Surface magnetisation of the Ising ferromagnet in a semi-infinite cubic lattice: renormalisation group approach

1989 J. Phys.: Condens. Matter 1 10129

(http://iopscience.iop.org/0953-8984/1/50/014)

J. Phys.: Condens. Matter **1** (1989) 10129–10142. Printed in the UK

Surface magnetisation of the Ising ferromagnet in a semi-infinite cubic lattice: renormalisation group approach

Anna Chame and Constantino Tsallis
Centro Brasileiro de Pesquisas Físicas—CBPF/CNPq, Rua Dr Xavier Sigaud 150, 22290 Rio de Janeiro, RJ, Brazil

Received 13 December 1988, in final form 4 May 1989

Abstract. Using a recently introduced renormalisation group method, we study the behaviour of the spontaneous surface and bulk magnetisations as functions of the temperature for an Ising ferromagnet in a semi-infinite cubic lattice for various J_S/J_B ratios (J_S and J_B respectively are the surface and bulk coupling constants). In particular we study the extraordinary transition where the surface maintains its magnetisation as the bulk disorders; we find a *discontinuity in the first derivative* of the surface magnetisation at the bulk transition temperature. The criticality of the system (universality classes, critical exponents and amplitudes) is discussed as well.

1. Introduction

Surface magnetism has attracted considerable interest during recent years due to its various applications (catalysis, corrosion, etc.) and its intrinsic theoretical and experimental richness [1]. Some experiments using techniques such as spin-polarised photoemission [2], spin-polarised low-energy electron diffraction [3] and electron-capture spectroscopy [4] are able to probe the surface critical behaviour of systems such as Ni, Cr, Gd and Tb, showing that the local magnetisation at the surface behaves, near the bulk transition temperature T_c^B, in a different way than the bulk magnetisation does. On theoretical grounds, surface magnetic order has been treated within different frameworks: the mean field approximation [5], effective field theories [6], Kikuchi-type theories [7], spin-fluctuation theories [8], the random-phase approximation [9], Monte Carlo techniques [10] and renormalisation group (RG) [11] methods (see [12] and [13] for reviews of reciprocal-space and real-space approaches respectively).

The RG techniques have been applied to semi-infinite magnetic solids usually to obtain critical exponents and phase diagrams [14, 15]; they have rarely been used to calculate surface thermodynamic functions [14, 16]. As far as we know, none of these techniques has yet been performed to obtain the surface magnetisation as function of the temperature; i.e., *the equation of state*. Recently, a real-space RG formalism was introduced [17] which allows the *direct* calculation (without going through the calculation of the thermodynamic energy [18]) of the equation of state for arbitrary values of the external parameters. In this work, we apply an extension of this formalism to the non-homogeneous case [19] (where we allow for different coupling constants in the system)

0953-8984/89/5010129 + 14 $02.50

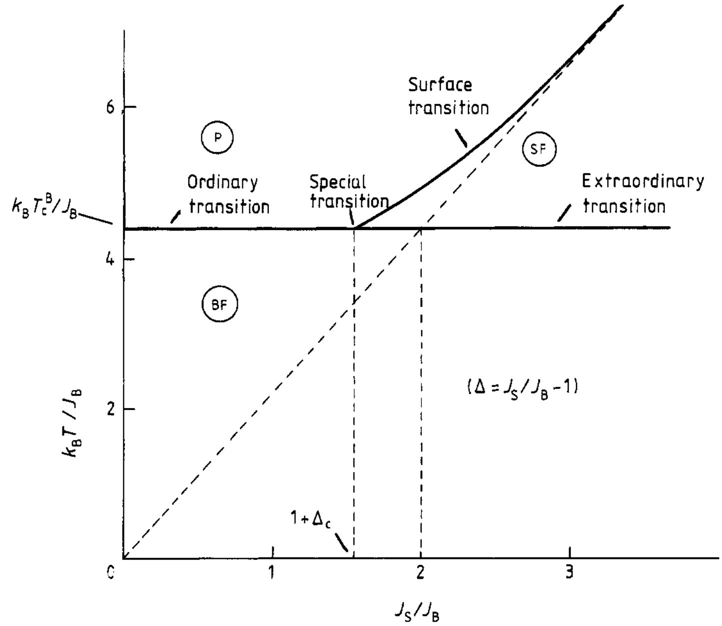


Figure 1. Phase diagram for the Ising ferromagnet in the semi-infinite cubic lattice with a (001) free surface. In the bulk ferromagnetic (BF) phase both the bulk and surface are magnetically ordered; in the surface ferromagnetic (SF) phase only the surface remains ordered; in the paramagnetic (P) phase both are disordered.

to study the Ising ferromagnet in a semi-infinite cubic lattice with a free surface (001). In our calculations the free surface coupling constant $J_S (J_S \geq 0)$ can be different from the bulk coupling constant $J_B > 0$.

We obtain the surface and bulk magnetisation curves as functions of the temperature and we study their behaviour as J_S/J_B varies. We also obtain the surface and bulk magnetisation exponents β and amplitudes A for the various types of transitions which may occur.

In § 2 we present the model and the formalism and in § 3 the results; finally, we present our conclusions in § 4.

2. The model and RG formalism

We consider a semi-infinite simple cubic lattice with a (001) free surface. The first-neighbouring sites interact according to

$$\mathcal{H} = -\sum_{\langle i,j \rangle} J_{ij} \sigma_i \sigma_j \qquad (\sigma_i = \pm 1, \forall i)$$

where the coupling constant J_{ij} equals J_S ($J_S \geq 0$) if both sites i and j belong to the free surface and equals J_B ($J_B > 0$) otherwise (let us introduce $\Delta \equiv J_S/J_B - 1$).

