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SURFACE MAGNETIZATION OF THE ISING FERROMAGNET IN SEMI-INFINITE CUBIC LATTICE: RENORMALIZATION GROUP APPROACH

by

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ABSTRACT

Through a recently introduced renormalization group method, we study the behaviour of the spontaneous surface and bulk magnetizations as functions of the temperature for the Ising ferromagnet in a semi-infinite cubic lattice for various ratios J_S/J_B (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 magnetization as the bulk disorders; we find a *discontinuity on the first derivative* of the surface magnetization at the bulk transition temperature. The criticality of the system (universality classes, critical exponents and amplitudes) is discussed as well. Finally, we observe an unexpected slight lack of monotonicity of the surface magnetization as a function of J_S/J_B for $J_S/J_B \lll 1$.

Key-words: Surface magnetism; Phase transitions; Renormalization group; Ising problems.

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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 polarized photo emission[2], spin-polarized low-energy electron diffraction[3] and electron-capture spectroscopy[4] are able to get information on the surface critical behaviour of ferromagnets such as Ni, Cr and Gd, showing that the local magnetization at the surface behaves, near the bulk transition temperature T_c^B, in a different way than the bulk magnetization does. On theoretical grounds, surface magnetic order has been treated within different frameworks: Mean Field approximation[5], effective field theories[6], Kikuchi type theories[7], Spin-fluctuation theories[8], random-phase-approximation[9], Monte Carlo techniques[10] and Renormalization Group[11] (RG) methods (see ref. 12 and 13 for reviews of reciprocal-space and real-space approaches respectively).

Usually RG techniques have been applied to semi-infinite magnetic solids to obtain critical exponents and phase diagrams[14]. Until now, RG calculations for these systems have not yet been performed to obtain the surface magnetization as function of the temperature, for *arbitrary* values of it, i.e., the equation of state. Recently, a real space RG formalism was introduced[15] which allows, for thermal systems, the *direct* calculation (without going through the calculation of the thermodynamic energy) of the equation of state for arbitrary values of the external parameters. In the present work, we use an extension of this formalism to the nonhomogeneous case[16] (where we allow for different coupling constants in the system) to study the Ising ferromagnet in semi-infinite cubic lattice with a free surface (001). The free surface coupling constant J_S ($J_S \geq 0$) is not necessarily equal to the bulk coupling constant $J_B > 0$.

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

In section 2 we present the model and the formalism and in section 3 the results; finally, we conclude in section 4.

2 MODEL AND RG FORMALISM

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

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

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 given in Fig. 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 magnetization. The bulk magnetization 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 magnetization 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 $\Delta > \Delta_c$, $M_S \sim A_S(1-T/T_c^B(\Delta))^{\beta^{2D}}$. 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

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

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

To obtain the surface and bulk spontaneous magnetizations 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 $K_B = J_B/k_BT$ in the bulk. 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 magnetization 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 choose $\mu = 1$, but we will rather leave it as a variable of our transformation just as K_B and K_S.

We transform (following Kadanoff ideas) the original system into a similar one of linear size L' (B ≡ linear expansion factor = L/L' > 1) with renormalized variables K_B', K_S' and μ'. Through renormalization, 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 system

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

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 $N^S_{L'}(K'_B,K'_S)$ and $N^S_L(K_B,K_S)$, taken at the sites associated with the surface. 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:

$$M_B(K'_B)\mu' = B^{d_B} M_B(K_B)\mu \tag{2}$$

where $M_B(K'_B) = N^B_{L'}(K'_B)/L'^{d_B}$.

Starting with K_B and $\mu^{(o)}$, and performing n iterations in (2), we have:

$$M_B(K_B^{(n)})\mu^{(n)} = B^{nd_B} M_B(K_B)\mu^{(o)} \tag{3}$$

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

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

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

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

The equations (4a) and (4b) are to be used together with the RG recurrence equations for K'_B and K'_S. 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 Fig. 1). In the paramagnetic region, (K_B,K_S) is attracted through successive renormalizations 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 (4a) and (4b))

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

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

in the *entire* paramagnetic region, thus reproducing the well known result. 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) gives

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

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

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 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 (4a) and (4b)

$$M_B(K_B) = 0 \qquad (7a)$$

$$M_S(K_B,K_S) = \lim_{n\to\infty} \frac{\mu^{(n)}}{B^{nd_S}} \qquad (7a)$$

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.

