Kac-type models of ferromagnetic thin films

1977 J. Phys. A: Math. Gen. 10 1009

(http://iopscience.iop.org/0305-4470/10/6/020)

J. Phys. A: Math. Gen., Vol. 10, No. 6, 1977. Printed in Great Britain. © 1977

Kac-type models of ferromagnetic thin films

Paul A Pearce

Department of Mathematics, University of Melbourne, Parkville, Victoria 3052, Australia

Received 19 November 1976

Abstract. The n-vector model of a thin film with free surfaces and Kac-type interactions is solved exactly. In zero field the system undergoes a phase transition of 'classical' type and, as conjectured by Costache, the critical temperature is independent of n. Unexpectedly, an examination of the $n \to \infty$ limit yields a generalized spherical model and not the ordinary spherical model. Although investigated for purposes of comparison, the ordinary spherical model is shown to be distinguished in that the distribution of the magnetization across the film can be calculated explicitly in a vanishing field. Moreover, in the bulk limit, as the width of the film becomes unbounded, the total magnetization of this spherical model depends on the boundary conditions.

1. Introduction and summary

Mean field theory has provided valuable insights into the understanding of phase transitions in ferromagnetic systems. Since the theory is properly a long-range theory, its predictions are of course insensitive to the geometry of the system. A simple way to overcome this problem for lattice models is to assume that the interaction matrix separates into a direct product of a long-range interaction matrix and a short-range interaction matrix. The long-range matrix then guarantees the tractability of the problem while the short-range matrix allows the introduction of geometrical structure. For purposes of exposition only we will consider the simplest possible geometry, a two-dimensional $N \times M$ square lattice. The ensuing analysis immediately extends to three- and higher-dimensional cubic lattices, which are finite in one direction, with exactly the same results; we are thus concerned with models of ferromagnetic thin films.

The interaction energy for the n-vector model of the system is

$$\mathscr{H}_n = -\tfrac{1}{2} \sum_{i,j=1}^{N} \sum_{t,s=1}^{M} \rho_{ij} A_{ts} \boldsymbol{S}_{it} \cdot \boldsymbol{S}_{js} - \sum_{i=1}^{N} \sum_{t=1}^{M} \boldsymbol{H}_t \cdot \boldsymbol{S}_{it}, \tag{1.1}$$

where the n-dimensional spins $\boldsymbol{S}_{it}$ have norm

$$\|\boldsymbol{S}_{it}\| = n^{1/2}. \tag{1.2}$$

On a cubic lattice i would be a lattice vector indicating the in-plane position and t would indicate the layer. Here we only explicitly consider a square lattice so that i simply indicates the column and t the row. Since we will be primarily concerned with a comparison with the corresponding spherical model we will assume parallel external fields of order $n^{1/2}$ (e.g. $\boldsymbol{H}_t = n^{1/2} H_t \hat{\boldsymbol{H}}$). The n-vector partition function is given by ($\beta = 1/kT$)

$$Z_n = A_n^{-NM} \int_{\|\boldsymbol{S}_{it}\| = n^{1/2}} \dots \int \mathrm{d}^{NM}\boldsymbol{S} \exp(-\beta \mathcal{H}_n) \tag{1.3}$$

with the normalization constant

$$A_n = (2\pi)^{n/2} n^{(n-1)/2} / \Gamma(n/2). \tag{1.4}$$

The spherical model of the same system has the interaction energy

$$\mathcal{H}_{\mathrm{sph}} = -\tfrac{1}{2} \sum_{i,j=1}^{N} \sum_{t,s=1}^{M} \rho_{ij} A_{ts} S_{it} S_{js} - \sum_{i=1}^{N} \sum_{t=1}^{M} H_t S_{it}. \tag{1.5}$$

Here the NM scalar spins are subject to the spherical constraint

$$\sum_{i=1}^{N} \sum_{t=1}^{M} S_{it}^2 = NM. \tag{1.6}$$

The spherical partition function is given by

$$Z_{\mathrm{sph}} = A_{NM}^{-1} \int_{\sum_{i=1}^{N} \sum_{t=1}^{M} S_{it}^2 = NM} \dots \int \mathrm{d}^{NM} S \exp(-\beta \mathcal{H}_{\mathrm{sph}}). \tag{1.7}$$

In these models we assume that the interaction parameters are ferromagnetic and of the Kac form (Kac and Helfand 1963)

$$\rho_{ij} = \gamma \rho(\gamma |i-j|) \geqslant 0, \tag{1.8}$$

$$A_{ts} = \delta_{t,s} + \tau(\delta_{t,s-1} + \delta_{t,s+1}), \qquad 0 \leqslant \tau \leqslant \tfrac{1}{2}, \tag{1.9}$$

that is, each spin in the lattice interacts with the spins in its own row and, to a weaker extent, with the spins in the two adjacent rows. The matrix ρ is the long-range interaction matrix with γ the inverse range. The form (1.9) for the short-range interaction matrix A is not essential but is assumed for mathematical simplicity. On a higher-dimensional partially finite lattice the long-range interaction needs to be suitably rescaled by factors of γ (see Thompson and Silver 1973). For M layers arranged on a simple cubic lattice, for example, the long-range interactions would be of the form $\rho_{ij} = \gamma^2 \rho(\gamma |i-j|)$, where i and j are in-plane lattice vectors.