The phase diagram for this system is known to be as indicated in figure 1. If $\Delta < \Delta_c$, for temperatures below the critical bulk temperature ($T < T_c^B$) we have the bulk ferromagnetic (BF) phase, where both the bulk and the surface are magnetically ordered; for

$T > T_c^B$, the bulk and the surface are disordered (paramagnetic (P) phase). If $\Delta > \Delta_c$, a third phase becomes possible at intermediate values of T, between the bulk ferromagnetic and paramagnetic phases. At this region, for T above T_c^B and up to $T_c^S(\Delta)$, the surface remains magnetically ordered while the bulk order is absent (surface ferromagnetic (SF) phase).

It is known that this system is associated with several universality classes. To illustrate them, we recall the thermal critical behaviour associated with the magnetisation. The bulk magnetisation M_B behaves near T_c^B, for all values of Δ, as $M_B(T) \sim A_{3D}(1 - T/T_c^B)^{\beta^{3D}}$. The critical behaviour associated with the surface magnetisation M_S is: (i) for $\Delta < \Delta_c$, $M_S(T) \sim A_{ord}(1 - T/T_c^B)^{\beta^{ord}}$; (ii) for $\Delta = \Delta_c$, $M_S(T) \sim A_{sp}(1 - T/T_c^B)^{\beta^{sp}}$; (iii) for $\Delta > \Delta_c$, $M_S \sim A_S(1 - T/T_c^S(\Delta))^{\beta^{2D}}$. We also expect a fifth non trivial singularity to be present in this problem: for $\Delta > \Delta_c$, M_S near T_c^B behaves as

$$M_S(T) - M_S(T_c^B) \sim \begin{cases} A_-(1 - T/T_c^B)^{\beta^{ex}} & \text{for } T \to T_c^B - 0 \\ -A_+(T/T_c^B - 1)^{\beta^{ex}} & \text{for } T \to T_c^B + 0, \end{cases}$$

since it is reasonable that it reflects somehow the bulk singularity.

To obtain the surface and bulk spontaneous magnetisations as functions of the temperature we will briefly summarize the RG method previously mentioned, while applying it to our system.

We first consider a d_B-dimensional bulk lattice of linear size L with a privileged surface in d_S-dimensions, the dimensionless coupling constants being $K_S = J_S/k_BT$ at this surface and $K_B = J_B/k_BT$ otherwise. We consider the special limit $L \to \infty$ such that the privileged surface gives rise to a free surface in a semi-infinite lattice. In this limit, we define the bulk and surface order parameters as $M_B = N_L^B(K_B)/L^{d_B}$ and $M_S = N_L^S(K_B, K_S)/L^{d_S}$, where $N_L^B(N_L^S)$ is the thermal average number of bulk (surface) sites whose spin is pointing along the easy magnetisation direction minus those whose spin is in the opposite direction. We associate with each site of the semi-infinite lattice a dimensionless magnetic dipole μ. We could in principle have a fixed μ but we will rather leave it as a variable of the RG transformation, just as K_B and K_S.

We transform (following Kadanoff ideas) the original system into a similar one of linear size L' ($l \equiv$ linear expansion factor $= L/L' > 1$) with renormalised variables K_B', K_S' and μ'. We impose the condition that through renormalisation, both the *total bulk magnetic moment* and the *total surface magnetic moment* must be preserved (since they are extensive quantities). We have, for the total bulk magnetic moment

$$N_{L'}^B(K_B')\mu' = N_L^B(K_B)\mu, \tag{1}$$

where the thermal averages $N_{L'}^B(K_B')$ and $N_L^B(K_B)$ are to be taken over the bulk sites of our system. We have a similar equation for the total surface magnetic moment, which involves thermal averages such as $N_{L'}^S(K_B', K_S')$ and $N_L^S(K_B, K_S)$ taken at the surface sites. We will work only with the bulk relation for simplicity and at the end we will recover the corresponding relation for the surface.

Dividing both sides of (1) by L^{d_B}, we obtain:

$$M_B(K_B')\mu' = l^{d_B} M_B(K_B)\mu, \tag{2}$$

where $M_B(K_B') = N_{L'}^B(K_B')/L'^{d_B}$.

At this point, it is worthy to discuss the connection between equation (2) and equation (2.64) of Niemeijer and van Leeuwen [18]. From a general expression for the free energy, they obtain the derivative of the free energy with respect to any odd-spin coupling. In particular, considering the magnetic field h as the odd-spin coupling, they have an expression for the magnetisation which is written as a sum of terms corresponding to all renormalised couplings that have been generated. This expression is similar to our equation (2) for an approximate renormalisation group in which no odd-spin couplings (besides the magnetic field) are generated (the summation then reduces to one term). Furthermore, to compare equations (2) and (2.64) we should identify $\mu'/\mu = \partial h'/\partial h$. However, we note that the assumptions we used to obtain equation (2) are quite different from theirs. Let us stress that μ is a variable introduced phenomenologically while h in [18] is a coupling which appears in the Hamiltonian. Let us anticipate here that the approximate RG we use preserves the two-body correlation function in a graph (see [21]). This is not strictly the same as to preserve, within some approximation, the partition function of the system [18]. In our case it is frequently possible to work in a closed parameter space.