We shall use the same kind of simple Migdal-Kadanoff - like cluster transformations already introduced[14] for the Potts (and related models) surface magnetism. The cells for the bulk and the free surface are shown respectively in Figs. 2(a) and 2(b). The transformation indicated in Fig. 2(a) approaches, through the standard bond-moving procedure, the bulk of our system. In Fig. 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 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 Fig. 2) the factors B^{d_B} and B^{d_S} in Eqs. 5,6 and 7 must be replaced by $B^{d_B^{bb'}}$ and $B^{d_S^{bb'}}$, which will be defined in what follows.

Suppose we are only interested in the homogeneous case $(K_B = K_S)$. The graph $G_1(G_2)$ with chemical distance between terminals $b_1 = 3(b_2 = 3)$ and $N_{b_1} = 27(N_{b_2} = 18)$ bonds is renormalized into the graph $G_1'(G_2')$, with chemical distance $b_1' = 1(b_2' = 1)$ and $N'_{b_1} = 1(N'_{b_2} = 1)$ bonds. The linear expansion factor B of these transformations is $B = b_1/b'_1 = b_2/b'_2 = 3$. The graph $G_1(G_2)$, through successive iterations, generates an hierarchical lattice with intrinsic fractal dimensionality[17] $d_{b_1} = \ln N_{b_1}/\ln b_1$ $(d_{b_2} = \ln N_{b_2}/\ln b_2)$; analogously, $G'_1(G'_2)$ is associated with $d'_{b_1} = \ln N'_{b'_1}/\ln b'_1$ $(d_{b'_2} = \ln N_{b'_2}/\ln b'_2)$ $(N_{b'_1} = b'_1 = N_{b'_2} = b'_2 = 1$ in Fig. 2, which leaves $d_{b'_1}$ and $d_{b'_2}$ undetermined; nevertheless it can be shown that the correct answer for this trivial case is $d_{b'_1} = d_{b'_2} = 1$). It is convenient[15] to define $d_B^{bb'}$ and $d_S^{bb'}$ through

$$B^{d_B^{bb'}} = \frac{N_{b_1}}{N_{b'_1}} \tag{8a}$$

$$B^{d_B^{bb'}} = \frac{N_{b_2}}{N_{b'_2}} \tag{8b}$$

hence

$$B^{d_B^{bb'}} = \frac{b_1^{d_{b_1}}}{b_1'^{d_{b_1}}} \tag{9a}$$

$$B^{d_S^{bb'}} = \frac{b_2^{d_{b_2}}}{b_2'^{d_{b'_2}}} \tag{9b}$$

and consequently

$$d_B^{bb'} = \frac{d_{b_1}\ln b_1 - d_{b'_1}\ln b'_1}{\ln b - \ln b'} \tag{10a}$$

$$d_S^{bb'} = \frac{d_{b_2}\ln b_2 - d_{b'_2}\ln b'_2}{\ln b_2 - \ln b'_2} \tag{10b}$$

In the inhomogeneous case (arbitrary K_B and K_S) we have extended[16] (8b) to

$$ {}_B d_S^{bb'} = \frac{N_{b_2}^B + N_{b_2}^S K_S/K_B}{N_{b_2'}^B + N_{b_2'}^S K_S/K_B} \tag{11} $$

where $N_{b_2}^B$ and $N_{b_2}^S$ ($N_{b_2'}^B$ and $N_{b_2'}^S$) are the numbers of bonds of graph G_2(G_2') respectively associated with K_B and K_S (K_B' and K_S'). Definition (11) is the simplest continuous expression which recovers the homogeneous definition (8b) in the particular cases $(K_S/K_B\,, K_S'/K_B') = (0,0,),(1,0),(0,1)$ and $(1,1)$.