The long-range limit ($\gamma \to 0$) must be taken after the thermodynamic limit. The limiting free energies then are given respectively by

$$-\beta\psi_n = \lim_{\substack{\gamma \to 0^+ \\ (M \text{ fixed})}} \lim_{N \to \infty} (NM)^{-1} \ln Z_n \tag{1.10}$$

and

$$-\beta\psi_{\mathrm{sph}} = \lim_{\substack{\gamma \to 0^+ \\ (M \text{ fixed})}} \lim_{N \to \infty} (NM)^{-1} \ln Z_{\mathrm{sph}}. \tag{1.11}$$

The interactions ($\gamma\rho(0)$ and $\tau\gamma\rho(0)$), specified by (1.8) and (1.9) between spins in the same column do not contribute to the free energies (1.10) and (1.11) in the long-range limit. Since the value of $\rho(0)$ is immaterial we assume that it is sufficiently large to ensure that the matrix ρ is positive definite. In addition we will assume that the sum

$$g(0,\gamma)=\gamma\sum_{i=-\infty}^{\infty}\rho(\gamma|i|), \tag{1.12}$$

over an infinite row, exists for all $\gamma>0$ and that

$$g(0)=\lim_{\gamma\to 0} g(0,\gamma)=\int \rho(|r|)\,\mathrm{d}r \tag{1.13}$$

exists (as a Riemann integral). In particular one could have $\rho(x)=J\exp(-x)$, as considered by Costache (1975), in which case $g(0)=2J$.

The layout of the remainder of the paper is as follows.

Our first result is presented in § 2. We show that, under the above assumptions on the interactions, the limiting n-vector free energy (1.10) is given by

$$\beta\psi_n=\min_{m_t}\frac{1}{M}\left[\tfrac{1}{2}n\beta g(0)\sum_{t,s=1}^{M}m_tA_{ts}m_s-\sum_{t=1}^{M}\ln\mathscr{I}_n\left(\beta g(0)\sum_{s=1}^{M}A_{ts}m_s+\beta H_t\right)\right] \tag{1.14}$$

where

$$\mathscr{I}_n(x)=\Gamma(n/2)I_{\frac{1}{2}n-1}(nx)/(\tfrac{1}{2}nx)^{\frac{1}{2}n-1} \tag{1.15}$$

and I_μ is a modified Bessel function of order μ. The minimum in (1.14) is attained for a solution of the system of equations

$$m_t=\mathscr{F}_n\left(\beta g(0)\sum_{s=1}^{M}A_{ts}m_s+\beta H_t\right),\qquad t=1,2,\ldots,M, \tag{1.16}$$

where

$$\mathscr{F}_n(x)=\mathscr{I}_n'(x)/n\mathscr{I}_n(x)=I_{\frac{1}{2}n}(nx)/I_{\frac{1}{2}n-1}(nx). \tag{1.17}$$

The minimizing solutions m_t of (1.16) are the layer (or row) magnetizations and the total magnetization is

$$m=\frac{1}{M}\sum_{t=1}^{M}m_t. \tag{1.18}$$

In § 3 the thermodynamic and critical properties of the n-vector model are briefly described. In particular, it is shown that for zero field ($H_t=0$) and for sufficiently high temperatures,

$$kT>kT_c=g(0)\left[1+2\tau\cos\left(\frac{\pi}{M+1}\right)\right], \tag{1.19}$$

there is only the trivial solution $m_t=0$, $t=1,2,\ldots,M$, of (1.16) corresponding to a state of zero spontaneous magnetization. T_c is identified as the critical temperature and is independent of n as conjectured by Costache (1975).

The $n\to\infty$ limit of the n-vector free energy (1.14) is evaluated in § 4. We find

$$\psi_\infty=\lim_{n\to\infty}n^{-1}\psi_n \tag{1.20}$$

is given by

$$\beta\psi_\infty = \min_{m_t} M^{-1}\left[\tfrac{1}{2}\beta g(0)\sum_{t,s=1}^{M} m_t A_{ts} m_s - \sum_{t=1}^{M} \ln \mathcal{I}_\infty\left(\beta g(0)\sum_{s=1}^{M} A_{ts}m_s + \beta H_t\right)\right]$$

$$= -\max_{|m_t|\leq 1} M^{-1}\left(\tfrac{1}{2}\beta g(0)\sum_{t,s=1}^{M} m_t A_{ts} m_s + \beta\sum_{t=1}^{M} H_t m_t + \tfrac{1}{2}\sum_{t=1}^{M}\ln(1-m_t^2)\right), \tag{1.21}$$

where the function $\mathcal{I}_\infty$ is defined by (cf (1.14) and (1.15))

$$\ln \mathcal{I}_\infty(x) = \lim_{n\to\infty} n^{-1}\ln \mathcal{I}_n(x) = \tfrac{1}{2}\{(1+4x^2)^{1/2} - 1 - \ln\tfrac{1}{2}[1+(1+4x^2)^{1/2}]\}. \tag{1.22}$$

The layer magnetizations are solutions of (cf (1.16))

$$m_t = \mathcal{F}_\infty\left(\beta g(0)\sum_{s=1}^{M} A_{ts}m_s + \beta H_t\right), \qquad t = 1, 2, \ldots, M, \tag{1.23}$$

where

$$\mathcal{F}_\infty(x) = \lim_{n\to\infty}\mathcal{F}_n(x) = \frac{2x}{1+(1+4x^2)^{1/2}}. \tag{1.24}$$

Contrary to expectation, the free energy (1.21) *does not agree* with the spherical model free energy, obtained in zero field, by Costache (1975). This surprise discovery demands a close scrutiny of the spherical model. This is done in § 5 where we show that

$$\beta\psi_{\text{sph}} = \min_{m_t}\left\{\tfrac{1}{2}\beta g(0)M^{-1}\sum_{t,s=1}^{M} m_t A_{ts} m_s - \ln \mathcal{I}_\infty\left(\left[M^{-1}\sum_{t=1}^{M}\left(\beta g(0)\sum_{s=1}^{M} A_{ts}m_s + \beta H_t\right)^2\right]^{1/2}\right)\right\}. \tag{1.25}$$

