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LETTER TO THE EDITOR

Spherical model for anisotropic ferromagnetic films

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Abstract. The corrections to the Curie temperature T_c of a ferromagnetic film consisting of N layers are calculated for $N \gg 1$ for the model of D-component classical spin vectors in the limit $D \to \infty$, which is exactly soluble and close to the spherical model. The present approach accounts, however, for the magnetic anisotropy playing the crucial role in the crossover from three to two dimensions in magnetic films. In the spatially inhomogeneous case with free boundary conditions the $D = \infty$ model is non-equivalent to the standard spherical one and always leads to the diminishing of $T_c(N)$ relative to the bulk.

The application of the spherical model [1] to spatially-inhomogeneous magnetic systems, such as ferromagnetic films with free boundary conditions by Barber and Fisher [2], has revealed the unphysical behaviour of the solution being the consequence of the global spin constraint. The dependence $T_c(N)$ for a d-dimensional hypercubic lattice infinite in $d' = (d-1)$ dimensions and having N layers in the dth dimension has been found to be for $d \geqslant 4$ a non-monotonic function with a maximum, i.e. $T_c(N)$ for $N \gg 1$ was larger than in the bulk. Other singular features of the spherical model were found by Abraham and Robert [3] by considering the problem of phase separation (i.e. the domain wall formation).

Besides the numerous publications using the spherical model for inhomogeneous systems in its original form (see, e.g., [4, 5]), there is a work by Costache *et al* [6] in which the global spin constraint was replaced for a ferromagnetic film by separate constraints in each layer. Although this model is less convenient for analytical calculations, it was shown that for $d \geqslant 4$ the value of $T_c(N)$ monotonically increases to its bulk value $T_c(\infty)$, as it should from physical grounds. Earlier Knops [7] had proved that in a general inhomogeneous situation the spherical model with a spin constraint on each lattice site is equivalent to the D-component classical vector model by Stanley [8] in the limit $D \to \infty$. The latter is not only more physically appealing than the original spherical model, but it also allows one to take into account the spin anisotropy [9] and to produce the $1/D$ expansions [10–12]. A convenient tool to handle the D-vector model is the classical spin diagram technique [12, 13].

The possibility of considering anisotropic systems makes the analytically soluble $D = \infty$ model, which can also be called for simplicity the spherical model, rather attractive for applications. In [14] it was used to investigate the role of fluctuations in the phase transition from Bloch to linear domain walls in *biaxial* ferromagnets. Anisotropy also plays a crucial role for ferromagnetic films in the actual case $d = 3$. For $N \neq \infty$

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the system is infinite in only $d' = 2$ dimensions, and cannot sustain a long-range order in the case of a continuous spin symmetry. Correspondingly, Barber and Fisher [2] have found diverging corrections to T_c for $N \gg 1$ for the standard spherical model. On the other hand, for a purely two-dimensional system ($N = 1$) T_c tends to zero only logarithmically slowly with vanishing anisotropy. One can expect that in the quasi three-dimensional case ($N \gg 1$) the characteristic anisotropy required to support the long-range order should be extremely small. The calculation of the T_c-corrections for three-dimensional ferromagnetic films, which strongly depend on the anisotropy, is the main purpose of this work. The Hamiltonian of the anisotropic classical D-vector model can be written in the form

$$\mathcal{H} = -\frac{1}{2}\sum_{ij} J_{ij}\left(m_{zi}m_{zj} + \eta\sum_{\alpha=2}^{D} m_{\alpha i}m_{\alpha j}\right) \tag{1}$$

where m_i is the normalized D-component vector, $|m_i| = 1$ and $\eta < 1$ is the dimensionless anisotropy factor. In the mean field approximation (MFA) the Curie temperature of this model is $T_c^{\rm MFA} = J_0/D$, where J_0 is the zero Fourier component of the exchange interaction. It is convenient to introduce the dimensionless temperature variable $\theta \equiv T/T_c^{\rm MFA}$ and the reduced correlation function (CF) of transverse ($\alpha \geqslant 2$) spin components: $s_{ij} \equiv D\langle m_{\alpha i}m_{\alpha j}\rangle$, which are well behaved in the limit $D \to \infty$. Using the diagram technique for classical spin systems [12–14], one arrives in the limit $D \to \infty$ at the closed system of equations for the average magnetization $m_i \equiv \langle m_{zi}\rangle$ and the CF s_{ij}. These are the magnetization equations

