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New effects in the magnetization profile of the spherical model in a step-like field

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Abstract. The ferromagnetic mean spherical model with a layer geometry of thickness L and Neumann–Dirichlet boundary conditions is investigated in the presence of a step-like $(+-)$ external field which changes sign at distance Lx $(0 \leqslant x \leqslant 1)$ from the Neumann boundary. The amplitude of the field can be taken to vanish in the thermodynamic limit as an inverse power of L. Exact expressions for the magnetization profile are derived and studied in three different temperature and field regimes: high-temperature bulk limit, critical finite-size scaling regime, and low-temperature moderate-field regime. It is found that in the critical finite-size scaling regime there exist two special values of x, denoted by $x_{1,2}$, $0 < x_1 < x_2 < 1$, which depend on the scaled temperature and field variables, and have the property that the magnetization changes sign only when $x_1 < x < x_2$. The magnetization is everywhere negative when $0 \leqslant x < x_1$ and everywhere positive when $x_2 < x \leqslant 1$. In the low-temperature moderate-field regime we establish that the field-induced critical point, in the case of periodic boundary conditions and a step-like field with $x = \frac{1}{2}$, appears at $x = \frac{1}{3}$.

1. Introduction

This study is motivated by the general interest in the interface properties of various spin models. Interfaces between domains of opposite mean spin orientation can be induced by imposing inhomogeneous fields and/or appropriate boundary conditions on the opposite faces of a system with layer geometry of finite thickness L. Within the spherical model introduced by Berlin and Kac, Abraham and Robert [1] have shown that the interface is diffuse (i.e. a nontrivial magnetization profile exists only on the macroscopic scale L) at all temperatures. The interface has been created by means of a bulk step-like $(+-)$ field which changes sign at the central layer of a system with Dirichlet–Dirichlet boundary conditions in the finite dimension and periodic in all the other $d-1$ dimensions. Angelescu *et al* [2] have proved that the interface is diffuse also in the case of the generalized spherical model, in which the overall spherical constraint is replaced by a set of layer mean spherical constraints. The model has been treated under the simplifying assumtion of a Kac–Helfand in-layer interaction and the profile has been induced by oppositely directed boundary fields the absolute value of which was let to infinity at the end of the calculations.

Surface and layer critical behaviour in different versions of the mean spherical model has been studied in a number of works. Here we refer to the classical paper by Barber [3] and the recent work [4] on the standard mean spherical model. The model with enhanced surface exchange has been considered in [5], and its modification by the addition of a new spherical constraint on the boundary spins has been studied in [6] and the recent paper [7].

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The case of vanishing in the thermodynamic limit inhomogeneous field perturbations, at fixed temperature, has been treated in detail by Patrick [8], [9]. In [8] the setting of Abraham and Robert [1] has been generalized to amplitudes h_L of the step-like field which vanish as inverse powers of L as $L \to \infty$. A new field-induced critical point has been discovered in the low-temperature moderate-field regime, when $h_L = \mathrm{O}(L^{-2})$. At the new critical point the leading-order asymptotic form of the free energy is analytic and the next-to-leading correction to it has a singularity. The magnetization profile has been studied on different length scales and it has been found that in an appropriate regime below the new critical temperature there exists a nontrivial frozen (temperature independent) profile on the scale of L. The paper [9] offers a systematic approach to the study of the influence of surface fields on different statistical properties of the spherical model.

The behaviour of different thermodynamic functions of the spherical and mean spherical models under inhomogeneous external fields has been studied also in the critical finite-size scaling regime under periodic, antiperiodic, free, and fixed boundary conditions, see [3, 4, 10, 11]. Note that here we will use the terms Dirichlet and Neumann instead of fixed (or open) and free boundary conditions, respectively. In the case of Dirichlet–Neumann boundary conditions, see [4], a whole family of layer critical exponents was found when the layer field is applied at a properly scaled distance from the Dirichlet boundary.

We emphasize that all the results obtained for the magnetization profile agree upon its diffuseness which implies the general conclusion that the limit Gibbs states of the spherical model are translation invariant at arbitrary high dimensionality.

The analysis of the shape of the nontrivial magnetization profile on the macroscopic scale has lead to some important, at least within the spherical model, conclusions as well. The fact that in the bulk limit the magnetization profile near the Dirichlet boundary is exactly the same as the one near the central layer of zero magnetization has been interpreted in [1] as a physically interesting decoupling effect. A similar effect has been noticed in the critical finite-size scaling regime for the mean spherical model under periodic and Dirichlet–Dirichlet boundary conditions in [11]. However, in [12] it was shown that in the case of an even number of layers L the decoupling effects take place only asymptotically, on the scale of the large bulk correlation length close to the critical point. In general, it has been found that the decoupling hypothesis breaks down since the mean square length of the spins at the Dirichlet (Neumann) boundary is different from the one at the central layers of a system in a step-like (uniform) field. On the other hand, in the low-temperature moderate-field regime, when the temperature is fixed below the critical one, and $h_L = \mathrm{O}(L^{-2})$ as $L \to \infty$, the magnetization profile is finite (nonvanishing) and decouples exactly on the macroscopic scale L [12].

One of the aims of this study is to establish if the new, field-induced critical point found by Patrick [8, 9] persists under more general conditions: (i) different, Neumann–Dirichlet boundary conditions at the opposite boundaries of the layer, and (ii) a step-like $(+-)$ external field perturbation which changes sign at a general position Lx $(0 \leqslant x \leqslant 1)$ from the Neumann boundary. In the low-temperature moderate-field regime we establish that the field-induced critical point $\tilde{T}_c$, found by Patrick [8] in the case of periodic boundary conditions and a step-like field with $x = \frac{1}{2}$, appears at $x = \frac{1}{3}$. We find that in an appropriate field regime below $\tilde{T}_c$ the magnetization profile has both a frozen component, as in the case of [8], and a temperature-dependent background term, which is absent in the case of periodic boundary conditions. Moreover, we report on some new effects which emerge in the critical finite-size scaling regime: there exist two special values of x, denoted by x_1 and x_2, which depend on the scaled temperature and field variables, and have the property that the magnetization changes sign only when $x_1 < x < x_2$. The magnetization is everywhere negative when $0 \leqslant x < x_1$ and everywhere positive when $x_2 < x \leqslant 1$.