Starting with K_B and $\mu^{(0)}$, let us now perform n iterations in (2), which leads to

$$M_B(K_B^{(n)})\mu^{(n)} = l^{nd_B} M_B(K_B)\mu^{(0)} \tag{3}$$

In the $n \to \infty$ limit, arbitrarily choosing [19] $\mu^{(0)} = 1$ we obtain

$$M_B(K_B) = \lim_{n\to\infty} \frac{M_B(K_B^{(n)})\mu^{(n)}}{l^{nd_B}}. \tag{4a}$$

Analogously, we also find a relation for the surface order parameter

$$M_S(K_B, K_S) = \lim_{n\to\infty} \frac{M_S(K_B^{(n)}, K_S^{(n)})\mu^{(n)}}{l^{nd_S}}. \tag{4b}$$

The equations (4a) and (4b) are to be used together with the RG recurrence equations for K_B' and K_S', to be described further. For Ising ferromagnetic systems with a free surface, these equations will give rise to a phase diagram with three distinct regions, namely the P, BF and SF ones (see figure 1). In the paramagnetic region, (K_B, K_S) is attracted through successive renormalisations towards $(K_B^{(\infty)}, K_S^{(\infty)}) = (0, 0)$. Since $M_B(K_B^{(\infty)}) = 0$ and $M_S(K_B^{(\infty)}, K_S^{(\infty)}) = 0$, we obtain (through (4$a$) and (4$b$))

$$M_B(K_B) = 0 \tag{5a}$$

$$M_S(K_B, K_S) = 0 \tag{5b}$$

in the *entire* paramagnetic region, as expected. If (K_B, K_S) is attracted towards $(K_B^{(\infty)}, K_S^{(\infty)}) = (\infty, \infty)$, which is associated with the bulk ferromagnetic phase, we have $M_B(K_B^{(\infty)}) = 1$ and $M_S(K_B^{(\infty)}, K_S^{(\infty)}) = 1$ (conventional value for the order parameters M_B and M_S when both the bulk and the surface are completely ordered). Then (4a) and (4b) give

$$M_B(K_B) = \lim_{n\to\infty} \frac{\mu^{(n)}}{l^{nd_B}}, \tag{6a}$$

$$M_S(K_B, K_S) = \lim_{n\to\infty} \frac{\mu^{(n)}}{l^{nd_S}}, \tag{6b}$$

for the bulk ferromagnetic phase. In the surface ferromagnetic region, (K_B, K_S) is attracted towards $(K_B^{(\infty)}, K_S^{(\infty)}) = (0, \infty)$ which corresponds to the situation where the

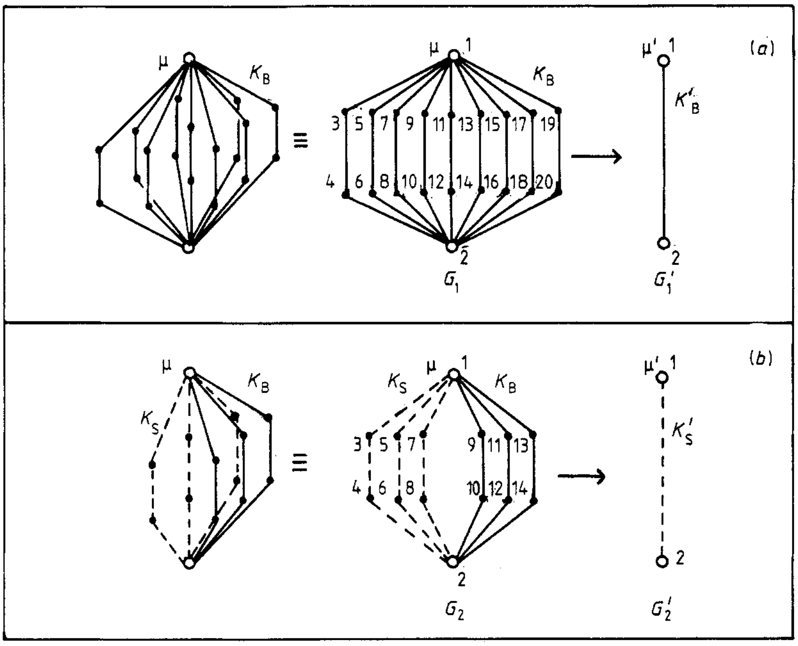


Figure 2. RG cell transformation: (*a*) associated with the bulk (coupling constant K_B); (*b*) associated with the surface (coupling constant K_S). The terminal sites are always denoted by 1 and 2; the other numerical labels denote internal sites. The lattice generated by iterative application of graph G_1 is an example of hierarchical lattice.

surface is completely ordered and the bulk disordered. Then we have $M_B(K_B^{(\infty)}) = 0$ and $M_S(K_B^{(\infty)}, K_S^{(\infty)}) = 1$ which yields, through (4*a*) and (4*b*)

$$M_B(K_B) = 0, \tag{7a}$$

$$M_S(K_B, K_S) = \lim_{n\to\infty} \frac{\mu^{(n)}}{l^{nd_S}}, \tag{7b}$$

for the surface ferromagnetic phase.

To close the procedure we must now specify how to obtain the RG recurrence relations for K_B, K_S and μ.

Following the Migdal–Kadanoff scheme (which was first introduced to study the semi-infinite Ising model in [14]), we shall use the same simple cluster transformations already introduced in [15] for the Potts (and related models) surface magnetism. The cells for the bulk and the free surface region are shown respectively in Figures 2(*a*) and 2(*b*). The transformation indicated in figure 2(*a*) simulates, through the standard bond-moving procedure, the renormalisation of the bulk of our system. In the left hand side of this figure we show an intermediate step in the construction of the final graph: a cluster composed of eight cubes in which the horizontal bonds have already been moved, and the sites at the top and at the bottom of the cluster have been collapsed into two terminals. In figure 2(*b*) the transformation is of the same type: the larger cell is assumed to lay on the free surface of our system in such a way that $\frac{1}{3}$ of its initial 27 bonds are outside the semi-infinite lattice, and therefore 9 bonds are absent.