Clarified this point, we come back to the determination of the recurrences for K_B, K_S and μ. 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, ref. 18),

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

$$ e^{-\beta \mathcal{H}'_{S_{12}}} = \operatorname*{Tr}_{3,\ldots,14} e^{-\beta \mathcal{H}_{S_{123\ldots14}}} \tag{13} $$

with

$$ -\beta \mathcal{H}'_{B_{12}} = K_B' \sigma_1 \sigma_2 + K_B^0 \tag{14a} $$

(associated with graph G_1'),

$$ -\beta \mathcal{H}_{B_{123\ldots20}} = K_B(\sigma_1\sigma_5 + \sigma_1\sigma_7 + \sigma_1\sigma_9 + \ldots + \sigma_5\sigma_4 + \sigma_7\sigma_8 + \sigma_9\sigma_{10} + $$

$$ \ldots + \sigma_4\sigma_2 + \sigma_6\sigma_2 + \sigma_8\sigma_2 + \ldots) \tag{14b} $$

(associated to graph G_1),

$$-\beta\mathcal{H}'_{S_{12}} = K'_S\sigma_1\sigma_2 + K^0_S \tag{14c}$$

(associated to graph G'_2) and

$$\begin{aligned}-\beta\mathcal{H}_{S_{123\ldots14}} &= K_S(\sigma_1\sigma_3+\sigma_1\sigma_5+\sigma_1\sigma_7+\sigma_3\sigma_4+\sigma_5\sigma_6+\sigma_7\sigma_8\\ &+\sigma_4\sigma_2+\sigma_6\sigma_2+\sigma_8\sigma_2) + K_B(\sigma_1\sigma_9+\sigma_1\sigma_{11}+\sigma_1\sigma_{13}+\sigma_9\sigma_{10}+\\ &\sigma_{11}\sigma_{12}+\sigma_{13}\sigma_{14}+\sigma_{10}\sigma_2+\sigma_{12}\sigma_2+\sigma_{14}\sigma_2)\end{aligned} \tag{14d}$$

(associated to graph G_2). K^0_B and K^0_S are two constants to be determined. Equations (12) and (13) uniquely determine

$$K_{B'} = f(K_B) \tag{15}$$

and

$$K'_S = g(K_B,K_S) \tag{16}$$

Following along the lines of Ref. 15, 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 Fig. 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. We obtain the magnetic moment m associated with a given configuration by adding the contributions from all sites. In the homogeneous case ($K_S/K_B = 1$) we know that each site contributes proportionally to its coordination number[15]. 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 nonhomogeneous 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 was already tested for the Potts ferromagnet in anisotropic square lattice[16], with results in good agreement with previously known ones. 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 Eq. (1a) and (1b), that the thermal average *total magnetic moment* in the original and renormalized clusters is preserved, for both the bulk and surface RG transformations respectively:

$$\langle m\rangle_{G_1} = \langle m\rangle_{G_1'} \tag{17}$$

$$\langle m\rangle_{G_2} = \langle m\rangle_{G_2'} \tag{18}$$

These equations have the form

$$\mu'_B = h(K_B)\mu_B \tag{19}$$

$$\mu'_S = \ell(K_B,K_S)\mu_S \tag{20}$$

as we can see inspecting Tables 1 and 2. Eq. (19) must enter into Eq. (6a), while Eq. (20) must enter into Eq. (6b) and Eq. (7b).

Summarizing, we use Eqs. (5),(6),(7) together with Eqs. (15),(16) and (19),(20) to obtain the surface and bulk spontaneous magnetizations. For the transformation of Fig. 2(a) ${}_{B}d_{B}^{bb'} = 27$ (homogeneous case) and for the one of Fig. 2(b) ${}_{B}d_{S}^{bb'} = \frac{9+9K_S/K_B}{K'_S/K'_B}$ (nonhomogeneous case).