In zero field this reduces to (cf (1.21))

$$\beta\psi_{\text{sph}} = -\max_{m_t}\left[\tfrac{1}{2}\beta g(0)M^{-1}\sum_{t,s=1}^{M} m_t A_{ts} m_s + \tfrac{1}{2}\ln\left(1 - M^{-1}\sum_{t=1}^{M} m_t^2\right)\right] \tag{1.26}$$

$$= \begin{cases} 0, & \eta < 1 \\ \tfrac{1}{2}(1-\eta+\ln\eta), & \eta > 1 \end{cases} \tag{1.27}$$

with

$$\eta = \beta g(0)\left[1 + 2\tau\cos\left(\frac{\pi}{M+1}\right)\right]. \tag{1.28}$$

The layer magnetizations are again the m_t that minimize the free energy. It is an extraordinary feature of the spherical model that the layer magnetizations can be calculated explicitly in a vanishing field. The result is

$$m_t = \begin{cases} 0, & \eta < 1 \\ (1-\eta^{-1})^{1/2}\left(\dfrac{M+1}{2M}\right)^{-1/2}\sin\left(\dfrac{t\pi}{M+1}\right), & \eta > 1. \end{cases} \tag{1.29}$$

Notice that the onset of spontaneous magnetization occurs at exactly the n-vector critical temperature (1.19). More importantly, observe that in the bulk limit the magnetization is given by

$$\lim_{M\to\infty} \frac{1}{M} \sum_{t=1}^{M} m_t = \frac{8^{1/2}}{\pi}(1-\eta^{-1})^{1/2}, \qquad \eta > 1. \tag{1.30}$$

This differs from the bulk value for periodic boundary conditions by the factor $8^{1/2}/\pi$, reflecting the dependence of the distribution of magnetization on the boundary conditions.

The discrepancy between the $n \to \infty$ model and spherical model arises because the interactions are *not* translationally invariant (i.e. the matrix A is not cyclic). Translational invariance figures prominently in the proof of the equivalence of these two models given by Kac and Thompson (1971). Although the Kac and Thompson theorem is not applicable an appeal can be made to the counterpart, for non-translationally invariant interactions, given by Knops (1973). Knops asserts that in the $n \to \infty$ limit the n-vector model approaches a generalized spherical model in which the single spherical constraint (1.6) is replaced by multiple spherical constraints. In § 6 we show that the $n \to \infty$ model is actually an M-spherical model (Bettoney and Mazo 1970) in which the single spherical constraint (1.6) is replaced by the M constraints

$$\sum_{i=1}^{N} S_{it}^2 = N, \qquad t = 1, 2, \ldots, M. \tag{1.31}$$

We remark finally that the failure of the Bettoney and Mazo theorem, stating the equivalence of the M-spherical model to the ordinary spherical model, is also due to the fact that the matrix A is not cyclic.

2. The *n*-vector model

In this section we derive the n-vector free energy (1.10)

$$\beta\psi_n = \min_{m_t} \frac{1}{M}\left[\tfrac{1}{2} n\beta g(0) \sum_{t,s=1}^{M} m_t A_{ts} m_s - \sum_{t=1}^{M} \ln \mathscr{I}_n\left(\beta g(0) \sum_{s=1}^{M} A_{ts} m_s + \beta H_t\right)\right]. \tag{2.1}$$

We adopt the coalescing bound method of Thompson and Silver (1973, to be referred to as TS) and refer the reader to their paper for most of the details which we prefer not to duplicate here.

The eigenvalues of the matrix A are given by

$$\lambda_t = 1 + 2\tau \cos\left(\frac{t\pi}{M+1}\right). \tag{2.2}$$

Thus for $0 \leqslant \tau \leqslant \frac{1}{2}$ the matrix A is positive definite. As a consequence the direct product matrix $\rho \otimes A$ is positive definite. We rely heavily on this fact in the sequel.

To obtain an upper bound we begin by imposing the semi-periodic boundary conditions

$$\sum_{i=1}^{N} \rho_{ij} = g_N(0, \gamma) \tag{2.3}$$

so that (see (1.12))

$$\lim_{N\to\infty} g_N(0,\gamma)=g(0,\gamma). \tag{2.4}$$

The n-vector Hamiltonian (1.1) can now be written as

$$\mathcal{H}_n=-\tfrac{1}{2}\sum_{i,j=1}^{N}\sum_{t,s=1}^{M}\rho_{ij}A_{ts}(\boldsymbol{S}_{it}-n^{1/2}m_t\hat{\boldsymbol{H}})\cdot(\boldsymbol{S}_{js}-n^{1/2}m_s\hat{\boldsymbol{H}})+\tfrac{1}{2}nNg_N(0,\gamma)\sum_{t,s=1}^{M}m_tA_{ts}m_s$$
$$-\sum_{i=1}^{N}\sum_{t=1}^{M}n^{1/2}\Big(g_N(0,\gamma)\sum_{s=1}^{M}A_{ts}m_s+H_t\Big)\hat{\boldsymbol{H}}\cdot\boldsymbol{S}_{it}, \tag{2.5}$$

where the values of the m_t are arbitrary. Recalling that the matrix $\rho\otimes A$ is positive definite, we obtain an immediate bound on the partition function (1.3):

$$Z_n\geqslant\exp\Big(-\tfrac{1}{2}n\beta Ng_N(0,\gamma)\sum_{t,s=1}^{M}m_tA_{ts}m_s\Big)$$
$$\times A_n^{-NM}\int_{\|\boldsymbol{S}_{it}\|=n^{1/2}}\cdots\int \mathrm{d}^{NM}\boldsymbol{S}\exp\Big[\sum_{i=1}^{N}\sum_{t=1}^{M}n^{1/2}\Big(\beta g_N(0,\gamma)\sum_{s=1}^{M}A_{ts}m_s+\beta H_t\Big)\hat{\boldsymbol{H}}\cdot\boldsymbol{S}_{it}\Big]. \tag{2.6}$$