At this point, we shall remark that as we are in fact approximating a Bravais lattice by hierarchical ones (see caption of figure 2) the factors l^{d_B} and l^{d_S} in equations (6) and (7) must be replaced [20] by $l^{d^{bb'}_\mathrm{B}}$ and $l^{d^{bb'}_\mathrm{S}}$, which will be defined in what follows.

For the transformation of figure 2(a), in which all the couplings constants are the same (homogeneous case, i.e., $K_\mathrm{B} = K_\mathrm{S}$), $l^{d^{bb'}_\mathrm{B}}$ is given by [17]

$$l^{d^{bb'}_\mathrm{B}} = \frac{N_{b_1}}{N_{b'_1}} \tag{8}$$

where N_{b_1} and $N_{b'_1}$ are respectively the number of bonds of graphs G_1 and G'_1 (which have chemical distances b_1 and b'_1 between their terminals).

For the transformations of figure 2(b) (inhomogeneous case) where we have arbitrary K_B and K_S, definition (8) has been extended [19] into

$$l^{d^{bb'}_\mathrm{S}} = \frac{N^\mathrm{B}_{b_2} + N^\mathrm{S}_{b_2} K_\mathrm{S}/K_\mathrm{B}}{N^\mathrm{B}_{b'_2} + N^\mathrm{S}_{b'_2} K'_\mathrm{S}\; K'_\mathrm{B}} \tag{9}$$

where $N^\mathrm{B}_{b_2}$ and $N^\mathrm{S}_{b_2}$ ($N^\mathrm{B}_{b'_2}$ and $N^\mathrm{S}_{b'_2}$) are the numbers of bonds of graph $G_2(G'_2)$ respectively associated with K_B and K_S (K'_B and K'_S), and $b_2(b'_2)$ is the chemical distance between terminals in the graph. Definition (9) is the simplest continuous expression which recovers the homogeneous definition (8) in the particular cases $(K_\mathrm{S}/K_\mathrm{B}, K'_\mathrm{S}/K'_\mathrm{B}) = (0, 0), (1, 0), (0, 1)$ and $(1, 1)$.

Let us come back to the determination of the K_B, K_S and μ recurrences relations. We impose that the correlation function between the two roots of the graphs G_1 and G'_1 (G_2 and G'_2) must be preserved, i.e. (see, for instance, reference [21]),

$$\mathrm{e}^{-\beta\mathcal{H}'_{\mathrm{B}_{12}}} = \operatorname*{Tr}_{3,\ldots,20} \mathrm{e}^{-\beta\mathcal{H}_{\mathrm{B}_{123\ldots20}}}, \tag{10}$$

$$\mathrm{e}^{-\beta\mathcal{H}'_{\mathrm{S}_{12}}} = \operatorname*{Tr}_{3,\ldots,14} \mathrm{e}^{-\beta\mathcal{H}_{\mathrm{S}_{123\ldots14}}}, \tag{11}$$

with

$$-\beta\mathcal{H}'_{\mathrm{B}_{12}} = K'_\mathrm{B}\sigma_1\sigma_2 + K^0_\mathrm{B}, \tag{12a}$$

(associated with graph G'_1),

$$-\beta\mathcal{H}_{\mathrm{B}_{123\ldots20}} = K_\mathrm{B}(\sigma_1\sigma_3 + \sigma_1\sigma_5 + \sigma_1\sigma_7 + \ldots + \sigma_3\sigma_4 + \sigma_5\sigma_6 + \sigma_7\sigma_8 + \ldots + \sigma_4\sigma_2 + \sigma_6\sigma_2 + \sigma_8\sigma_2 + \ldots), \tag{12b}$$

(associated with graph G_1),

$$-\beta\mathcal{H}'_{\mathrm{S}_{12}} = K'_\mathrm{S}\sigma_1\sigma_2 + K^0_\mathrm{S}, \tag{12c}$$

(associated with graph G'_2) and

$$-\beta\mathcal{H}_{\mathrm{S}_{123\ldots14}} = K_\mathrm{S}(\sigma_1\sigma_3 + \sigma_1\sigma_5 + \sigma_1\sigma_7 + \sigma_3\sigma_4 + \sigma_5\sigma_6 + \sigma_7\sigma_8 + \sigma_4\sigma_2 + \sigma_6\sigma_2 + \sigma_8\sigma_2) + K_\mathrm{B}(\sigma_1\sigma_9 + \sigma_1\sigma_{11} + \sigma_1\sigma_{13} + \sigma_9\sigma_{10} + \sigma_{11}\sigma_{12} + \sigma_{13}\sigma_{14} + \sigma_{10}\sigma_2 + \sigma_{12}\sigma_2 + \sigma_{14}\sigma_2) \tag{12d}$$