3 RESULTS

The curves we have obtained for the surface spontaneous magnetization for $J_S/J_B = 0, 0.5, 1$ and 1.5 are presented in Fig. 3. We also present the curve for the bulk spontaneous magnetization. Since $\Delta < \Delta_c$ ($\Delta_c \simeq 0.74$ in the present RG procedure[14]), the surface and bulk order at, for decreasing temperatures, the same temperature T_c^B (*ordinary* transition). We observe that the surface magnetization 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 caracterized by a different set of critical exponents.

The corresponding surface magnetization curve is presented in Fig. 4 with the bulk curve.

In Fig. 5 we present the surface magnetization 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 T_c^B, where the surface magnetization curve is believed to present some kind of soft singularity. We obtain that the temperature first derivative of the surface magnetization 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

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

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

with $\tilde{m} \propto M_s$ and $\tilde{t} \propto (T - T_c^{MF})$, i.e., the leading singularity would occur at $0(t^2)$ (the discontinuity only appears in the *second* derivative at $\tilde{t}= 0$). Furthermore, experimental data of Rau and Robert[4] in Gd (which seems to be close to a Heisenberg ferromagnet) give support to the possible *continuity*, at T_c^B, of the first derivative of $M_S(T)$. However, an effective field theory with correlation for an Ising model[6] has suggested a discontinuity. On the other hand, accurate experiments[19] measuring surface tension at the λ transition on liquid ^4H_e (whose criticality is expected to be the same as that of some surface magnetic systems) suggest a *discontinuity* in the first derivative, conflicting with the the theoretical predictions for the system. The point is still controversial. Let us present some qualitative arguments favoring what we find, i.e., a *discontinuity* in the first derivative of $M_S(T)$. The bulk acts on the surface magnetization through two different physical channels. The first one is the obvious fact that the bulk magnetization, 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. In the neighbourhood of T_c^B, the paramagnetic-side amplitude of the bulk susceptibility is higher (*two* times higher in standard mean-field calculations) than that of the ferromagnetic-side bulk susceptibility. The effect of the paramagnetic-side bulk susceptibility overcomes both the effects of the vanishing bulk field and of the bulk susceptibility just below T_c^B, thus suggesting 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.

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 exponents for each transition and the corresponding amplitudes A. They are shown in Table 3 and compared with other estimates whenever available.

Let us mention an interesting feature that appears as J_S/J_B decreases, for $J_S/J_B << 1$: a slight non-monotonicity of the surface magnetization. At first sight it might seem that, for a given value of J_S/J_B, we must always have a surface magnetization curve which is below the one associated with a greater value of J_S/J_B. Instead of that, at J_S/J_B 0.35 we find that the surface magnetization begins to increase, as J_S/J_B is lowered. We can see in Fig. 3 the surface magnetization curve for $J_S/J_B =$ 0.5 which is *below* the curves for $J_S/J_B = 1, 1.5$, as expected. But the surface magnetization curve for $J_S/J_B = 0$, for instance, is *above* the $J_S/J_B = 0.5$ 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 magnetization 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 magnetization. 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 the renormalization-group results presented here for an Ising ferromagnet, we see that the result $A_+/A_- = 1$ experimentally obtained by Rau and Robert either is due to the fact that Gd seems to be closer to a Heisenberg ferromagnet than to a Ising one, or it should not be considered the generic situation, and its comprehension should be searched elsewhere. We have also observed that the surface magnetization as a function of J_S/J_B, for $J_S/J_B << 1$, presents an unexpected slight non-monotonicity.

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.

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CAPTION FOR FIGURES AND TABLES

Fig. 1 - (a) 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. (b) Phase diagram with the convenient variables $t_B = \tanh(J_B/k_BT)$ and $t_S = \tanh(J_S/k_BT)$, the bulk and surface transmissivities for the Ising model. The RG flow is indicated; ■ , ● and O respectively denote the trivial (fully stable), critical (semi-stable) and multicritical (fully unstable) fixed points.