Evaluation of the integrals (TS, equation (2.11)) and the taking of limits then gives the desired bound on the free energy (1.10)

$$\beta\psi_n\leqslant\frac{1}{M}\Big[\tfrac{1}{2}n\beta g(0)\sum_{t,s=1}^{M}m_tA_{ts}m_s-\sum_{t=1}^{M}\ln\mathcal{I}_n\Big(\beta g(0)\sum_{s=1}^{M}A_{ts}m_s+\beta H_t\Big)\Big] \tag{2.7}$$

where $g(0)$ is given by (1.13) and $\mathcal{I}_n(x)$ by (1.15).

To obtain the reverse inequality, with suitably chosen m_t, we start with a well known representation (TS) for the partition function

$$Z_n=(2\pi)^{-NMn/2}(\det\rho)^{-Mn/2}(\det A)^{-Nn/2}$$
$$\times\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty}\mathrm{d}^{NM}\boldsymbol{x}\exp\Big(-\tfrac{1}{2}\sum_{i,j=1}^{N}\sum_{t,s=1}^{M}\rho_{ij}^{-1}A_{ts}^{-1}\boldsymbol{x}_{it}\cdot\boldsymbol{x}_{js}\Big)$$
$$\times A_n^{-NM}\int_{\|\boldsymbol{S}_{it}\|=n^{1/2}}\cdots\int\mathrm{d}^{NM}\boldsymbol{S}\exp\Big(\sum_{i=1}^{N}\sum_{t=1}^{M}(\beta^{1/2}\boldsymbol{x}_{it}+\beta\boldsymbol{H})\cdot\boldsymbol{S}_{it}\Big). \tag{2.8}$$

This formula is valid because the matrices ρ and A are positive definite. Imitation of the procedure in TS now leads readily to the inequality

$$Z_n\leqslant(2\pi)^{-NMn/2}(\det\rho)^{-Mn/2}(\det A)^{-Nn/2}$$
$$\times\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty}\mathrm{d}^{NM}\boldsymbol{x}\exp\Big(-\tfrac{1}{2}\sum_{i,j=1}^{N}\sum_{t,s=1}^{M}(\rho_{ij}^{-1}-z^{-1}\delta_{i,j})A_{ts}^{-1}\boldsymbol{x}_{it}\cdot\boldsymbol{x}_{js}\Big)$$
$$\times\max_{\boldsymbol{x}_{it}}\prod_{i=1}^{N}\exp\Big(-\tfrac{1}{2}z^{-1}\sum_{t,s=1}^{M}A_{ts}^{-1}\boldsymbol{x}_{it}\cdot\boldsymbol{x}_{is}+\sum_{t=1}^{M}\ln\mathcal{I}_n(\beta^{1/2}n^{-1/2}\|\boldsymbol{x}_{it}\|+\beta H_t)\Big) \tag{2.9}$$

where z is chosen to make the quadratic form in the simple Gaussian integral positive definite. With the long-range limit ($\gamma \to 0$), after the thermodynamic limit ($N \to \infty$), we will take $z \to g(0)+$.

It can be shown, as in TS, that in the final limit only the maximized term in (2.9) contributes to the bound. Moreover, the maximum in (2.9) is attained for $\boldsymbol{x}_{it} = \boldsymbol{x}_t$ a solution of the stationary condition

$$\boldsymbol{x}_t = \beta^{1/2} z \sum_{s=1}^{M} A_{ts} \mathscr{F}_n (\beta^{1/2} n^{-1/2} \|\boldsymbol{x}_s\| + \beta H_s) \frac{\boldsymbol{x}_s}{\|\boldsymbol{x}_s\|}, \tag{2.10}$$

where $\mathscr{F}_n(x)$ is given by (1.17). Using the actual form (1.9) of the matrix A in (2.10) it can be seen, by a recursive process, that the maximizing $\boldsymbol{x}_t$ are mutually parallel. Setting

$$n^{-1/2} \|\boldsymbol{x}_t\| = \beta^{1/2} g(0) \sum_{s=1}^{M} A_{ts} m_s \tag{2.11}$$

we obtain from (2.9) our final bound on the n-vector free energy (1.10) in the form

$$\beta \psi_n \geqslant \min_{m_t} \frac{1}{M} \left[\tfrac{1}{2} n \beta g(0) \sum_{t,s=1}^{M} m_t A_{ts} m_s - \sum_{t=1}^{M} \ln \mathscr{I}_n \left(\beta g(0) \sum_{t=1}^{M} A_{ts} m_s + \beta H_t \right) \right]. \tag{2.12}$$

This establishes the equality (2.1).