This paper is organized as follows. In section 2 we specify the notation used in the description of the mean spherical model with layer geometry, under Neumann–Dirichlet boundary conditions, and write down the basic expressions necessary for our further investigations. The asymptotic behaviour of the solution of the mean spherical constraint in three different temperature and field regimes is derived in section 3. The magnetization profile is analysed in section 4. The results are summarized and discussed in section 5.

2. Description of the model

Following [4], we 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 spin variable $\sigma(\boldsymbol{r}) \in \mathbb{R}$. The energy of a configuration $\sigma_\Lambda = \{\sigma(\boldsymbol{r}), \boldsymbol{r} \in \Lambda\}$ in a finite region $\Lambda \subset \mathbb{Z}^3$, containing $|\Lambda|$ sites, is given by

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

Here $\beta = 1/k_B T$ is the inverse temperature, $K = \beta J$ is the dimensionless coupling constant, $h_\Lambda = \{h(\boldsymbol{r}),\ \boldsymbol{r} \in \Lambda\}$, with $h(\boldsymbol{r}) \in \mathbb{R}$, is an external magnetic field, s is the spherical field which satisfies the mean spherical constraint, see equation (2.11) below, $Q_\Lambda(\boldsymbol{r}-\boldsymbol{r}')$, with $\boldsymbol{r}, \boldsymbol{r}' \in \mathbb{Z}^3$, is the adjacency matrix for the infinite cubic lattice: $Q_\Lambda(\boldsymbol{r}-\boldsymbol{r}') = 1$ if and only if $|\boldsymbol{r}-\boldsymbol{r}'| = 1$ and $Q_\Lambda(\boldsymbol{r}-\boldsymbol{r}') = 0$ otherwise. The first sum on the right-hand side of (2.1) describes the pairwise interaction between the spins in Λ, while the boundary conditions (denoted by the superscript τ) are taken into account by the second sum: it describes the interaction of the spins in Λ with a specified configuration $\{\sigma(\boldsymbol{r}), \boldsymbol{r} \in \Lambda^c\}$ in the complement $\Lambda^c = \mathbb{Z}^3 \setminus \Lambda$. Hereafter we take Λ to be the parallelepiped $\Lambda = \mathcal{L}_1 \times \mathcal{L}_2 \times \mathcal{L}_3$, with $\mathcal{L}_i = \{1, \ldots, L_i\}$, and explicitly study the case of a film geometry which results in the limit $L_2, L_3 \to \infty$ at finite values of $L_1 = L$. In the finite r_1 direction it suffices to specify the values of $\sigma(0, r_2, r_3)$ and $\sigma(L+1, r_2, r_3)$ for all $(r_2, r_3) \in \mathcal{L}_2 \times \mathcal{L}_3$. For given boundary conditions $\tau = (\tau_1, \tau_2, \tau_3)$, defined for each pair of opposite faces of Λ, the eigenfunctions of the interaction matrix in (2.1) have the form

$$u_\Lambda^{(\tau)}(\boldsymbol{r}, \boldsymbol{k}) = u_{L_1}^{(\tau_1)}(r_1, k_1)u_{L_2}^{(\tau_2)}(r_2, k_2)u_{L_3}^{(\tau_3)}(r_3, k_3) \qquad \boldsymbol{k} \in \Lambda \tag{2.2}$$

and the corresponding eigenvalues are

$$\mu_\Lambda^{(\tau)}(\boldsymbol{k}) = 2\sum_{\nu=1}^{3} \cos\varphi_{L_\nu}^{(\tau_\nu)}(k_\nu) \qquad \boldsymbol{k} \in \Lambda. \tag{2.3}$$

Here we consider the case of Neumann–Dirichlet boundary conditions ($\tau_1 = c$), when

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

The corresponding eigenfunctions are given by

$$u_L^{(c)}(r, k) = 2(2L+1)^{-1/2}\cos[(r-\tfrac{1}{2})\varphi_L^{(c)}(k)] \tag{2.5}$$

where

$$\varphi_L^{(c)}(k) = \frac{\pi(2k-1)}{2L+1}. \tag{2.6}$$

Note that all the eigenvalues $-K\mu_\Lambda^{(\tau)}(\boldsymbol{k})+s$, $\boldsymbol{k}\in\Lambda$, of the quadratic form on the right-hand side of equation (2.1) are positive if the spherical field s satisfies the inequality

$$s > K\max_{\boldsymbol{k}\in\Lambda}\mu_\Lambda^{(\tau)}(\boldsymbol{k}) := K\mu_\Lambda^{(\tau)}(\boldsymbol{k}_0). \tag{2.7}$$

It is convenient to introduce a shifted and rescaled spherical field $\phi > 0$ by setting $s = s(\phi)$, where

$$s(\phi) := K[\phi + \mu_\Lambda^{(\tau)}(\boldsymbol{k}_0)]. \tag{2.8}$$

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

$$\beta f_\Lambda^{(\tau)}(K, h_\Lambda) := \sup_\phi\{-|\Lambda|^{-1}\ln Z_\Lambda^{(\tau)}(K, h_\Lambda;\phi) - s(\phi)\} \tag{2.9}$$

where

$$Z_\Lambda^{(\tau)}(K, h_\Lambda;\phi) = \int_{\mathbb{R}^{|\Lambda|}}\exp[-\beta\mathcal{H}_\Lambda^{(\tau)}(\sigma_\Lambda|K, h_\Lambda; s(\phi))]\prod_{\boldsymbol{r}\in\Lambda}\mathrm{d}\sigma\,(\boldsymbol{r}) \tag{2.10}$$

is the partition function. The supremum is attained at the solution $\phi = \phi_\Lambda^{(\tau)}(K, h_\Lambda)$ of the mean spherical constraint

$$|\Lambda|^{-1}\sum_{\boldsymbol{r}\in\Lambda}\langle\sigma^2(\boldsymbol{r})\rangle_\Lambda^{(\tau)}(K, h_\Lambda;\phi) = 1 \tag{2.11}$$