Fig. 2 - RG cell transformation (a) associated to the bulk (coupling constant K_B); (b) associated to the surface (coupling constant K_S). The lattice generated by iterative application of graph G_1 is an example of hierachical lattice.

Fig. 3 - Surface spontaneous magnetization M_S as a function of the temperature for the Ising ferromagnet in 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 magnetization M_B is also shown as a reference.

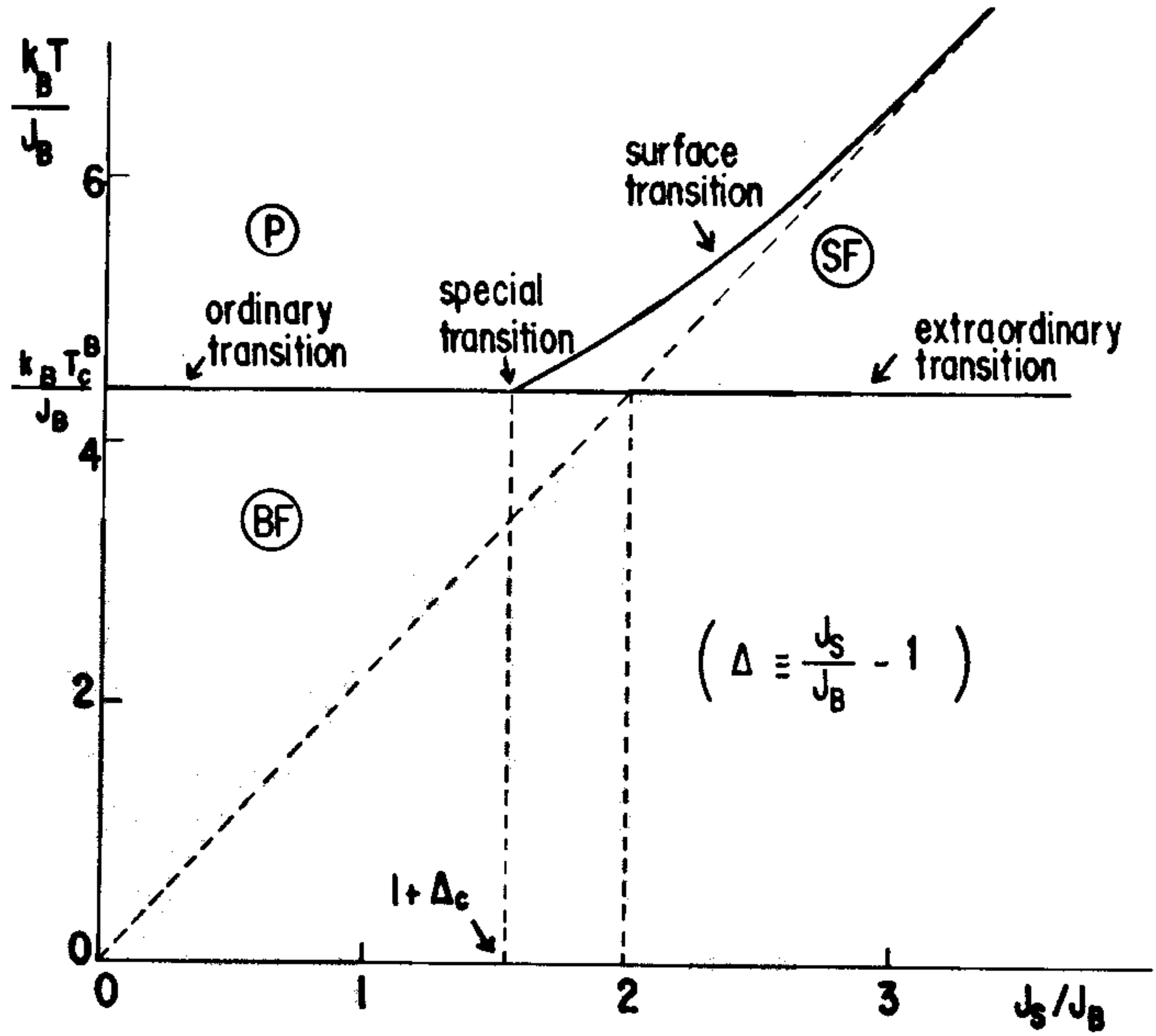
Fig. 4 - Surface magnetization M_S as a function of the temperature for $\Delta = \Delta_c$. The bulk magnetization M_B is also shown.