To investigate the layer magnetizations we notice that the stationary equations (cf (2.10)) now have the scalar form (cf (1.16))

$$m_t = \mathscr{F}_n \left(\beta g(0) \sum_{s=1}^{M} A_{ts} m_s + \beta H_t \right). \tag{2.13}$$

The magnetization (in the direction of the field) of row t is defined by the thermodynamic average

$$\lim_{\gamma \to 0} \lim_{N \to \infty} \left\langle \frac{1}{N} \sum_{i=1}^{N} \boldsymbol{S}_{it} \right\rangle \cdot \hat{\boldsymbol{H}}. \tag{2.14}$$

To evaluate this average we calculate the derivative (see (1.10))

$$-M \frac{\partial \psi_n}{\partial (\|\boldsymbol{H}_t\|)} = -n^{1/2} M \frac{\partial \psi_n}{\partial (n H_t)}. \tag{2.15}$$

Differentiating (2.1), using (1.17) and (2.13) we conclude that the magnetization of row t is $n^{1/2} m_t$. That is, m_t is the normalized layer magnetization. The scaling factor $n^{1/2}$ guarantees finite normalized magnetizations (i.e. solutions of (2.13)) in the limit $n \to \infty$. We will return to this matter in § 4.

The total magnetization (in the direction of the field) is defined as

$$\lim_{\gamma \to 0} \lim_{N \to \infty} \left\langle \frac{1}{NM} \sum_{i=1}^{N} \sum_{t=1}^{M} \boldsymbol{S}_{it} \right\rangle \cdot \hat{\boldsymbol{H}} = \frac{1}{M} \sum_{t=1}^{M} n^{1/2} m_t. \tag{2.16}$$

In a uniform field ($H_t = H$) this is precisely the derivative

$$-\partial \psi_n / \partial (\|\boldsymbol{H}\|). \tag{2.17}$$

This establishes that

$$m=\frac{1}{M}\sum_{t=1}^{M} m_t \tag{2.18}$$

is the total normalized magnetization.

3. Thermodynamics and critical behaviour

The behaviour of the n-vector system is determined entirely by the equations of state (2.13). Unfortunately these coupled transcendental equations for the layer magnetizations cannot be solved explicitly. Nonetheless, it should be possible to establish the existence of a phase transition in zero field with classical singularities for the magnetization and susceptibility. Since the behaviour of the n-vector system is exemplified by the Ising system we will not deliberate on these matters here. The interested reader is referred to Angelescu *et al* (1972) where the Ising case is studied extensively. With considerable effort they also prove certain properties (e.g. symmetry and concavity) of the distribution of magnetization across the film. A similar situation prevails for the closely related equivalent-neighbour model of Falk and Ruijgrok (1974) (see also Thompson 1974).

To determine the critical temperature we show that for sufficiently high temperatures,

$$kT>kT_c=g(0)\left[1+2\tau\cos\left(\frac{\pi}{M+1}\right)\right], \tag{3.1}$$

there is only the trivial solution $m_t=0$, $t=1,2,\ldots,M$, of the equations of state (2.13) in zero field. The equations (2.13) can be written in the matrix form ($\nu=\beta g(0)$)

$$A^{-1}|m\rangle=|\mathscr{F}_n(\nu m)\rangle \tag{3.2}$$

where the state vector

$$|m\rangle=(m_1,m_2,\ldots,m_M) \tag{3.3}$$

and

$$|\mathscr{F}_n(\nu m)\rangle=(\mathscr{F}_n(\nu m_1),\mathscr{F}_n(\nu m_2),\ldots,\mathscr{F}_n(\nu m_M)). \tag{3.4}$$

Clearly $|m\rangle=0$ is always a solution of the equation (3.2). But suppose $|m\rangle\neq 0$ is a solution of (3.2) for $T>T_c$ given by (3.1), that is from (2.2), $\nu\lambda_1<1$ where λ_1 is the maximum eigenvalue of the matrix A. Then forming inner products in (3.2) we obtain

$$\frac{1}{\lambda_1}\leqslant\frac{\langle m|A^{-1}|m\rangle}{\langle m|m\rangle}=\frac{\langle m|\mathscr{F}_n(\nu m)\rangle}{\langle m|m\rangle}\leqslant\frac{\langle\mathscr{F}_n(\nu m)|\mathscr{F}_n(\nu m)\rangle^{1/2}}{\langle m|m\rangle^{1/2}}\leqslant\nu. \tag{3.5}$$

The inequalities result respectively from the minimax principle, the Cauchy–Schwarz inequality and the modified Bessel function inequality

$$|\mathscr{F}_n(x)|=|I_{\frac{1}{2}n}(nx)/I_{\frac{1}{2}n-1}(nx)|\leqslant|x|. \tag{3.6}$$

The inequality (3.5) contradicts the assumption $\nu\lambda_1<1$ and hence $|m\rangle=0$ is the only solution of (3.2) for $T>T_c$.

For $T<T_c$ the situation is more complicated and indeed there are many solutions of the equation of state (3.2). To complete the identification of T_c as the critical temperature, though, it should be shown that the absolute minimum of the free energy functional (2.1), for $T<T_c$, occurs for a non-trivial solution of (3.2). This program has been carried out for the prototype Ising system by Angelescu *et al* (1972), who furthermore isolated the unique (non-trivial) ferromagnetic ($m_t \geqslant 0$, $t=1,2,\ldots,M$) solution as the minimizing solution determining the distribution of magnetization. This course will not be pursued here for the n-vector model. Instead we will return to these matters for the tractable and more transparent spherical model in § 5.