$$m_i = G_i\sum_j \lambda_{ij}m_j \tag{2}$$

the Dyson equation for the correlation function

$$s_{ii'} = \theta G_i\delta_{ii'} + \eta G_i\sum_j \lambda_{ij}s_{ji'} \tag{3}$$

and the kinematic relation playing the role of the spin constraint on a lattice site i

$$s_{ii} + m_i^2 = 1. \tag{4}$$

Here $\lambda_{ij} \equiv J_{ij}/J_0$ and G_i is the one-site spin average $D\langle m_{\alpha i}m_{\alpha i}\rangle\theta$ renormalized by fluctuations, which should be eliminated from the equations.

In the Ising case ($\eta = 0$) the influence of the fluctuations of the transverse spin components disappear. Since, additionally, the longitudinal fluctuations dying out as $1/D$ are not present in the equations above, the situation is in this case exactly described by the MFA. Equation (3) has for $\eta = 0$ the trivial solution $s_{ii} = \theta G_i$; then from constraint (4) one gets $G_i = (1-m_i^2)/\theta$, and the elimination of G_i in (2) leads to a closed equation for the magnetization.

In the homogeneous case $m_i = m$ and $G_i = G$ are constants, and equation (3) can be easily solved with the help of the Fourier transformation, which results in

$$s_{ii} = v_0\int\frac{d^d\boldsymbol{k}}{(2\pi)^d}s_{\boldsymbol{k}} = \theta GP(\eta G) \qquad P(X) \equiv v_0\int\frac{d^d\boldsymbol{k}}{(2\pi)^d}\frac{1}{1 - X\lambda_{\boldsymbol{k}}}. \tag{5}$$

Here v_0 is the unit cell volume and $\lambda_{\boldsymbol{k}} \equiv J_{\boldsymbol{k}}/J_0$. For the d-dimensional hypercubic lattices $v_0 = a_0^d$, a_0 is the lattice spacing,

$$\lambda_{\boldsymbol{k}} = \frac{1}{d}\sum_{i=1}^{d}\cos(a_0k_i) \tag{6}$$

and the lattice integral $P(X)$ has the following properties:

$$P(X) \cong \begin{cases} 1 + X^2/(2d) & X \ll 1 \\ (1/\pi)\ln[8/(1-X)] & 1-X \ll 1; d=2 \\ W_3 - c_3(1-X)^{1/2} & 1-X \ll 1; d=3 \\ W_4 - c_4(1-X)\ln[c_4'/(1-X)] & 1-X \ll 1; d=4 \end{cases} \tag{7}$$

where $W_3 = 1.516\,39$ and $W_4 = 1.239\,47$ are the Watson integrals, $c_3 = (2/\pi)(3/2)^{3/2}$ and $c_4 = (2/\pi)^2$. For $d \geqslant 5$ the leading terms of the expansion of $P(X)$ about $X = 1$ are non-singular. Since in the homogeneous case the sum on the right-hand side of (2) equals m, it is satisfied only if $m = 0$ (above θ_c) or $G = 1$ (below θ_c). Then from equation (4) one obtains the temperature-dependent magnetization:

$$m = (1 - \theta/\theta_c)^{1/2} \qquad \theta \leqslant \theta_c \equiv 1/P(\eta). \tag{8}$$

In the isotropic case ($\eta = 1$) for $d \geqslant 3$ the value of the temperature in the bulk θ_c reduces to the well known result $\theta_c = 1/W$ [1]. For $d = 2$ one obtains $\theta_c(\eta) \cong \pi/\ln[8/(1-\eta)]$ vanishing for $\eta \to 1$. In the Ising case $\eta = 0$, the MFA result $\theta_c = 1$ is reproduced.