Fig. 5 - Surface magnetization 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 magnetization M_B curve is also shown.

Table 1 - Establishment of Eq. 17 for the bulk RG transformation. (a) Possible configurations for the graph G_1'; $\langle m\rangle_{G_1'} = e^{K_B'} 2\mu' / (e^{K_B'} + e^{-K_B'})$ (b) 3 of the 2^{19} possible configurations for the graph G_1; $\langle m\rangle_{G_1} = (54e^{27K_B} + 50e^{23K_B} + 32e^{5K_B} + \ldots)\mu/(e^{27K_B} + e^{23K_B} + e^{5K_B} + \ldots)$.

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

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



k_BT/J_B
6
4
2
0
$k_BT_c^B/J_B$
P
ordinary transition
special transition
surface transition
SF
extraordinary transition
BF
$\left(\Delta \equiv \frac{J_S}{J_B} - 1 \right)$
$1+\Delta_c$
0
1
2
3
J_S/J_B

FIG. 1

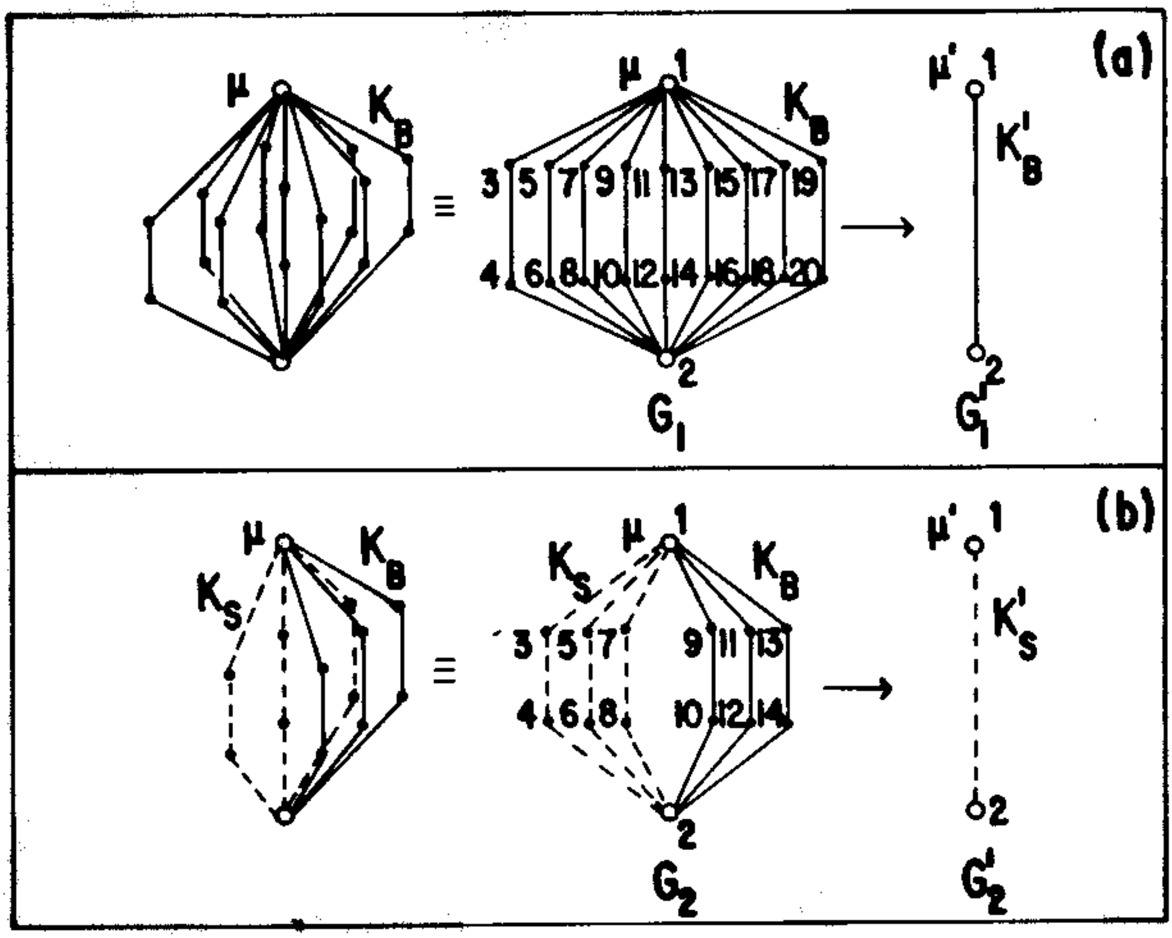

(a)
μ
K_B
≡
μ 1
3 5 7 9 11 13 15 17 19
4 6 8 10 12 14 16 18 20
2
G_1
μ' 1
K'_B
2
G'_1
(b)
μ
K_S
K_B
≡
μ 1
K_S
K_B
3 5 7 9 11 13
4 6 8 10 12 14
2
G_2
μ' 1
K'_S
2
G'_2