4. The $n\to\infty$ limit

To evaluate the free energy

$$\psi_\infty = \lim_{n\to\infty} n^{-1}\psi_n \tag{4.1}$$

we use the asymptotic formula (Pearce and Thompson 1976)

$$\lim_{n\to\infty} n^{-1}\ln \mathscr{I}_n(x) = \tfrac{1}{2}\{(1+4x^2)^{1/2}-1-\ln\tfrac{1}{2}[1+(1+4x^2)^{1/2}]\}. \tag{4.2}$$

From (2.1) it follows that ($\nu=\beta g(0)$)

$$\beta\psi_\infty = \min_{m_t} \frac{1}{2M}\left(\nu\sum_{t,s=1}^{M} m_t A_{ts} m_s - \sum_{t=1}^{M}\{(1+4z_t^2)^{1/2}-1-\ln\tfrac{1}{2}[1+(1+4z_t^2)^{1/2}]\}\right), \tag{4.3}$$

with

$$z_t = \nu\sum_{s=1}^{M} A_{ts} m_s + \beta H_t. \tag{4.4}$$

The expression (4.3) to be extremized can be somewhat simplified (Pearce and Thompson 1977). We show that

$$\beta\psi_\infty = -\max_{|m_t|\leqslant 1}\frac{1}{M}\left(\tfrac{1}{2}\nu\sum_{t,s=1}^{M} m_t A_{ts} m_s + \beta\sum_{t=1}^{M} H_t m_t + \tfrac{1}{2}\sum_{t=1}^{M}\ln(1-m_t^2)\right). \tag{4.5}$$

The demonstration relies on the fact that the extremum in (4.3) occurs for a solution of the equations

$$m_t = \frac{2z_t}{1+(1+4z_t^2)^{1/2}}, \tag{4.6}$$

in conjunction with the fact that the extremum equations for (4.5) are

$$z_t = \frac{m_t}{1-m_t^2}. \tag{4.7}$$

The roots of the latter equations (4.7) in the range $|m_t|\leqslant 1$ are given precisely by the former equations (4.6), that is,

$$m_t = \frac{-1+(1+4z_t^2)^{1/2}}{2z_t}. \tag{4.8}$$

The equivalence of (4.3) and (4.5) is now established straightforwardly by using the relations:

$$\frac{1}{1-m_t^2}=\frac{z_t}{m_t}=\tfrac{1}{2}[1+(1+4z_t^2)^{1/2}], \tag{4.9}$$

$$\nu\sum_{t,s=1}^{M} m_tA_{ts}m_s+\beta\sum_{t=1}^{M} H_tm_t=\sum_{t=1}^{M} m_tz_t=\tfrac{1}{2}\sum_{t=1}^{M}[-1+(1+4z_t^2)^{1/2}]. \tag{4.10}$$

It is immediately apparent, by differentiating (4.5) with respect to the field H_t, that m_t is the magnetization of row t. Moreover, the magnetizations can be obtained from the normalized n-vector magnetizations (2.13). This is verified by the formula

$$\lim_{n\to\infty}\mathscr{F}_n(x)=\lim_{n\to\infty}\frac{I_{\frac{1}{2}n}(nx)}{I_{\frac{1}{2}n-1}(nx)}=\frac{2x}{1+(1+4x^2)^{1/2}} \tag{4.11}$$

which follows readily from the modified Bessel function identity (Abramowitz and Stegun 1964)

$$I_{\mu-1}(\mu x)-I_{\mu+1}(\mu x)=2x^{-1}I_\mu(\mu x). \tag{4.12}$$

Although it would be desirable to study the equations of state (4.7) numerically, we bypass this concern here and, for the sake of comparison, immediately investigate the spherical model.

5. The spherical model

The derivation of the spherical model free energy proceeds along very similar lines to § 2. For the sake of completeness, however, it is given here. The result to be proved is

$$\beta\psi_{\mathrm{sph}}=\min_{m_t}\Big\{\tfrac{1}{2}\beta g(0)M^{-1}\sum_{t,s=1}^{M} m_tA_{ts}m_s -\ln\mathscr{I}_\infty\Big(\Big[M^{-1}\sum_{t=1}^{M}\Big(\beta g(0)\sum_{s=1}^{M}A_{ts}m_s+\beta H_t\Big)^2\Big]^{1/2}\Big)\Big\}. \tag{5.1}$$

The spherical model interaction energy (1.5) can be recast as

$$\mathscr{H}_{\mathrm{sph}}=-\tfrac{1}{2}\sum_{i,j=1}^{N}\sum_{t,s=1}^{M}\rho_{ij}A_{ts}(S_{it}-m_t)(S_{js}-m_s) +\tfrac{1}{2}Ng_N(0,\gamma)\sum_{t,s=1}^{M}m_tA_{ts}m_s-\sum_{i=1}^{N}\sum_{t=1}^{M}\Big(g_N(0,\gamma)\sum_{s=1}^{M}A_{ts}m_s+H_t\Big)S_{it}. \tag{5.2}$$

Discarding the first term leads to a bound on the partition function (1.7):

$$Z_{\mathrm{sph}}\geq\exp\Big(-\tfrac{1}{2}\beta Ng_N(0,\gamma)\sum_{t,s=1}^{M}m_tA_{ts}m_s\Big) \times A_{NM}^{-1}\int_{\sum_{i=1}^{N}\sum_{t=1}^{M}S_{it}^2=NM}\cdots\int d^{NM}S\exp\Big[\sum_{i=1}^{N}\sum_{t=1}^{M}\Big(\beta g_N(0,\gamma)\sum_{s=1}^{M}A_{ts}m_s+\beta H_t\Big)S_{it}\Big]. \tag{5.3}$$