where $\langle\cdots\rangle_\Lambda^{(\tau)}(K, h_\Lambda;\phi)$ denotes expectation value with respect to the Gibbs distribution with Hamiltonian (2.1). Now we set $\tau_1 = c$ (Neumann–Dirichlet), $\tau_2 = \tau_3 = p$ (periodic), note that for these boundary conditions $\boldsymbol{k}_0 = \{1, L_2, L_3\}$, and take the limit $L_2, L_3 \to \infty$ at fixed $L_1 = L$. In the case of an inhomogeneous external field which depends on the first coordinates only and has the step-like form (L is assumed even, Lx integer, and $0 \leqslant x \leqslant 1$)

$$h(\boldsymbol{r}, x) = h_L\,\mathrm{sgn}(Lx + \tfrac{1}{2} - r_1) \tag{2.12}$$

one obtains for the free energy per spin

$$\begin{aligned}\beta f_\Lambda^{(c)}(K, h_\Lambda) &= \tfrac{1}{2}\log(K/\pi) - K\mu_\Lambda^{(c)}(\boldsymbol{k}_0)\\ &\quad+\frac{1}{L}\frac{1}{8\pi^2}\int_0^{2\pi}\mathrm{d}\theta_1\int_0^{2\pi}\mathrm{d}\theta_2\sum_{k=1}^{L}\log[\phi + 2\cos\varphi_L^{(c)}(1) - 2\cos\varphi_L^{(c)}(k)]\\ &\quad-\tfrac{1}{2}P_L^{(c)}(K, h_L, x;\phi) - K\phi.\end{aligned} \tag{2.13}$$

Here $P_L^{(c)}(K, h_L, x;\phi)$ is the field term which reads

$$\begin{aligned}P_L^{(c)}(K, h_L, x;\phi) &= \frac{h_L^2}{2KL(2L+1)}\\ &\quad\times\sum_{k=1}^{L}\frac{\{2\cos[((1-x)L+\frac{1}{2})\varphi_L^{(c)}(k)] - \cos[\varphi_L^{(c)}(k)/2]\}^2}{\{1-\cos[\varphi_L^{(c)}(k)]\}\{\phi/2 + \cos[\varphi_L^{(c)}(1)] - \cos[\varphi_L^{(c)}(k)]\}}.\end{aligned} \tag{2.14}$$

The mean spherical constraint (2.11) takes the form

$$W_{L,3}^{(c)}(\phi) - \frac{\partial}{\partial\phi}P_L^{(c)}(K, h_L, x;\phi) = 2K \tag{2.15}$$

where the spin–spin interaction term $W_{L,3}^{(c)}(\phi)$ is given by

$$W_{L,3}^{(c)}(\phi) := \frac{1}{L}\sum_{k=1}^{L}W_2[\phi + 2\cos\varphi_L^{(c)}(1) - 2\cos\varphi_L^{(c)}(k)] \tag{2.16}$$

with the function

$$W_2(z) = (2\pi)^{-2} \int_0^{2\pi} \mathrm{d}\theta_1 \int_0^{2\pi} \mathrm{d}\theta_2 \left[z + 2 \sum_{\nu=1}^{2} (1 - \cos\theta_\nu) \right]^{-1}. \tag{2.17}$$

Now we pass to the analysis of the mean spherical constraint (2.15).

3. The mean spherical constraint

Here we study the asymptotic behaviour of the solution $\phi = \phi_L$ of equation (2.15) in the case of a step-like field (2.12) with arbitrary value of the parameter $x \in [0, 1]$. The field term (2.14) is evaluated exactly with the aid of a 'contour summation' technique [8]. The resulting analytic expressions depend on whether $\phi/2 + \cos\varphi_L^{(c)}(1)$ is greater, or less than unity. We give the derivation of the relevant results for $\phi/2 + \cos\varphi_L^{(c)}(1) > 1$; the opposite case is obtained by analytical continuation [4].

Assuming $\phi/2 + \cos\varphi_L^{(c)}(1) > 1$, we set

$$\phi/2 + \cos\varphi_L^{(c)}(1) = \cosh z. \tag{3.1}$$

By performing the summation in the field term one obtains

$$\begin{aligned} P_L^{(c)}(K, h_L, x; \phi) = {} & \frac{h_L^2}{8K\sinh^2(z/2)} \left\{ \frac{2(L+1)}{2L+1} + \frac{1}{2L(2L+1)\cosh^2(z/2)} \right. \\ & \left. - \frac{3\sinh[(L+\frac{1}{2})z] - 2\sinh[(1-2x)Lz + \frac{1}{2}z] - 4\cosh(z/2)\sinh(xLz)}{L\sinh(z)\cosh[(L+\frac{1}{2})z]} \right\} \\ & - \frac{h_L^2}{8K} \left\{ \frac{\tanh[(L+\frac{1}{2})z] - (2L+1)^{-1}\tanh(z/2)}{L\sinh(z)} \right\}. \end{aligned} \tag{3.2}$$

Note that in the bulk limit, $L \to \infty$, $h_L = h$ and $\phi > 0$ fixed, the above expression reduces to

$$P_\infty^{(c)}(K, h_L, x; \phi) = \frac{h^2}{2K\phi} \tag{3.3}$$

independently of $x \in [0, 1]$. Therefore, the bulk mean spherical constraint is

$$W_3(\phi) + \frac{h^2}{2K\phi^2} = 2K \tag{3.4}$$

where

$$W_3(\phi) = \frac{1}{\pi^3} \int_0^{\pi} \mathrm{d}\theta_1 \int_0^{\pi} \mathrm{d}\theta_2 \int_0^{\pi} \mathrm{d}\theta_3 \left[\phi + 2 \sum_{\mathrm{i}=1}^{3} (1 - \cos\theta_{\mathrm{i}}) \right]^{-1} \tag{3.5}$$

is the three-dimensional Watson integral.

The two interesting regimes, the critical finite-size scaling regime and the low-temperature moderate-field one, require a more detailed separate treatment.