To solve the equations of the spherical model for a d-dimensional hypercubic ferromagnetic film it is convenient to use the Fourier representation in $d' = d - 1$ translationally-invariant dimensions and the site representation in the dth dimension. The Dyson equation (3) for the Fourier-transformed CF $\sigma_{nn_0}(\boldsymbol{k})$ takes on the form of a system of the second-order finite-difference equations

$$2b_n\sigma_n - \sigma_{n+1} - \sigma_{n-1} = (2d\theta/\eta)\delta_{nn_0} \qquad n = 1, 2, ..., N \tag{9}$$

where the mute index n_0 of σ was dropped. For the free and periodic boundary conditions (fbc and pbc) in (9) we set

$$\begin{aligned} &\sigma_0 = \sigma_{N+1} = 0 && \text{(fbc)} \\ &\sigma_0 = \sigma_N \qquad \sigma_{N+1} = \sigma_1 && (\text{pbc}, N \geqslant 3). \end{aligned} \tag{10}$$

The coefficient b_n in (9) reads

$$b_n = 1 + d[(\eta G_n)^{-1} - 1] + d'(1 - \lambda'_{\boldsymbol{k}}) \tag{11}$$

where $\lambda'_{\boldsymbol{k}}$ is given by (6) with $d \Rightarrow d'$. The magnetization equation (2) takes on the form

$$2\bar{b}_n m_n - m_{n+1} - m_{n-1} = 0 \tag{12}$$

with $\bar{b}_n \equiv b_n(\eta = 1, \boldsymbol{k} = 0)$ and the boundary conditions similar to (10). The constraint equations (4) can now be written as

$$s_{nn} + m_n^2 = 1 \qquad s_{nn} = a_0^{d'} \int \frac{\mathrm{d}^{d'}\boldsymbol{k}}{(2\pi)^{d'}} \sigma_{nn}(\boldsymbol{k}) \qquad n = 1, 2, ..., N. \tag{13}$$

The solution of equation (9) is governed by the effective $\boldsymbol{k}$-dependent correlation length, which in the long wavelength region, $a_0 k \ll 1$, is given by

$$r_c(k) = a_0/\sqrt{2d[(\eta G)^{-1} - 1] + (a_0 k)^2} \tag{14}$$

and which should be compared with the film thickness $L = Na_0$. In the region of parameters $r_c(k) \ll L$ one can expect the d-dimensional quasi-bulk behaviour perturbed due to the finite L. In the opposite limit a behaviour corresponding to the reduced dimensionality $d' = d - 1$ is to be expected. For $d \geqslant 3$ in situations where the finite-size corrections to θ_c are small, the main contribution to the integral (13) comes from the region $a_0 k \sim 1$. For such wave vectors the correlation length (14) is of the order of the lattice spacing a_0, and

$\sigma_{nn}(\boldsymbol{k})$ are the functions of G_n in several neighbouring layers. Then from the constraint equations (13) it follows (at least in the paramagnetic state, $m_n = 0$) that the inhomogeneity of G_n in the fbc case is confined to the boundary regions $n, N - n \lesssim n_{\rm c} \sim 1$. Due to this inhomogeneity an analytical solution of the problem is possible only in limiting cases. In the subsequent we shall restrict ourselves to the calculation of the Curie temperature $\theta_{\rm c}$ of ferromagnetic films with $N \gg 1$.

In the Ising limit $\eta = 0$ we have $G = 1/\theta$ above $\theta_{\rm c}$, and $\theta_{\rm c}$ can be found from the condition that the determinant of the linear system of equations (12) turns to zero. This leads to the MFA result [15]

$$\theta_{\rm c} = 1 - \frac{1}{d}\left(1 - \cos\frac{\pi}{N+1}\right). \qquad (15)$$

For the model with pbc, G is also independent of n due to the symmetry of the problem, and for $\theta \leqslant \theta_{\rm c}$, where $m \neq 0$, one finds $G = 1$ from (2) or (12). The homogeneous solution of the finite-difference equation (9) with $b_n = b$ has the form $\sigma_n = c_1\mu^n + c_2\mu^{-n}$, and the result for the one-layer correlator σ_{nn} reads

$$\sigma_{nn}(\boldsymbol{k}) = \frac{d\theta}{\eta\sqrt{b^2-1}}\frac{1+\mu^{-N}}{1-\mu^{-N}} \qquad \mu = b + \sqrt{b^2-1}. \qquad (16)$$