(associated with graph G_2). K_B^0 and K_S^0 are two constants to be determined. Equations (10) and (11) uniquely determine

$$K_B' = f(K_B), \tag{13}$$

and

$$K_S' = g(K_B, K_S). \tag{14}$$

Following [17], we will now establish the recurrence equation for μ. In order to break the symmetry (a condition needed for establishing the equations for the order parameter) we impose that in all graphs of figure 2 one of the terminal spins, say spin 1, is fixed. We consider all possible configurations for the other sites and associate with each configuration the corresponding Boltzmann weight and magnetic moment. We obtain the magnetic moment m associated with a given configuration adding all sites contributions. In the homogeneous case ($K_S/K_B = 1$) we know that each site contributes proportionally to its coordination number [17]. This is due to the fact that we are approaching a Bravais lattice (translationally invariant and consequently having a spatially uniform order parameter) by a hierarchical one (scale invariant and having a non uniform order parameter in space). In the non-homogeneous case ($K_S \neq K_B$) each site contributes proportionally to its *average coordination number*, which is defined by attributing to each bond a weight proportional to its coupling constant (this is the simplest continuous definition which recovers that of the homogeneous case for $K_S/K_B = 1$). This definition has already been tested for the Potts ferromagnet in anisotropic square lattice [19], yielding results in good agreement with other calculations. In table 1 we present, as an example, a few configurations for graphs G_1 and G_1' (associated with the bulk, where we only have the coupling constant K_B). In table 2 we illustrate the same procedure for graphs G_2 and G_2', which are associated with the surface, where we have both coupling constants K_B and K_S. Finally we impose, as we did in equation (1), that the thermal average *total magnetic moment* in the original and renormalised clusters is preserved, for both the bulk and surface RG transformations respectively:

$$\langle m \rangle_{G_1} = \langle m \rangle_{G_1'} \tag{15}$$

$$\langle m \rangle_{G_2} = \langle m \rangle_{G_2'} \tag{16}$$

These equations have the form

$$\mu_B' = j(K_B)\mu_B \tag{17}$$

$$\mu_S' = k(K_B, K_S)\mu_S \tag{18}$$

as we can see inspecting tables 1 and 2. Equation (17) must enter into equation (6*a*), while equation (18) must enter into equation (6*b*) and equation (7*b*).

Summarising, we use equations (5), (6), (7) together with equations (13), (14) and (17), (18) to obtain the surface and bulk spontaneous magnetisations. For the transformation of figure 2(*a*), $l^{d_B^{bb'}} = 27$ (homogeneous case) and for the one of figure 2(*b*), $l^{d_S^{bb'}} = (9 + 9K_S/K_B)/(K_S'/K_B')$ (non-homogeneous case).

3. Results

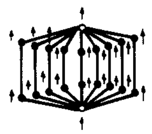
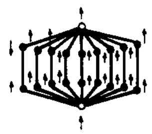
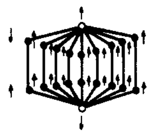
The curves we have obtained for the surface spontaneous magnetisation for $J_S/J_B = 0, 0.5, 1$ and 1.5 are presented in figure 3. We also present the curve for the bulk

Table 1. Establishment of equation (15) for the bulk RG transformation. (*a*) Possible configurations for the graph G_1'; $\langle m \rangle_{G_1'} = e^{K_B'} 2\mu_B'/(e^{K_B'} + e^{-K_B'})$. (*b*) Three of the 2^{19} possible configurations for the graph G_1; $\langle m \rangle_{G_1} = (54e^{27K_B} + 50e^{23K_B} + 32e^{5K_B} + \ldots)\mu_B/(e^{27K_B} + e^{23K_B} + e^{5K_B} + \ldots)$.

(*a*)

G_1' configuration	Weight	m
	$e^{K_B'}$	$2\mu_B'$
	$e^{-K_B'}$	0

(*b*)

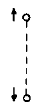
G_1 configuration	Weight	m
	e^{27K_B}	$54\mu_B$
	e^{23K_B}	$50\mu_B$
	e^{5K_B}	$32\mu_B$

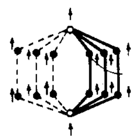
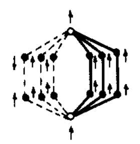
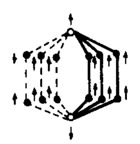
spontaneous magnetisation. Since $\Delta < \Delta_c$ ($\Delta_c = 0.74$ in the present RG procedure [15]), the surface and bulk order at, for decreasing temperatures, the same temperature T_c^B (*ordinary* transition). We observe that the surface magnetisation curve, as Δ is increased, gradually approaches the bulk one and, for $\Delta \lesssim \Delta_c$, it lays *above* this curve.

If $\Delta = \Delta_c$, the surface still disorders at the same temperature T_c^B than the bulk, but this transition (*special transition*) is characterised by a different set of critical exponents. The corresponding surface magnetisation curve is presented in figure 4 with the bulk curve.

In figure 5 we present the surface magnetisation curves for $J_S/J_B = 2, 2.5$ and 3; these values of J_S/J_B correspond to $\Delta > \Delta_c$. In this case the bulk orders in the presence of an already ordered surface. We have the *surface* transition at $T_c^S(\Delta) > T_c^B$ from a ferromagnetic surface phase to a paramagnetic phase and the *extraordinary* transition at

Table 2. Establishment of equation (16) for the surface RG transformation. (*a*) Possible configurations for the graph G_2'; $\langle m\rangle_{G_2'} = e^{K_S'} 2\mu_S'/(e^{K_S'} + e^{-K_S'})$. (*b*) Three of the 2^{13} possible configurations for the graph G_2; $\langle m\rangle_{G_2} = (e^{9K_B+9K_S}(18 + 18K_S/K_B) + e^{9K_B+5K_S}(18 + 14 K_S/K_B) + e^{3K_B-K_S}(12 + 8K_S/K_B) + \ldots)\mu_S/(e^{9K_B+9K_S} + e^{9K_B+5K_S} + e^{3K_B-K_S} + \ldots)$.