3.1. *Critical finite-size scaling regime*

In the critical finite-size scaling limit, when

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

equation (3.1) yields that for fixed $y > \pi/2$

$$zL \cong (y^2 - \pi^2/4)^{1/2} \equiv y_1. \tag{3.7}$$

Then, the asymptotic behaviour of expression (3.2) is given by

$$P_L^{(c)}(K, h_L, x; \phi) \cong \frac{h_L^2 L^2}{2K y_1^2}[1 - Y(x, y_1)] \tag{3.8}$$

where

$$Y(x, y_1) = \frac{3\sinh y_1 - 4\sinh(xy_1) - 2\sinh[(1-2x)y_1]}{y_1 \cosh y_1}. \tag{3.9}$$

Hence, the field term in the mean spherical constraint has the leading-order asymptotic form

$$-\frac{\partial}{\partial\phi} P_L^{(c)}(K, h_L, x; \phi) \cong \frac{h_L^2 L^4}{2K y_1^4}[1 - Y(x, y_1) + \tfrac{1}{2} y_1 Y'(x, y_1)] \tag{3.10}$$

where $Y'(x, y_1) = \mathrm{d}Y(x, y_1)/\mathrm{d}y_1$.

The interaction term in the mean spherical constraint has been obtained in [4] and reads:

$$W_{L,3}^{(c)}(\phi) = 2K_{c,L}^{(c)} - \frac{1}{4\pi L}\ln[\cosh y_1] + \mathrm{O}(L^{-2}) \tag{3.11}$$

where

$$K_{c,L}^{(c)} = K_c + \frac{1}{2L}\left[K_c - \frac{1}{2}W_2(4) - \frac{\ln 2}{4\pi}\right] \tag{3.12}$$

is the shifted critical coupling. By combining (3.10) and (3.11), and ignoring the $\mathrm{O}(L^{-2})$ corrections, equation (2.15) can be written in the finite-size scaling form

$$\frac{1}{4\pi}\ln[\cosh y_1] - \frac{h_L^2 L^5}{2K y_1^4}[1 - Y(x, y_1) + \tfrac{1}{2} y_1 Y'(x, y_1)] = 2(K_{c,L}^{(c)} - K)L. \tag{3.13}$$

In terms of the scaled variables,

$$v_1 = (K_{c,L}^{(c)} - K)L \qquad v_2 = K^{-1/2} h_L L^{5/2} \tag{3.14}$$

the solution $y_1 = y_1(x, v_1, v_2)$ of the mean spherical constraint (3.13) in the neighbourhood of the critical point defined by $v_1 = \mathrm{O}(1)$ and $v_2 = \mathrm{O}(1)$ yields the following asymptotic form of the spherical field,

$$\phi_L \simeq L^{-2} X^{(c)}(x, v_1, v_2). \tag{3.15}$$

Note that in the bulk limit equation (3.13) yields

$$\frac{\phi^{1/2}}{4\pi} - \frac{h^2}{2K\phi^2} = 2(K_c - K) \tag{3.16}$$

which is the leading-order expansion in small ϕ of the bulk spherical constraint (3.4).

3.2. Low-temperature moderate-field regime

Next we study the mean spherical constraint in the so-called low-temperature moderate-field regime, when $K > K_c$ and $h_L L^2 = \mathrm{O}(1)$ ([8, 12]). In this case the leading-order correction to the free energy density is

$$\beta f_L^{(c)}(K, h_L, x) \cong \text{constant} + \frac{1}{L^2}\sup_{z\geqslant 0}[(K_c - K)(z - \pi^2/4) - \tfrac{1}{2}\eta^2 g^{(c)}(x, z)]. \tag{3.17}$$

Here, we have introduced the function

$$g^{(c)}(x, z) = \frac{1}{2(z - \pi^2/4)}\left[1 - Y\left(x, \sqrt{z - \pi^2/4}\right)\right] \tag{3.18}$$

and the scaled magnetic field variable

$$\eta = K^{-1/2} h_L L^2. \tag{3.19}$$

Note that for all $x \in [0, 1]$, $g^{(c)}(x, z)$ is a positive, continuous function of $z > 0$, which monotonically decreases with $z \geqslant 0$. We mention that it has a removable singularity at $z = \pi^2/4$, where

$$\begin{aligned} g^{(c)}(x, \pi^2/4) &= \tfrac{1}{6}[1 - 6x(1 - x)^2] > 0 \\ g'^{(c)}(x, \pi^2/4) &= -\tfrac{1}{15} + \tfrac{1}{12}x(1 - x)^2[5 + 2x - 3x^2] < 0. \end{aligned} \tag{3.20}$$

When $z \to \infty$, it is easily seen that

$$g^{(c)}(x, z) \to 0 \qquad \text{and} \qquad g'^{(c)}(x, z) \to 0 \qquad \text{as } z \to \infty \tag{3.21}$$

where $g'^{(c)}(x, z) = \mathrm{d}g^{(c)}(x, z)/\mathrm{d}z$. On the other hand, when $z \to 0$ and $x \neq \frac{1}{3}$,

$$g^{(c)}(x, z) \to \infty \qquad g'^{(c)}(x, z) \to -\infty \qquad \text{as } z \to 0. \tag{3.22}$$

Therefore, if $K > K_c$ and $x \neq \frac{1}{3}$, the supremum in (3.17) is reached at some finite value $z = z^*(K, \eta; x)$, which is the unique solution of the equation

$$-\eta^2 g'^{(c)}(x, z) = 2(K - K_c). \tag{3.23}$$

Hence, for the spherical field one obtains $\phi_L = z^* L^{-2}$.

In the special case of $x = \frac{1}{3}$, both the function $g^{(c)}(\frac{1}{3}, 0)$ and its derivative are finite at $z = 0$:

$$g^{(c)}(\tfrac{1}{3}, 0) = \frac{2}{\pi^2}\left(\frac{2\sqrt{3}}{\pi} - 1\right) \qquad \text{and} \qquad g'^{(c)}(\tfrac{1}{3}, 0) = -\frac{40}{3\pi^4}\left(1 - \frac{9\sqrt{3}}{5\pi}\right). \tag{3.24}$$