FIG. 2

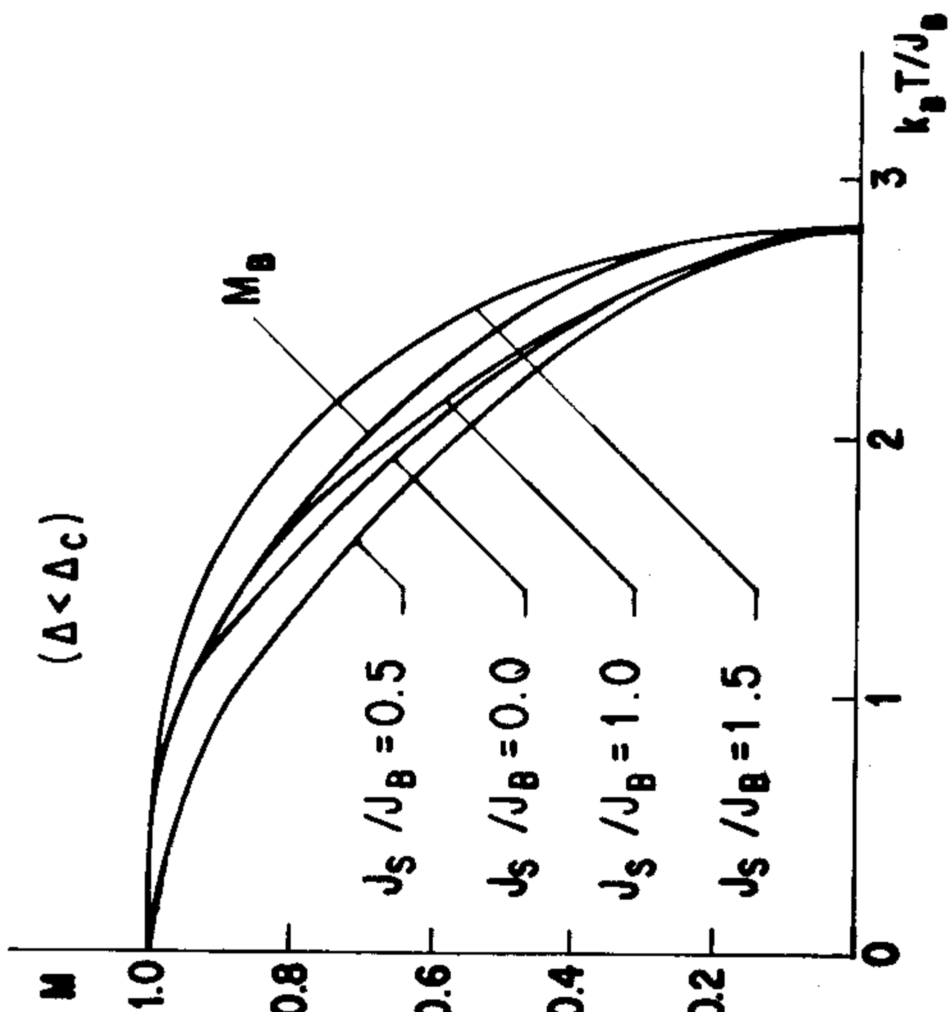