(*a*) G_2' configuration	Weight	m
	$e^{K_S'}$	$2\mu_S'$
	$e^{-K_S'}$	0

(*b*) G_2 configuration	Weight	m
	$e^{9K_B+9K_S}$	$(18+18\,K_S/K_B)\mu_S$
	$e^{9K_B+5K_S}$	$(18+14\,K_S/K_B)\mu_S$
	$e^{3K_B-K_S}$	$(12+8\,K_S/K_B)\mu_S$

T_c^B, where the surface magnetisation curve is believed to present some kind of weak singularity. We obtain that the temperature first derivative of the surface magnetisation is *discontinuous* at T_c^B, and that just above T_c^B the tendency of the surface to disorder is weaker than just below. This result might surprise at first sight since we know that bulk order must enhance surface order. We verify that $\beta^{ex} = 1$ and that A_-/A_+ is roughly equal to 4, for typical ratios of J_S/J_B. Mean-field (MF) theories [5] for the extraordinary transition give

$$\tilde{m} = 1 - \tfrac{1}{2}\tilde{t} - \tfrac{1}{8}\tilde{t}^2 + 0(\tilde{t}^3), \qquad \tilde{t} > 0$$

$$\tilde{m} = 1 - \tfrac{1}{2}\tilde{t} - \tfrac{1}{9}\tilde{t}^2 + 0(\tilde{t}^3), \qquad \tilde{t} < 0$$

with $\tilde{m} \propto M_S$ and $\tilde{t} \propto (T - T_c^{MF})$, i.e., the leading singularity would occur at $0(\tilde{t}^2)$ (the discontinuity only appears in the *second* derivative at $\tilde{t} = 0$). Bray and Moore [5] define

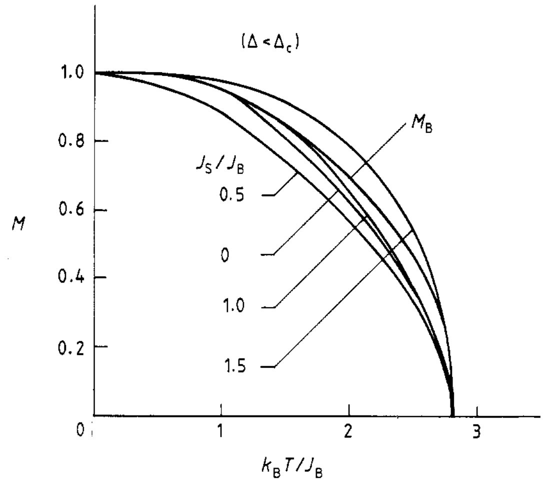


Figure 3. Surface spontaneous magnetisation M_S as a function of the temperature for the Ising ferromagnet in a semi-infinite simple cubic lattice with free surface (001). $J_S/J_B = 0$, 0.5, 1 and 1.5 ($\Delta < \Delta_c$). The bulk magnetisation M_B is also shown as a reference.

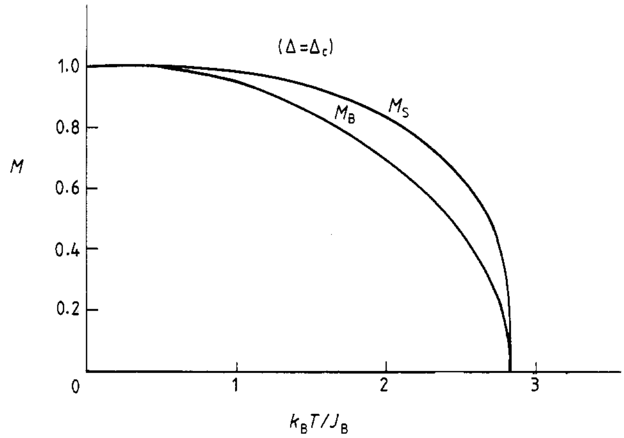


Figure 4. Surface magnetisation M_S as a function of the temperature for $\Delta = \Delta_c$. The bulk magnetisation M_B is also shown.

a β-exponent (β_1^e according to their notation) which is identified with the exponent of the term which presents the singularity. They find $\beta_1^e = 2$ (as we have found different amplitudes above and below T_c^B for the *linear* term, we have $\beta_1^e = \beta^{ex} = 1$). Based on scaling arguments, Bray and Moore state that the singularity in the surface magnetisation is identical to that in the bulk free energy (hence it is valid *outside* mean-field theory) and consequently $\beta_1^e = 2 - \alpha$, where α is the bulk specific heat exponent. Giving support to the possible *continuity*, at T_c^B, of the first derivative of $M_S(T)$, there are also experimental data of Rau and Robert [4] in Gd (which seems to be close to a Heisenberg ferromagnet). On the other hand, a result similar to ours has been obtained, using RPA, for a Heisenberg semi-infinite ferromagnet [9]. Also effective field theories with

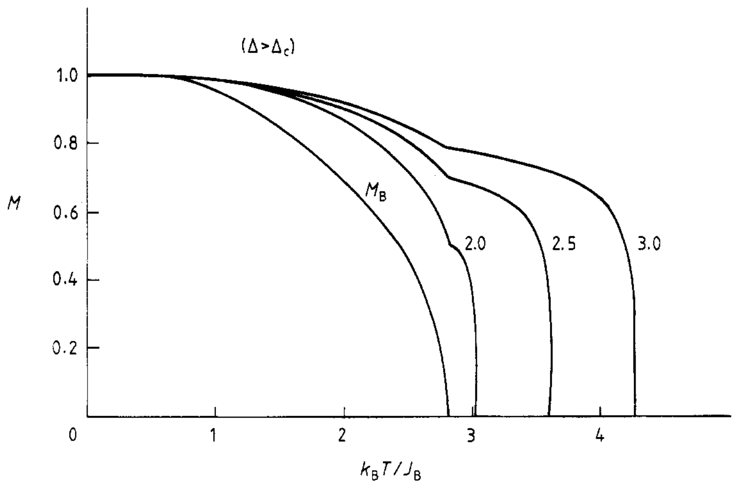


Figure 5. Surface magnetisation M_S as a function of the temperature for $\Delta > \Delta_c$; $J_S/J_B = 2$, 2.5 and 3. At T_c^B there is a discontinuity in the first temperature derivative of M_S. The bulk magnetisation M_B is also shown.