Therefore, when

$$\eta^2 \leqslant \frac{2(K - K_c)}{-g'^{(c)}(\frac{1}{3}, 0)} \tag{3.25}$$

the supremum in (3.17) is reached at $z = 0$, which implies $\phi = 0$. Actually, if one takes into account the higher-order corrections in L^{-1}, one obtains $\phi_L = \mathrm{O}(L^{-3})$. Indeed, let us assume $\phi = \mathrm{O}(L^{-3})$ and expand the solution of equation (3.1) for sufficiently large L, when $\phi/2 + \cos\varphi_L^{(c)}(1) < 1$, up to terms of order $\mathrm{O}(L^{-2})$:

$$z = \mathrm{i}\left[\frac{\pi}{2L} - \frac{\phi L}{\pi} - \frac{\pi}{4L^2} + \mathrm{O}(L^{-3})\right]. \tag{3.26}$$

Then, by expanding the exact expression (3.2) for the field term at $x = \frac{1}{3}$, we obtain

$$P_L^{(c)}(K, h_L, \tfrac{1}{3}; \phi) = \frac{h_L^2 L^2}{K} \left\{ \left(\frac{2}{\pi^2} + \frac{3}{\pi^2 L} \right) \left(\frac{2\sqrt{3}}{\pi} - 1 \right) + \frac{1}{12\phi L^4} - \frac{40}{3\pi^4} \left(1 - \frac{9\sqrt{3}}{5\pi} \right) \phi L^2 + \mathrm{O}(L^{-2}) \right\}. \tag{3.27}$$

Hence, the solution $\phi = \phi_L$ of the mean spherical constraint (2.15) takes the leading-order asymptotic form

$$\phi_L = \frac{|\eta|}{2\sqrt{3}[2(K - K_c) + \eta^2 g'^{(c)}(\frac{1}{3}, 0)]^{1/2}} L^{-3}. \tag{3.28}$$

In the complementary domain

$$\eta^2 > \frac{2(K - K_c)}{-g'^{(c)}(\frac{1}{3}, 0)} \tag{3.29}$$

the supremum in (3.17) is reached again at some finite value $z = z^*(K, \eta; \frac{1}{3})$, which obeys equation (3.23) at $x = \frac{1}{3}$. This implies again $\phi_L = z^* L^{-2}$.

4. Analysis of the magnetization profile

The mean spherical model permits one to obtain exact finite-size expressions for the magnetization profile. We start from the general expression

$$\langle \sigma(\boldsymbol{r}) \rangle = K^{-1} \sum_{\boldsymbol{k} \in \Lambda} U_\Lambda^{(c)}(\boldsymbol{r}, \boldsymbol{k}) [\phi + \omega_\Lambda^{(c)}(\boldsymbol{k})]^{-1} \hat{h}_\Lambda^{(c)}(\boldsymbol{k}) \tag{4.1}$$

where $\langle \cdots \rangle$ denotes a Gibbs canonical average with the Hamiltonian (2.1), and $\hat{h}_\Lambda^{(c)}(\boldsymbol{k})$ is the projection of the magnetic field configuration on the corresponding eigenfunction. In the case under consideration, with a field given by (2.12), the right-hand side of (4.1) depends on the coordinate r_1 only. By evaluating exactly the spin average value, we obtain the result

$$\langle \sigma(\boldsymbol{r}) \rangle = \frac{h_L}{2K(2L+1)} \times \sum_{k=1}^{L} \frac{\sin[(L + 1 - r_1)\varphi_L^{(c)}(k)]\{2\cos[((1-x)L + \frac{1}{2})\varphi_L^{(c)}(k)] - \cos[\varphi_L^{(c)}(k)/2]\}}{\sin[\varphi_L^{(c)}(k)/2]\{\phi/2 + \cos[\varphi_L^{(c)}(1)] - \cos[\varphi_L^{(c)}(k)]\}}. \tag{4.2}$$

As in the previous section, the resulting analytic expression depends on the value of $\phi/2 + \cos[\varphi_L^{(c)}(1)]$ compared with unity. Assuming $\phi/2 + \cos[\varphi_L^{(c)}(1)] = \cosh(z) > 1$, the summation in expression (4.2) yields

$$\langle \sigma(\boldsymbol{r}) \rangle = \frac{h_L \mathrm{sgn}(h)}{8K \sinh^2(z/2)} \left\{ 1 - \frac{\cosh[L + \frac{1}{2} - |r_1 - \frac{1}{2} - xL|]z}{\cosh(z/2)\cosh[(L + \frac{1}{2})z]} - \mathrm{sgn}(h) \frac{\cosh[(r_1 - (1-x)L - 1)z] - \cosh(z/2)\cosh[(r_1 - \frac{1}{2})z]}{\cosh(z/2)\cosh[(L + \frac{1}{2})z]} \right\}. \tag{4.3}$$

First we check if the coordinate-dependent magnetization profile obeys some extended version of the finite-size scaling, which is expected to include an additional dependence on the coordinate r_1 through the ratio $\rho = r_1/L$, $0 \leqslant \rho \leqslant 1$.

4.1. Critical finite-size scaling regime

By substituting $z = (y^2 - \pi^2/4)^{1/2}L^{-1} \equiv y_1 L^{-1}$ into (4.3), the exact expression for the scaled magnetization profile,

$$m_L(K, h_L, x; \rho) = \langle \sigma(\rho L, r_2, r_3) \rangle \tag{4.4}$$

simplifies to

$$\begin{aligned} m_L(K, h_L, x; \rho) \cong \operatorname{sgn}(h) \frac{h_L L^2}{2K y_1^2} \bigg\{ 1 - \frac{\cosh[(1-|\rho - x|)y_1]}{\cosh(y_1)} \\ - \operatorname{sgn}(h) \frac{\cosh[(x-1+\rho)y_1] - \cosh(\rho y_1)}{\cosh(y_1)} \bigg\}. \end{aligned} \tag{4.5}$$

From equation (4.5) we obtain for $0 \leqslant \rho \leqslant x$

$$m_L(K, h_L, x; \rho) \cong \frac{h_L L^2}{2K y_1^2} \left\{ 1 - \left[\frac{2\cosh[(1-x)y_1] - 1}{\cosh(y_1)} \right] \cosh(\rho y_1) \right\}. \tag{4.6}$$

From the above expression it is clear that the magnetization vanishes in the interval $\rho \in (0, x)$, at the point $\rho = \rho_0(x, y_1)$,

$$\rho_0(x, y_1) = \frac{1}{y_1} \cosh^{-1} \left[\frac{\cosh y_1}{2\cosh[(1-x)y_1] - 1} \right] \tag{4.7}$$

if and only if $x_1(y_1) \leqslant x \leqslant \frac{1}{3}$, where

$$x_1(y_1) = 1 - y_1^{-1} \cosh^{-1}[\tfrac{1}{2}(\cosh y_1 + 1)]. \tag{4.8}$$

When $0 \leqslant x < x_1(y_1)$ the magnetization turns out negative everywhere.