After evaluating the integral (TS, equation (2.11)) we ultimately obtain

$$\beta\psi_{\text{sph}} \leq \tfrac{1}{2}\beta g(0) M^{-1} \sum_{t,s=1}^{M} m_t A_{ts} m_s - \lim_{N\to\infty} (NM)^{-1} \ln \mathcal{I}_{NM}\left(\left(M^{-1} \sum_{t=1}^{M} z_t^2\right)^{1/2}\right) \tag{5.4}$$

with

$$z_t = \beta g(0) \sum_{s=1}^{M} A_{ts} m_s + \beta H_t. \tag{5.5}$$

The functional integral representation (TS) for the spherical partition function (1.7) is

$$\begin{aligned} Z_{\text{sph}} = {} & (2\pi)^{-NM/2} (\det\rho)^{-M/2} (\det A)^{-N/2} \\ & \times \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} \mathrm{d}^{NM}x \, \exp\left(-\tfrac{1}{2} \sum_{i,j=1}^{N} \sum_{t,s=1}^{M} \rho_{ij}^{-1} A_{ts}^{-1} x_{it} x_{js}\right) \\ & \times A_{NM}^{-1} \int_{\sum_{i=1}^{N}\sum_{t=1}^{M} S_{it}^2 = NM} \cdots \int \mathrm{d}^{NM}S \, \exp\left(\sum_{i=1}^{N} \sum_{t=1}^{M} (\beta^{1/2} x_{it} + \beta H_t) S_{it}\right). \end{aligned} \tag{5.6}$$

It follows that for large enough z $(z > g_N(0, \gamma))$

$$\begin{aligned} Z_{\text{sph}} \leq {} & (2\pi)^{-NM/2} (\det\rho)^{-M/2} (\det A)^{-N/2} \\ & \times \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} \mathrm{d}^{NM}x \, \exp\left(-\tfrac{1}{2} \sum_{i,j=1}^{N} \sum_{t,s=1}^{M} (\rho_{ij}^{-1} - z^{-1}\delta_{i,j}) A_{ts}^{-1} x_{it} x_{js}\right) \\ & \times \max_{x_{it}} \Bigg\{ \exp\Bigg[-\tfrac{1}{2} z^{-1} \sum_{i=1}^{N} \sum_{t,s=1}^{M} A_{ts}^{-1} x_{it} x_{is} \\ & + \ln \mathcal{I}_{NM}\left((NM)^{-1/2} \left(\sum_{i=1}^{N} \sum_{t=1}^{M} (\beta^{1/2} x_{it} + \beta H_t)^2\right)^{1/2}\right)\Bigg]\Bigg\}. \end{aligned} \tag{5.7}$$

Again only the maximized term contributes to the bound in the final limit. Moreover the maximum occurs for $x_{it} = x_t$, $i = 1, 2, \ldots, N$. Setting

$$x_t = \beta^{1/2} g(0) \sum_{s=1}^{M} A_{ts} m_s \tag{5.8}$$

and taking into account (5.4) we deduce finally that (remember $z \to g(0)+$)

$$\beta\psi_{\text{sph}} = \min_{m_t} \left[\tfrac{1}{2}\beta g(0) M^{-1} \sum_{t,s=1}^{M} m_t A_{ts} m_s - \lim_{N\to\infty} (NM)^{-1} \ln \mathcal{I}_{NM}\left(\left(M^{-1} \sum_{t=1}^{M} z_t^2\right)^{1/2}\right)\right]. \tag{5.9}$$

Appealing to the asymptotic formula (4.2) we obtain the general expression (5.1) for the spherical free energy. The magnetization in row t for the spherical model is now given by

$$\lim_{\gamma\to 0} \lim_{N\to\infty} \left\langle \frac{1}{N} \sum_{i=1}^{N} S_{it} \right\rangle = -M \frac{\partial \psi_{\text{sph}}}{\partial H_t}. \tag{5.10}$$

As before, comparison of the derivative with the stationary equations for (5.9) identifies m_t as the magnetization in row t.

In *zero field* the free energy assumes the simple form ($\nu = \beta g(0)$)

$$\beta\psi_{\mathrm{sph}} = \min_{r_t} \tfrac{1}{2}\left(\nu \sum_{t,s=1}^{M} r_t A_{ts}^{-1} r_s - (1+4\nu^2 r^2)^{1/2} + 1 + \ln \tfrac{1}{2}[1+(1+4\nu^2 r^2)^{1/2}]\right) \tag{5.11}$$

where

$$r_t = M^{-1/2} \sum_{s=1}^{M} A_{ts} m_s \tag{5.12}$$

and

$$r = \left(\sum_{t=1}^{M} r_t^2\right)^{1/2}. \tag{5.13}$$

The minimum is attained for a scalar multiple of the normalized principal eigenvector of the matrix A, that is,

$$r_t = r\left(\frac{M+1}{2}\right)^{-1/2} \sin\left(\frac{t\pi}{M+1}\right). \tag{5.14}$$

The free energy is consequently given by

$$\beta\psi_{\mathrm{sph}} = \min_{r} \tfrac{1}{2}\{\nu\lambda_1^{-1} r^2 - (1+4\nu^2 r^2)^{1/2} + 1 + \ln \tfrac{1}{2}[1+(1+4\nu^2 r^2)^{1/2}]\} \tag{5.15}$$

$$= \begin{cases} \tfrac{1}{2}(1-\eta+\ln\eta), & \eta > 1 \\ 0, & \eta < 1, \end{cases} \tag{5.16}$$

where

$$\eta = \beta g(0)\lambda_1, \tag{5.17}$$

with the principal eigenvalue of A (cf (2.2)) given by

$$\lambda_1 = 1 + 2\tau \cos\left(\frac{\pi}{M+1}\right). \tag{5.18}$$

The Curie–Weiss form (5.15) for the zero-field spherical model has been obtained by Costache (1975) using a steepest-descents method. A distinct advantage of the present method is that it allows for the calculation of the layer magnetizations. From (5.12) and (5.14) the layer magnetizations are given by

$$m_t = \lambda_1^{-1} M^{1/2} r_t = \lambda_1^{-1} r\left(\frac{M+1}{2M}\right)^{-1/2} \sin\left(\frac{t\pi}{M+1}\right) \tag{5.19}$$

where r minimizes (5.15), that is (Pearce and Thompson 1976)

$$\lambda_1^{-1} r = \begin{cases} (1-\eta^{-1})^{1/2}, & \eta > 1 \\ 0, & \eta < 1. \end{cases} \tag{5.20}$$

