phi \downarrow 0$ and $\omega \uparrow 0$, so that $\omega > \omega_1(\phi)$, is readily obtained from the exact representation (3.6) and expansions (3.11) and (3.19):

$$G_3^-(\phi,\omega) = 2K_c\rho_c - (2\pi)^{-1}\phi^{1/2} - (|\omega|/2\pi)\ln(\phi^{1/2} - |\omega|) + \mathrm{O}(\phi) + \mathrm{O}(\omega). \tag{3.22}$$

At fixed $\Delta\rho > 0$ the leading-order equation for the surface spherical field becomes

$$-(|\omega_0|/2\pi)\ln(8\pi|\Delta K| - |\omega_0|) = 2K_c\Delta\rho. \tag{3.23}$$

Assuming $|\omega_0| = 8\pi|\Delta K| - x$, where $x = \mathrm{o}(|\Delta K|)$, one obtains

$$\omega_0 \simeq -8\pi|\Delta K| + \exp\left(-\frac{K_c\Delta\rho}{2|\Delta K|}\right). \tag{3.24}$$

Therefore, in this critical regime the local surface susceptibility diverges exponentially as the bulk critical temperature is approached from above:

$$\chi_{1,1}(T;\rho) \simeq \frac{1}{2K}\exp\left(\frac{K_c\Delta\rho}{2|\Delta K|}\right). \tag{3.25}$$

This behaviour reminds us of the one of a two-dimensional system close to $T = 0$. The fact that the surface is coupled to an infinite three-dimensional system is reflected in the replacement of $T = 0$ by the bulk critical temperature $T = T_c$.

Finally, if $\rho < \rho_c$ it is easy to see that (3.4) has a finite solution $\omega_0(\rho, K)$, where $0 < \omega_0 < 1$, when $\Delta K \uparrow 0$. The last actually follows from the inequalities

$$G_3(0,\phi) > W_3(\phi) > G_3(1,\phi). \tag{3.26}$$

Thus, if $\rho = 1$ the local surface susceptibility, $\chi_{1,1}(T_c; 1)$ is finite.

3.2. Critical behaviour of the local susceptibility around the middle of the system

For the local susceptibility $\chi_{l,l}(T;\rho)$ from (2.17) and (2.19) one explicitly obtains

$$\chi_{l,l}(T;\rho) = \frac{1}{K}\lim_{L\to\infty}\frac{1}{L}\sum_{k=1}^{L}\frac{\{\sin[l\varphi_L^n(k;\omega)] - (1-\omega)\sin[(l-1)\varphi_L^n(k;\omega)]\}^2}{\phi + 2[1-\cos\varphi_L^n(k;\omega)]}$$
$$\times\{1 - 2(1-\omega)\cos\varphi_L^n(k;\omega) + (1-\omega)^2 + [1-(1-\omega)^2]/L\}^{-1}. \tag{3.27}$$

We will only be interested in the behaviour of this quantity around the middle of the system. Let us set $l = (L+1)/2$. Then, from (3.27) it follows

$$\chi_{l,l}(T;\rho) = \frac{1}{K}\lim_{L\to\infty}\frac{1}{L}\sum_k[\phi + 2[1-\cos\varphi_L^n(k;\omega)]]^{-1}$$
$$\times\left\{1 - \frac{1-(1-\omega)^2}{L\left[1-2(1-\omega)\cos\varphi_L^n(k;\omega) + (1-\omega)^2\right] + 1 - (1-\omega)^2}\right\} \tag{3.28}$$

where the summation is only over the roots of equation (2.14). Having in mind the properties of the roots $\varphi_L^n(k;\omega)$, it is easy to see that in the limit $L \to \infty$ this equation leads to

$$\chi_{\infty,\infty}(T;\rho) = \frac{1}{2K}W_1(\phi_0) \tag{3.29}$$

for any ω. We recall now that considering ω as a free parameter, at $\omega = 0$ one has the standard spherical model under the Neumann–Neumann boundary condition and at $\omega = 1$ the corresponding one with Dirichlet–Dirichlet boundary conditions. The above result shows that the behaviour of $\chi_{\infty,\infty}(T;\rho)$ does not actually depend on the boundary conditions. From the temperature dependence of ϕ_0 around the bulk critical temperature $\phi_0 \simeq [8\pi(K_c - K)]^2$ [17] and the expansion of $W_1(\phi)$ for small values of the argument [17],