For $x \leqslant \rho \leqslant 1$ equation (4.5) can be written in the form

$$m_L(K, h_L, x; \rho) \cong \frac{h_L L^2}{2K y_1^2} \sinh[(1-\rho)y_1] \left\{ \frac{2\sinh(x y_1) - \sinh y_1}{\cosh y_1} + \tanh[\tfrac{1}{2}(1-\rho)y_1] \right\}. \tag{4.9}$$

It is clear that in the interval under consideration the magnetization not only vanishes at the Dirichlet boundary $\rho = 1$, but also at the internal point $\rho = \rho_0(x, y)$ given by

$$\rho_0(x, y_1) = 1 - \frac{2}{y_1} \tanh^{-1} \left[\tanh y_1 - \frac{2\sinh(x y_1)}{\cosh y_1} \right] \tag{4.10}$$

if and only if $\frac{1}{3} \leqslant x \leqslant x_2(y_1)$, where

$$x_2(y_1) = y_1^{-1} \sinh^{-1}(\tfrac{1}{2} \sinh y_1). \tag{4.11}$$

Under these conditions one can rewrite equation (4.9) in the transparent form

$$m_L(K, h_L, x; \rho) \cong \frac{h_L L^2}{K y_1^2} \frac{\sinh[\frac{1}{2}(1-\rho)y_1] \sinh[\frac{1}{2}(\rho_0(x, y_1) - \rho)y_1]}{\cosh[\frac{1}{2}(1 - \rho_0(x, y_1))y_1]}. \tag{4.12}$$

When $x_2(y_1) < x \leqslant 1$ the magnetization turns out positive everywhere.

The behaviour of $x_1(y_1)$ and $x_2(y_1)$, where $y_1 = (y^2 - \pi^2/4)^{1/2}$, as a function of $y = \phi^{1/2}L \in [0, \infty)$ is illustrated in figure 1. We note that $x_1(y_1) \uparrow \frac{1}{3}$ and $x_2(y_1) \downarrow \frac{1}{3}$ as $y \to 0$. Clearly, upon leaving the finite-size scaling regime towards the high-temperature bulk limit, when $y = \phi^{1/2}L \to \infty$, one obtains $x_1(y_1) \downarrow 0$ and $x_2(y_1) \uparrow 1$.

The shape of the magnetization profile $m_L(K, h_L, x; \rho)$, $\rho \in [0, 1]$, is shown in figure 2 for different values of x and y. Obviously, on approaching the high-temperature bulk limit, $y \to \infty$, the magnetization tends to follow more closely the (vanishing in the

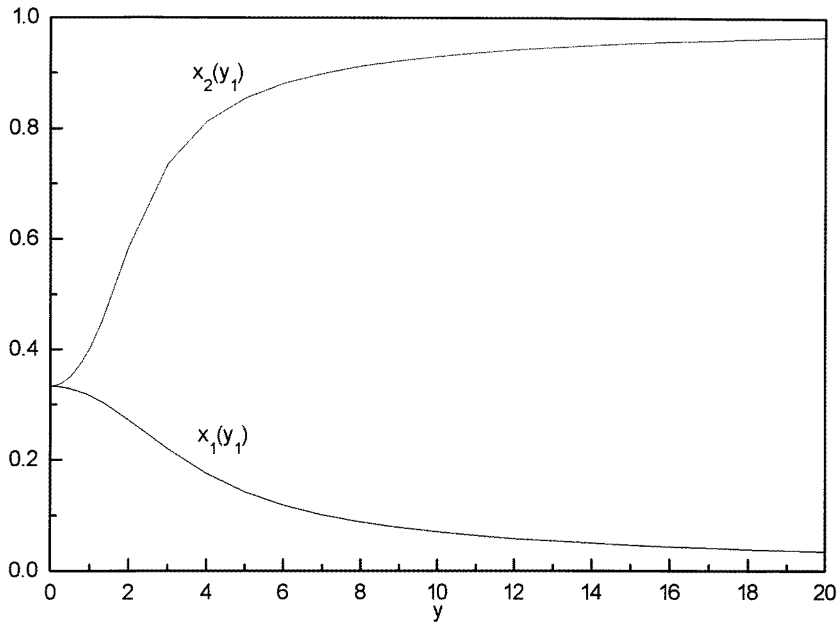

Figure 1. Plot of the functions $x_1(y_1)$ and $x_2(y_1)$ given by equations (4.8) and (4.11) respectively.

thermodynamic limit) step-like external field. For finite values of y, however, there is a pronounced deviation from the external field. This can be understood as a manifestation of a more coherent, dominated by the exchange interaction behaviour of the spin system as the finite-size correlation length becomes comparable with the layer thickness L.

4.2. High-temperature bulk limit

In the high-temperature bulk limit, $L \to \infty$, $h_L = h$ fixed, $K < K_c$, one has $\phi_L \to \phi_\infty > 0$, hence, $y \to \infty$. Then, equations (4.6) and (4.12) yield an exponentially fast approach of the magnetization per spin to the bulk limit, $\pm m_\infty(K, h)$, where

$$m_\infty(K, h) = \frac{|h|}{2K\phi_\infty} \tag{4.13}$$

provided ρ is fixed and $\rho \neq x$, $\rho < 1$. Close to the point $\rho = x$ one obtains

$$\lim_{L\to\infty} m_L(K, h_L, x; \rho) \cong \operatorname{sgn}(\rho - x) m_\infty(K, h)\{1 - \exp(-|\rho - x|L/\xi_\infty)\} \tag{4.14}$$

and close to $\rho = 1$,

$$\lim_{L\to\infty} m_L(K, h_L, x; \rho) \cong -m_\infty(K, h)\{1 - \exp[-(1-\rho)L/\xi_\infty]\} \tag{4.15}$$

where $\xi_\infty = \phi_\infty^{-1/2}$ is the bulk correlation length.