correlation have suggested a discontinuity of the first derivative of $M_S(T)$ at T_c^B for an Ising model and for this model in a transverse field [6]. Furthermore, there are accurate experiments [22] measuring surface tension at the λ transition on liquid ^{4}He (whose criticality is expected to be the same as that of some surface magnetic systems), which suggests a *discontinuity* in the first derivative, conflicting with some theoretical predictions for the system. The point is still controversial. Let us present some qualitative arguments which could enlighten the cause of what we find, i.e., a *discontinuity* in the first derivative of $M_S(T)$. The bulk acts on the surface magnetisation through two different physical channels. The first one is the obvious fact that the bulk magnetisation, as long as non-vanishing, acts as an effective field on the surface. The second channel, more subtle, refers to bulk susceptibility effects near T_c^B, where the bulk susceptibility diverges ($\chi(T) \sim C_-(1 - T_c^B)^{-\gamma}$ for $T \rightarrow T_c - 0$ and $\chi(T) \sim C_+(T/T_c^B - 1)^{-\gamma}$ for $T \rightarrow T_c + 0$). In the neighbourhood of T_c^B, the paramagnetic-side amplitude of the bulk susceptibility (C_+) is greater (*two* times greater in standard mean-field calculations) than that of the ferromagnetic-side bulk susceptibility (C_-). The effect of the paramagnetic-side bulk susceptibility might overcome both the effects of the vanishing bulk field and of the bulk susceptibility just below T_c^B. This suggests an explanation for the *decrease* in the tendency of the surface to disorder in the region just above T_c^B (i.e., $A_- > A_+$). The fact that mean-field calculation yield $A_+ = A_-$ would be fortuitous and possibly related to the factor 2 mentioned above. Our results are in disagreement with those obtained by Bray and Moore [5], where some scaling arguments have been assumed.

The present RG formalism yields the values of T_c^B, $T_c^S(\Delta)$ (through the recurrence relations for K_B' and K_S' in the standard way), the β exponent for each transition and the corresponding amplitude A. They are shown in table 3 and compared with other estimates whenever available.

Let us mention an unexpected feature which appears as J_S/J_B decreases, for $J_S/J_B \ll 1$: a slight non-monotonicity of the surface magnetisation. We expect [25] that, for a given value of J_S/J_B, we must always have a surface magnetisation curve which is below

Table 3. Present RG values for the critical temperatures, exponents β and the corresponding amplitudes A for each transition. Other estimates are also shown whenever available.

Bulk magnetisation			
β^{3D}	$k_B T_c^B / J_B$		A_{3D}
0.46 (present RG)	2.82 (present RG)		1.24 (present RG)
0.312[24]	2.3062 (Series[23])		—

Surface magnetisation			
Ordinary transition			
β^{ord}	J_S/J_B		A_{ord}
0.55 (present RG)	0.5		1.1
0.78 (Monte Carlo[10])	1.0		1.2
0.82 (ε expansion[12])	1.5		1.8
Special transition			
β^{sp}	J_S/J_B		A_{sp}
0.21 (present RG)	1.74 (present RG)		
0.175 (Monte Carlo[10])	1.6 (Series[10])		0.6
0.25 (ε expansion[12])	1.5 (Monte Carlo[10])		
Surface transition			
β^{2D}	J_S/J_B	$T_c^S(J_S/J_B)$	A_S
0.17 (present RG)	2	3.03	0.8
0.125 (exact[23])	2.5	3.61	0.92
	3	4.26	0.96
Extraordinary transition			
β^{ex}	J_S/J_B	A_-	A_+
1.0 (present RG)	2	3.0	0.8
1 (Mean field[5])	2.5	1.1	0.3
	3.0	0.6	0.17

the one associated with a greater value of J_S/J_B. Instead of that, at $J_S/J_B \simeq 0.35$ we find that the surface magnetisation begins to increase, as J_S/J_B is lowered. We can see in figure 3 the surface magnetisation curve for $J_S/J_B = 0.5$ which is *below* the curves for $J_S/J_B = 1$ and 1.5, as expected. But the surface magnetisation curve for $J_S/J_B = 0$, for instance, is *above* the $J_S/J_B = 0.5$ one. This regime change at $J_S/J_B \simeq 0.35$ is directly connected with a RG flow regime change in the corresponding phase diagram. Indeed the flow line connecting the BF and P phases attractors as well as the fixed point which lies on the P–BF critical frontier precisely corresponds to $J_S/J_B \simeq 0.35$. As we are using an approximate RG procedure, this effect could be a spurious one.

4. Conclusion

A real-space RG scheme has been applied to the Ising model in a semi-infinite cubic lattice in order to obtain the equations of state for this system. The surface and bulk spontaneous magnetisation curves as functions of the temperature present the qualitative behaviour expected for $\Delta < \Delta_c$, $\Delta = \Delta_c$ and $\Delta > \Delta_c$. We find for the extraordinary transition ($\Delta > \Delta_c$) the critical exponent $\beta^{ex} = 1$ and a *discontinuity* in the first derivative of the surface magnetisation. This last result differs from the mean-field prediction (*continuity* in the first derivative). Bulk susceptibility effects on the surface at T_c^B may explain this discrepancy since mean-field theories do not properly take into account fluctuations. At the light of our renormalisation-group results for an Ising ferromagnet we see that the result $A_+/A_- = 1$ experimentally obtained by Rau and Robert might either be due to the fact that Gd seems to be closer to a Heisenberg ferromagnet than to an Ising one, or it should not be considered the generic situation, and its comprehension should be searched elsewhere. To clarify this point, it would be interesting to study, within the present RG scheme extended to quantum systems [26] or some other technique, the anisotropic Heisenberg model with particular focus on the Heisenberg ↔ Ising crossover.