$$W_1(\phi) = \tfrac{1}{2}\phi^{-1/2} + \mathrm{O}(\phi^{1/2}) \tag{3.30}$$

we obtain $\gamma_{\infty,\infty} = 1$. It is clear that the same will be true for any layer at a finite distance from the middle of the system. The above result was derived in [10] for a spherical model under Dirichlet–Dirichlet boundary conditions (see equation (82) in [10]). Here we simply show that it does not depend on the boundary conditions if they are identical at both the boundaries: just due to the symmetry the system models by itself an analogue of the Neumann boundary at the middle layers.

4. Discussion

In this paper the surface critical behaviour of a modified three-dimensional mean spherical model with a L-layer film geometry under Neumann–Neumann boundary conditions is considered. The standard spherical model is modified in the sense that in addition to the usual bulk spherical constraint a second spherical field is included in the Hamiltonian to fix the mean square value of the spins at the boundaries at some value $\rho > 0$. We are mainly interested in the upper critical behaviour of the local susceptibilities $\chi_{1,1}$ and $\chi_{l,l}$ with l close to the middle of the system. The surface susceptibility $\chi_{1,1}$ and the local susceptibility $\chi_{\infty,\infty}$ are evaluated exactly and the corresponding results are given by equations (3.3) and (3.29), respectively.

It is shown that the behaviour of $\chi_{1,1}(T;\rho)$ depends crucially on ρ. At $\rho = 1$ we find that $\chi_{1,1}$ is finite at the bulk critical temperature T_c, in contrast to the recently derived value $\gamma_{1,1} = 1$ in the case of just one global spherical constraint. The result $\gamma_{1,1} = 1$ is only recovered if $\rho = \rho_c = 2 - (12K_c)^{-1}$, where K_c is the dimensionless critical coupling. When $\rho > \rho_c$, the local surface susceptibility $\chi_{1,1}$ diverges exponentially as $T \to T_c^+$, see equation (3.25). The calculation of the mean square value ρ_s of the spins at the Neumann boundary in the standard spherical model elucidates the appearance of the critical value of $\rho = \rho_c$: it turns out that at the bulk critical point $\rho_c = \rho_s$, see equation (3.15), at $K = K_c$, $\phi = 0$ and $L = \infty$. As it is expected, the behaviour of the local susceptibility $\chi_{\infty,\infty}$ turns out to be independent of the boundary conditions if they are the same at both boundaries. Just due to the symmetry, the system models by itself an analogue of the Neumann boundary at the middle layers which leads to $\gamma_{\infty,\infty} = 1$ (see section 3.2 for details). By considering the second spherical field as an independent free parameter, we rederive in a uniform way the previously known critical properties of the local surface susceptibility. They follow directly from equation (3.3) at $\omega = 0$, for Neumann–Neumann (see (3.12)), and $\omega = 1$, for Dirichlet–Dirichlet boundary conditions. For $\omega \neq 0, 1$ equation (3.3) gives the corresponding result for the so-called 'intermediate' [15] boundary conditions. From these results one concludes that $\chi_{1,1}$ diverges at $T = T_c$ only under Neumann boundary conditions. Finally, an effective Hamiltonian which leads to an exactly solvable model with $\gamma_{1,1} = 2$, the value for the $n \to \infty$ limit of the corresponding $O(n)$ model, is proposed. It is given by equation (2.1) where one has to set $v = -8\pi K(K_c - K)$, see (3.16).

We emphasize that the spherical model under nonperiodic boundary conditions is not in the same surface universality class as the corresponding $O(n)$ model in the limit $n \to \infty$, in contrast to the bulk universality classes. For example $\Delta_1^{o} = 1$ and $\Delta_1^{sb} = 2$ for the $O(\infty)$ model, but $\Delta_1^{o} = \frac{1}{2}$ and $\Delta_1^{sb} = \frac{3}{2}$ for the spherical model. The results presented above show that the properties of the model are improved by introducing a second spherical constraint in the sense that they are closer, in a certain way, to the corresponding ones for the $O(n)$, $n \to \infty$, model. It seems clear that in order to obtain 'correct' surface critical properties, one has to impose a separate spherical constraint on each layer parallel to the surface.

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