4.3. Low-temperature moderate-field regime

Note that in the domain

$$\eta^2 > \frac{2(K - K_c)}{-g'^{(c)}(x, \pi^2/4)} \tag{4.16}$$

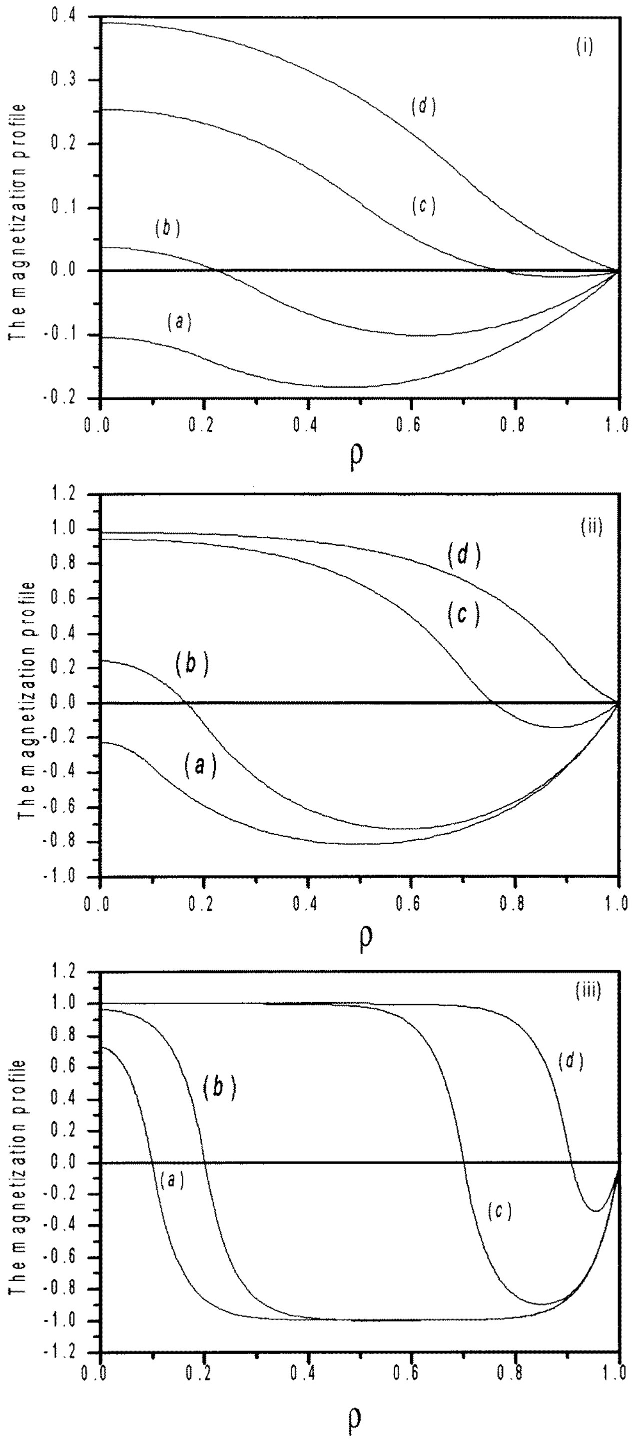

Figure 2. The magnetization profile of equations (4.6) and (4.12) when: (i) $y = 2$ and (a) $x = 0.2$ (b) $x = 0.3$ (c) $x = 0.5$ (d) $x = 0.7$; (ii) $y = 5$ and (a) $x = 0.1$ (b) $x = 0.2$ (c) $x = 0.7$ (d) $x = 0.9$; (iii) $y = 20$ and (a) $x = 0.1$ (b) $x = 0.2$ (c) $x = 0.7$ (d) $x = 0.9$.

one has $\pi/2 < y^* < \infty$, and the magnetization profile is given by equations (4.6) and (4.12) at $y_1 = [(y^*)^2 - \pi^2/4]^{1/2}$. In the complemetary domain,

$$\eta^2 \leqslant \frac{2(K - K_c)}{-g'^{(c)}(x, \pi^2/4)} \tag{4.17}$$

when $x \neq \frac{1}{3}$, one obtains $0 < y^* < \pi/2$, and the magnetization profile is given by equations (4.6) and (4.12) at $y_1 = \mathrm{i}[\pi^2/4 - (y^*)^2]^{1/2}$. The borderline between these two regions is given explicitly by the equation

$$\eta = \pm \frac{\sqrt{30}}{\sqrt{1 - \frac{5}{4}x(1-x)^2(5 + 2x - 3x^2)}}(K - K_c)^{1/2}. \tag{4.18}$$

On this line one has $y^* = \pi/2$, hence $y_1 = 0$, and the magnetization profiles (4.6) and (4.12), respectively, reduce to

$$m_L(K, h_L, x; \rho) \cong \frac{h_L L^2}{4K}[1 - \rho^2 - 2(1-x)^2] \qquad 0 \leqslant \rho \leqslant x \tag{4.19}$$

and

$$m_L(K, h_L, x; \rho) \cong -\frac{h_L L^2}{4K}(1 - \rho)[1 + \rho - 4x] \qquad x \leqslant \rho \leqslant 1. \tag{4.20}$$

By substituting $x = 0$ or 1 into (4.18), one obtains equation (4.48) in [12] (after a shift by $\frac{1}{2}$ in ρ which is due to a different definition of that variable) for the mean spherical constraint of a system of L layers under Neumann–Dirichlet boundary conditions and uniform field.