In the vicinity of the various critical temperatures we have obtained the correspondent β exponents (according to what is expected on the basis of universality arguments) and amplitudes A in reasonable agreement with other estimates whenever available.

Acknowledgments

We acknowledge fruitful discussions with E V L de Mello, E M F Curado, N Majlis, S Selzer, J L Móran-López, J M Sanchez and F Y Wu as well as useful remarks from H Herrmann and G Schwacchheim.

References

[1] Binder K 1983 in *Phase Transitions and Critical Phenomena* ed. C Domb and J L Lebowitz, vol 8 (Academic Press)
[2] Cerri A, Mauri D and Landolt M 1983 *Phys. Rev.* B **27** 6526
[3] Alvarado S, Campagna M and Hopster H 1982a *Phys. Rev. Lett.* **48** 51
Alvarado S F, Campagna M, Ciccacci F and Hopster H 1982b *J. Appl. Phys.* **53** 7920
Weller D, Alvarado S F, Gudat W, Schröder K and Campagna M 1985 *Phys. Rev. Lett.* **54** 1555
[4] Rau C and Eichner S 1980 in *Nuclear Methods in Materials Research* ed. K Bethge, H Bauman, H Jex and F Rauch (Vieweg: Braunscheig)
Rau C and Eichner S 1986 *Phys. Rev.* B **34** 6347
Rau C and Robert M 1987 *Phys. Rev. Lett.* **58** 2714
Rau C, Jin C and Robert M 1988 *J. Appl. Phys.* **63** 3667
[5] Mills D L 1971 *Phys. Rev.* B **3** 3887
Lubensky T C and Rubin M H 1975 *Phys. Rev.* B **12** 3885
Bray A J and Moore M A 1977 *J. Phys. A: Math. Gen.* **10** 1927
[6] Tamura I, Sarmento E F, Fittipaldi I P and Kaneyoshi T 1983 *Phys. Stat. Sol.* B **118** 409
Sarmento E F, Tamura I and Kaneyoshi T 1984 *Z. Phys.* B **54** 241; Kaneyoshi T, preprint
[7] Sánchez J M, and Morán-López J L 1986 in *Magnetic Properties of Low-Dimensional Systems* ed. L M Falicov and J L Móran-López (Springer-Verlag)
Sanchez J M and Móran-López J L 1987 *Phys. Rev. Lett.* **58** 1120

[8] Bennemann K H in *Magnetic Properties of Low-Dimensional Systems* ed. L M Falicov and J L Morán-López (Springer-Verlag)
[9] Selzer S and Majlis N 1983 *Phys. Rev.* B **27** 544
[10] Binder K and Hohenberg P C 1974 *Phys. Rev.* B **9** 2194
Binder K and Landau D P 1984 *Phys. Rev. Lett.* **52** 318
[11] Svrakić N M and Wortis M 1977 *Phys. Rev.* B **15** 396
Burkhadt T W and Eisenriegler E 1978 *Phys. Rev.* B **17** 318
Diehl H W and Dietrich S 1980 *Phys. Lett.* **80** A408
[12] Diehl W 1986 in *Phase Transitions and Critical Phenomena* ed. C Domb and J L Lebowitz, vol 10 (Academic Press)
[13] Tsallis C 1986 in *Magnetic Properties of Low-Dimensional Systems* ed. L M Falicov and J L Morán-López (Springer-Verlag)
[14] Lipowsky R and Wagner H 1981 *Z. Phys.* B **42** 355
[15] Tsallis C and Sarmento E F 1985 *J. Phys. C: Solid State Phys.* **18** 2777
[16] Svrakić N M, Pandit R and Wortis M 1980 *Phys. Rev.* B **22** 1286
[17] Caride A O and Tsallis C 1987 *J. Phys. A: Math. Gen.* **20** L665
[18] Niemeijer Th and van Leeywen J M J 1976 in *Phase Transitions and Critical Phenomena* ed. C Domb and M S Green, vol 6 (New York: Academic)
[19] Chame A, Tsallis C and Costa U M S 1988 *Phys. Rev.* B **37** 7549
[20] Melrose J R 1983 *J. Phys. A: Math. Gen.* **16** 3077; **16** L407
[21] Essam J W and Tsallis C 1986 *J. Phys. A: Math. Gen.* **19** 409
[22] Magerlein J H and Sanders T M 1976 *Phys. Rev. Lett.* **36** 258
[23] See, for example Wu F Y 1982 *Rev. Mod. Phys.* **54** 235
[24] See, for example Domb C 1974 in *Phase Transitions and Critical Phenomena* ed. C Domb and M S Green, vol 3 (New York: Academic)
[25] Griffiths R B 1972 in *Phase Transitions and Critical Phenomena* ed. C Domb and M S Green, vol 1 (New York: Academic)
[26] Caride A O, Tsallis C and Zanette S I 1983 *Phys. Rev. Lett.* **51** 145; **51** 616
Mariz A M, Tsallis C and Caride A O 1985 *J. Phys. C: Solid State Phys.* **18** 4189