In the region $1 - \eta \ll 1$ and $a_0 k \ll 1$ this expression has the limiting forms

$$\sigma_{nn}(\boldsymbol{k}) \cong \begin{cases} \dfrac{2d\theta}{\eta N}\dfrac{1}{2d(1-\eta)+(a_0k)^2} & L/r_{\rm c}(k) = N\sqrt{2d(1-\eta)+(a_0k)^2} \ll 1 \\ \dfrac{d\theta}{\eta}\dfrac{1}{\sqrt{2d(1-\eta)+(a_0k)^2}} & L/r_{\rm c}(k) \gg 1 \end{cases} \qquad (17)$$

demonstrating the crossover from d- to d'-dimensional behaviour mentioned above. The second of these limiting expressions corresponds to the bulk and can also be obtained by the integration of the bulk CF $s_{\boldsymbol{k}}$ (5) over the dth component of the wave vector. For $N \gg 1$ and $d = 3$ the integral in (13) with $\sigma_{nn}(\boldsymbol{k})$ (16) can be calculated analytically, and the result for $\theta_{\rm c}$ reads (pbc)

$$\theta_{\rm c}^{-1} \cong W_3 + \frac{3}{\pi N}\ln\frac{1}{1-\exp[-N\sqrt{6(1-\eta)}]}. \qquad (18)$$

In the limit of extremely small anisotropies $1 - \eta$ the transition temperature $\theta_{\rm c}$ becomes logarithmically small,

$$\theta_{\rm c} \cong \left(\frac{2\pi N}{3}\right) \Big/ \ln\frac{1}{6N^2(1-\eta)} \ll 1 \qquad (19)$$

but this limit is very difficult to reach for $N \gg 1$. The minimal value of $1-\eta$ required to support $\theta_{\rm c} \sim 1$ diminishes exponentially fast with the increase of N, $1 - \eta^* \sim N^{-2}\exp(-2\pi N/3)$. For $d = 4$ the results have the form (pbc)

$$\theta_{\rm c}^{-1} \cong \begin{cases} W_4 + \dfrac{2}{3N^2} & 1 \ll N^2 \ll 1/(1-\eta) \\ W_4 + \dfrac{4[2(1-\eta)]^{1/4}}{(\pi N)^{3/2}}\exp\left[-2N\sqrt{2(1-\eta)}\right] & N^2(1-\eta) \gg 1. \end{cases} \qquad (20)$$

The first of these limiting expressions coinsides with that of Barber and Fisher [2].

Now we proceed to the investigation of the more complicated case of a ferromagnetic film with free boundary conditions. Here the solution of the Dyson equation (9) with $n = n_0$ can be represented by the recurrence formula

$$\sigma_{nn} = \frac{2d\theta}{\eta}\frac{1}{2b_n - \alpha_n - \alpha'_n} \qquad \alpha_{n+1} = \frac{1}{2b_n - \alpha_n} \qquad \alpha'_{n-1} = \frac{1}{2b_n - \alpha'_n} \tag{21}$$

with the initial conditions

$$\alpha_1 = \alpha'_N = 0 \qquad \alpha_2 = 1/(2b_1) \qquad \alpha'_{N-1} = 1/(2b_N). \tag{22}$$

Now all quantities G_n entering b_n (11) can be determined numerically as functions of θ from the N constraint equations (13). Finally, θ_c can be found from the condition $D_N = 0$, where D_N is the determinant of the linear system (12). The problem can be solved analytically in two limiting cases depending on the value of $N^2(1-\eta)$ (see (17)). In the limit $N^2(1-\eta) \gg 1$ the system shows a d-dimensional (bulk) behaviour in the whole range of $\boldsymbol{k}$, and in the main part of a sample all $\sigma_{nn}(\boldsymbol{k})$ are equal to each other and determined by the value of G far from the boundaries. Indeed, in this region the recurrence relations in (21) converge in the depth of the sample to $\alpha = \alpha' = b - \sqrt{b^2 - 1}$, which leads to a bulk expression for $\sigma_{nn}(\boldsymbol{k})$ analogous to the second one in (17). The value of G in the depth of the film is in our limit insensitive to its behaviour in the boundary regions n, $N - n \lesssim n_c \sim 1$, and can be found from the condition $D_N = 0$ using $G_n = G = \text{constant}$. To see that, one can simply cut the boundary regions and require $D_{N-n_c} = 0$, which introduces corrections of the order $1/N \ll 1$. The calculation analogous to that in the MFA case yields $G \cong 1 + (\pi/N)^2/(2d)$. After integration over $\boldsymbol{k}$ in (13) one arrives at the obvious expression $s_{nn} = \theta G P(\eta G)$ (see (5)), and the value of θ_c determined from the condition $s_{nn} = 1$ reads (fbc, $N^2(1-\eta) \gg 1$)

$$\theta_c \cong \frac{1}{P(\eta)}\left[1 - \frac{1}{2d}\left(\frac{\pi}{N}\right)^2 I(\eta)\right] \qquad I(\eta) = 1 + \frac{\eta P'(\eta)}{P(\eta)}. \tag{23}$$