At $x = \frac{1}{3}$, in the region (3.25) one obtains $\phi = \mathrm{O}(L^{-3})$, which is given by (3.28), and the explicit expression of the magnetization profile (4.3) takes the form

$$\begin{aligned} m_L(K, h_L, \tfrac{1}{3}; \rho) \cong{}& \frac{8}{\pi^2}\left(\frac{h}{4J}\right)\left[\frac{2}{\sqrt{3}}\cos\left(\frac{\pi\rho}{2}\right) - 1\right] \\ &- \left[m_0(K) - \frac{320}{3\pi^4}\left(1 - \frac{9\sqrt{3}}{5\pi}\right)\left(\frac{h}{4J}\right)^2\right]\sqrt{2}\cos(\pi\rho/2) \end{aligned} \tag{4.21}$$

for $0 \leqslant \rho \leqslant \frac{1}{3}$, and

$$\begin{aligned} m_L(K, h_L, \tfrac{1}{3}; \rho) \cong{}& -\frac{8}{\pi^2}\left(\frac{h}{4J}\right)\left[\frac{2}{\sqrt{3}}\cos\left(\frac{\pi\rho}{2} - \frac{\pi}{3}\right) - 1\right] \\ &- \left[m_0(K) - \frac{320}{3\pi^4}\left(1 - \frac{9\sqrt{3}}{5\pi}\right)\left(\frac{h}{4J}\right)^2\right]\sqrt{2}\cos(\pi\rho/2) \end{aligned} \tag{4.22}$$

for $\frac{1}{3} \leqslant \rho \leqslant 1$, where $h = h_L L^2/\beta$ is fixed, and $m_0(K) = (1 - K_c/K)^{1/2}$ is the spontaneous magnetization.

5. Discussion

In this paper we have treated the somewhat simpler case of the mean spherical model, as compared with the Berlin–Kac spherical model considered in [8]. In both cases the system is taken to have a layer geometry of thickness L and the spins are subjected to a step-like (+−) external field with a vanishing (as $L \to \infty$) amplitude h_L. We have generalized the setting in three aspects: (i) non-symmetric, Neumann–Dirichlet boundary conditions, instead of periodic [8], have been imposed at the opposite boundaries of the layer; (ii) the step-like $(+-)$ external field has been taken to change sign at an arbitrary distance Lx $(0 \leqslant x \leqslant 1)$ from the Neumann boundary; (iii) the critical finite-size scaling regime has been studied, along with the low-temperature moderate-field regime. We have derived an exact expressions for the magnetization profile, see equation (4.3), and analysed its leading-order behaviour in the different temperature and field regimes.

We have found that in the critical finite-size scaling regime $v_1 = \mathrm{O}(1)$, and $v_2 = \mathrm{O}(1)$, due to the asymmetry of the boundary conditions, the magnetization profile does not closely follow the external field which changes sign at distance xL from the Neumann boundary, see equations (4.6) and (4.12). Two special values of x, $0 < x_1 < x_2 < 1$, have been found to exist, which are dependent on the scaled temperature and field variables, see figure 1, and have the property that the magnetization changes sign only when $x_1 < x < x_2$. The magnetization is negative everywhere when $0 \leqslant x < x_1$ and positive everywhere when $x_2 < x \leqslant 1$, see figure 2. When $x_1 < x < \frac{1}{3}$ the point of zero magnetization $\rho = \rho_0(x, y_1)$ is shifted towards the Neumann boundary, see equation (4.7), and when $1/3 < x < x_2$ the shift takes place towards the Dirichlet boundary, see equation (4.10).

In the low-temperature moderate-field regime, when $K > K_c$ and $\eta := K^{-1/2}h_L L^2 = \mathrm{O}(1)$, the magnetization profile has a nonvanishing limit as $L \to \infty$. In contrast to the case of periodic boundary conditions [8], the profile freezes and exhibits an algebraic dependence on the macroscopic distance ρ, see equations (4.19) and (4.20), only on the line (4.18) in the half-plane of parameters $K > K_c$, $\eta \in (-\infty, +\infty)$. On crossing that special line the ρ-dependence of the profile, given by hyperbolic functions in the domain (4.16), changes into a dependence given by trigonometric functions in the complementary domain (4.17), provided $x \neq \frac{1}{3}$.

The point $x = \frac{1}{3}$ is the counterpart of the point $x = \frac{1}{2}$ in the case of symmetric boundary conditions. It is characterized by the fact that the leading-order contribution of the ground-state eigenfunction in the field term (2.14),

$$P_L^{(c)}(K, h_L, x; \phi) \cong \frac{4h_L^2[1 - 2\sin(\pi x/2)]^2}{\pi^2 K \phi} \tag{5.1}$$

vanishes. However, the cancellation is not exact in all orders of L^{-1} and the field term $P_L^{(c)}(K, h_L, \frac{1}{3}; \phi)$ remains singular at $\phi = 0$, as can be seen from equation (3.27). As a consequence, when $x = \frac{1}{3}$ and the parameters are in the region given by inequality (3.25), the asymptotic behaviour of the spherical field changes from $\phi_L = \mathrm{O}(L^{-2})$ to $\phi_L = O(L^{-3})$, see equation (3.28). The borderline between these two regimes can be interpreted as a new, field induced critical temperature, $\tilde{T} = \tilde{\beta}^{-1}$, given by

$$\tilde{\beta}_c = \frac{\beta_c}{1 - 8|g'^{(c)}(\frac{1}{3}, 0)|(\frac{h}{4J})^2}. \tag{5.2}$$

In the appropriate field regime below $\tilde{T}_c$, the magnetization profile has both a frozen component, such as in the case of [8], and a temperature-dependent background term, see equations (4.21) and (4.22)), which is absent in the case of periodic boundary conditions.

In contrast, the field term for periodic boundary conditions and antisymmetric external field, $x = \frac{1}{2}$, contains no contribution from the ground state, and due to that it is regular at $\phi = 0$, see [11],

$$P_L^{(p)}(K, h_L, \tfrac{1}{2}; \phi) \cong \frac{h_L^2 L^2}{K}\left(\frac{1}{96} - \frac{1}{3840}\phi L^2\right). \tag{5.3}$$

Hence, in the moderate-field regime the solution $\phi = \phi_L$ of the mean spherical constraint takes the leading-order asymptotic form

$$\phi_L = \frac{1}{2(K - K_c) - \frac{1}{3840}\eta^2} L^{-3} \tag{5.4}$$

below Patrick's [8] critical temperature

$$\tilde{\beta}_c = \frac{\beta_c}{1 - \frac{1}{480}(\frac{h}{4J})^2}. \tag{5.5}$$

The results obtained here can be easily extended to obtain explicit probability distributions for single (or layer) spin variables, as well as for properly normalized block-spin variables, by following the lines of [8, 9].

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