We conclude that the distribution of magnetization across the film in zero field is sinusoidal and given by

$$m_t = \begin{cases} (1-\eta^{-1})^{1/2}\left(\dfrac{M+1}{2M}\right)^{-1/2} \sin\left(\dfrac{t\pi}{M+1}\right), & \eta > 1 \\ 0, & \eta < 1, \end{cases} \tag{5.21}$$

with

$$\eta = \beta g(0)\left[1 + 2\tau \cos\left(\frac{\pi}{M+1}\right)\right]. \tag{5.22}$$

Notice that the distribution has the expected symmetry and concavity properties. The total magnetization is given by

$$m = M^{-1} \sum_{t=1}^{M} m_t = \begin{cases} (1-\eta^{-1})^{1/2}\left(\frac{M+1}{2M}\right)^{-1/2} M^{-1} \sum_{t=1}^{M} \sin\left(\frac{t\pi}{M+1}\right), & \eta < 1 \\ 0, & \eta > 1. \end{cases} \tag{5.23}$$

In the bulk limit, $M \to \infty$, the sum is replaced by an integral and the bulk magnetization below T_c is

$$m_0 = \lim_{M\to\infty} M^{-1} \sum_{t=1}^{M} m_t = \frac{8^{1/2}}{\pi}(1-\eta^{-1})^{1/2}. \tag{5.24}$$

This is remarkable because if the free boundary condition is replaced by periodic boundary conditions the matrix A becomes cyclic; the equation (5.14) becomes $r_t = r$ and clearly the bulk magnetization is given by

$$m_0 = \begin{cases} (1-\eta^{-1})^{1/2}, & \eta < 1 \\ 0, & \eta > 1. \end{cases} \tag{5.25}$$

The bulk magnetization is thus seen to be sensitive to the boundary conditions. A similar phenomenon has been observed by Kac (unpublished) for the Bose gas concerning the single-particle distribution function.

6. The M-spherical model

The M-spherical partition function is given by

$$Z_M = A_N^{-M} \underset{\sum_{i=1}^{N} S_{it}^2 = N}{\int \cdots \int} \mathrm{d}^{MN}S \exp(-\beta \mathscr{H}_{\text{sph}}) \tag{6.1}$$

where $\mathscr{H}_{\text{sph}}$ is the spherical interaction energy given by (1.5). We will show that the M-spherical free energy ψ_M satisfies

$$\psi_M = \psi_\infty, \tag{6.2}$$

where ψ_M is defined by

$$-\beta\psi_M = \lim_{\gamma\to 0+} \lim_{N\to\infty} (NM)^{-1} \ln Z_M \tag{6.3}$$

and ψ_∞ is given by (1.21).

Repetition of the arguments presented in the previous section for the spherical model, with the appropriate replacements for the configurational integrals, leads to coalescing bounds establishing the equality

$$\beta\psi_M = \min_{m_t}\left[\tfrac{1}{2}\beta g(0)M^{-1}\sum_{t,s=1}^{M} m_t A_{ts} m_s - \lim_{N\to\infty}(NM)^{-1}\sum_{t=1}^{M}\ln \mathscr{I}_N\left(\beta g(0)\sum_{s=1}^{M} A_{ts}m_s + \beta H_t\right)\right]. \tag{6.4}$$

The asymptotic formula (4.2) then establishes the desired result

$$\beta\psi_M = \min_{m_t} M^{-1}\left[\tfrac{1}{2}\beta g(0)\sum_{t,s=1}^{M} m_t A_{ts} m_s - \sum_{t=1}^{M}\ln \mathscr{I}_\infty\left(\beta g(0)\sum_{s=1}^{M} A_{ts}m_s + \beta H_t\right)\right], \tag{6.5}$$

proving that the $n\to\infty$ model considered in § 4 is equivalent to an M-spherical model.

Acknowledgments

The author would like to thank Professor Colin J Thompson for continued advice and encouragement, as well as for a critical reading of the manuscript. The author also acknowledges support from a Commonwealth Postgraduate Research Award.

References

Abramowitz M and Stegun I A 1964 *Handbook of Mathematical Functions* (Washington: National Bureau of Standards) p 376
Angelescu N, Costache G and Nenciu G 1972 *Phys. Stat. Solidi* B **51** 205–14
Bettoney G V and Mazo R M 1970 *J. Math. Phys.* **11** 1147–9
Costache G 1975 *Phys. Lett.* **54A** 128–30
Falk H and Ruijgrok Th W 1974 *Physica* **78** 73–90
Kac M and Helfand E 1963 *J. Math. Phys.* **4** 1078–88
Kac M and Thompson C J 1971 *Physica Norv.* **5** 163–8
Knops H J F 1973 *J. Math. Phys.* **14** 1918–20
Pearce P A and Thompson C J 1976 *Prog. Theor. Phys.* **55** 665–71
—— 1977 *J. Phys. A: Math. Gen.* **10** 571–81
Thompson C J 1974 *Physica* A **79** 113–9
Thompson C J and Silver H 1973 *Commun. Math. Phys.* **33** 53–60