For $d = 3$ the limiting forms of $I(\eta)$ obtained from (7) are given by

$$I(\eta) \cong \begin{cases} 1 + \eta^2/d & \eta \ll 1 \\ \dfrac{(3/2)^{3/2}}{\pi W_3}\dfrac{1}{\sqrt{1-\eta}} & 1 - \eta \ll 1. \end{cases} \tag{24}$$

One can see that (23) generalizes the MFA result (15), and for $1 - \eta \ll 1$ corrections to θ_c due to the finite-size effects are much greater than in the MFA.

For $d \geqslant 5$ the derivative $P'(\eta)$ is finite for $\eta \to 1$ (see (7)) and the results obtained above can be applied for all values of η. The reason for this is that the region of small wave vectors, $k \lesssim k_N \equiv a_0^{-1}/N$, where for $N^2(1-\eta) \lesssim 1$ the quasi-bulk expression for the CF $\sigma_{nn}(\boldsymbol{k})$ becomes invalid (see (17)), is suppressed by the phase-volume factor in the integral (13). The marginal case is $d = 4$, where for $1 - \eta \lesssim (a_0 k_N)^2 \sim 1/N^2$ with logarithmic accuracy it is sufficient to calculate the integral over the Brillouin zone down to k_N. As a result one gets (fbc)

$$\theta_c^{-1} \cong \begin{cases} W_4 + \dfrac{1}{N^2}\ln N + \mathrm{O}\left(\dfrac{1}{N^2}\right) & 1 \ll N^2 \lesssim 1/(1-\eta) \\ W_4 + \dfrac{1}{2N^2}\ln\dfrac{c'_4}{1-\eta} & N^2(1-\eta) \lesssim 1 \end{cases} \tag{25}$$

(cf (20)). An asymptotic dependence of the type $\ln(N)/N^2$ in the isotropic limit with a coefficient close to unity was obtained numerically for the spherical model with the layer constraint in [6]. In contrast, for the standard spherical model [1] with fbc $\theta_c^{-1} \cong W_4 + a/N$ with $a < 0$ [2].

For a three-dimensional ferromagnetic film in the limit $N^2(1-\eta) \ll 1$ the leading correction to the $\boldsymbol{k}$-integral (13) and hence to θ_c comes from the long wavelength region $k \lesssim k_N = a_0^{-1}/N$, where $\sigma_{nn}(\boldsymbol{k})$ behaves two-dimensionally. The form of $\sigma_{nn}(\boldsymbol{k})$ in this region can be determined from the general formula (21). Beyond the narrow boundary regions the quantities $\bar{b}_n \equiv b_n(\eta = 1, \boldsymbol{k} = 0)$, etc, satisfy $\bar{b}_n \cong \bar{\alpha}_n \cong \bar{\alpha}'_n \cong 1$, and the values of α_n and α'_n can be found from the recurrence relations (21) with the help of the expansion with respect to small $1-\eta$ and $(a_0k)^2$. As a result one gets the same expression (17) in the same wave vector range $k \lesssim k_N$. This region yields the contribution of the order $(1/N)\ln[1/(N^2(1-\eta))]$ into s_{nn} (13). The contribution of the region $k \gtrsim k_N$ into the correction to s_{nn} can be estimated in the following way. For $1-\eta \ll 1$ the finite-size correction described by (23) and (24) comes from the region of small wave vectors $a_0k \sim \sqrt{1-\eta}$. In our case, however, $a_0k_N \gg \sqrt{1-\eta}$, and the corresponding contribution is reduced to the value of the order $1/N$. With logarithmic accuracy the latter can be neglected in comparison to that of the two-dimensional region $k \lesssim k_N$. The final result for θ_c of the three-dimensional model with free boundary conditions can be written as (fbc, $N^2(1-\eta) \ll 1$)

$$\theta_c^{-1} \cong W_3 + \frac{3}{2\pi N} \ln \frac{1}{N^2(1-\eta)} + \mathrm{O}\left(\frac{1}{N}\right). \tag{26}$$

The similarity of this result with (18) is not surprising since in the relevant region $k \lesssim k_N$, where $r_c(k) \gtrsim L$, all N layers are strongly correlated with each other and the type of boundary conditions plays no role in the leading approximation.

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