FIG. 3

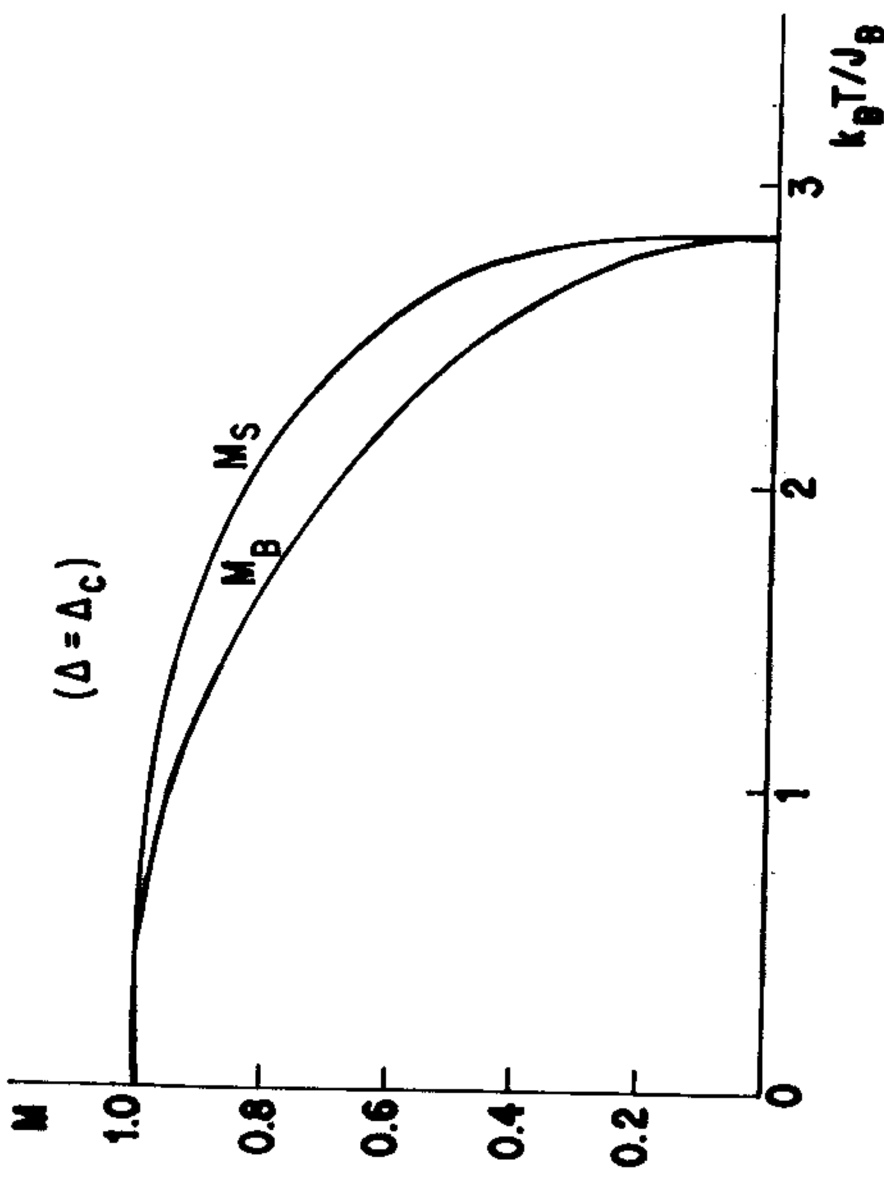


FIG. 4

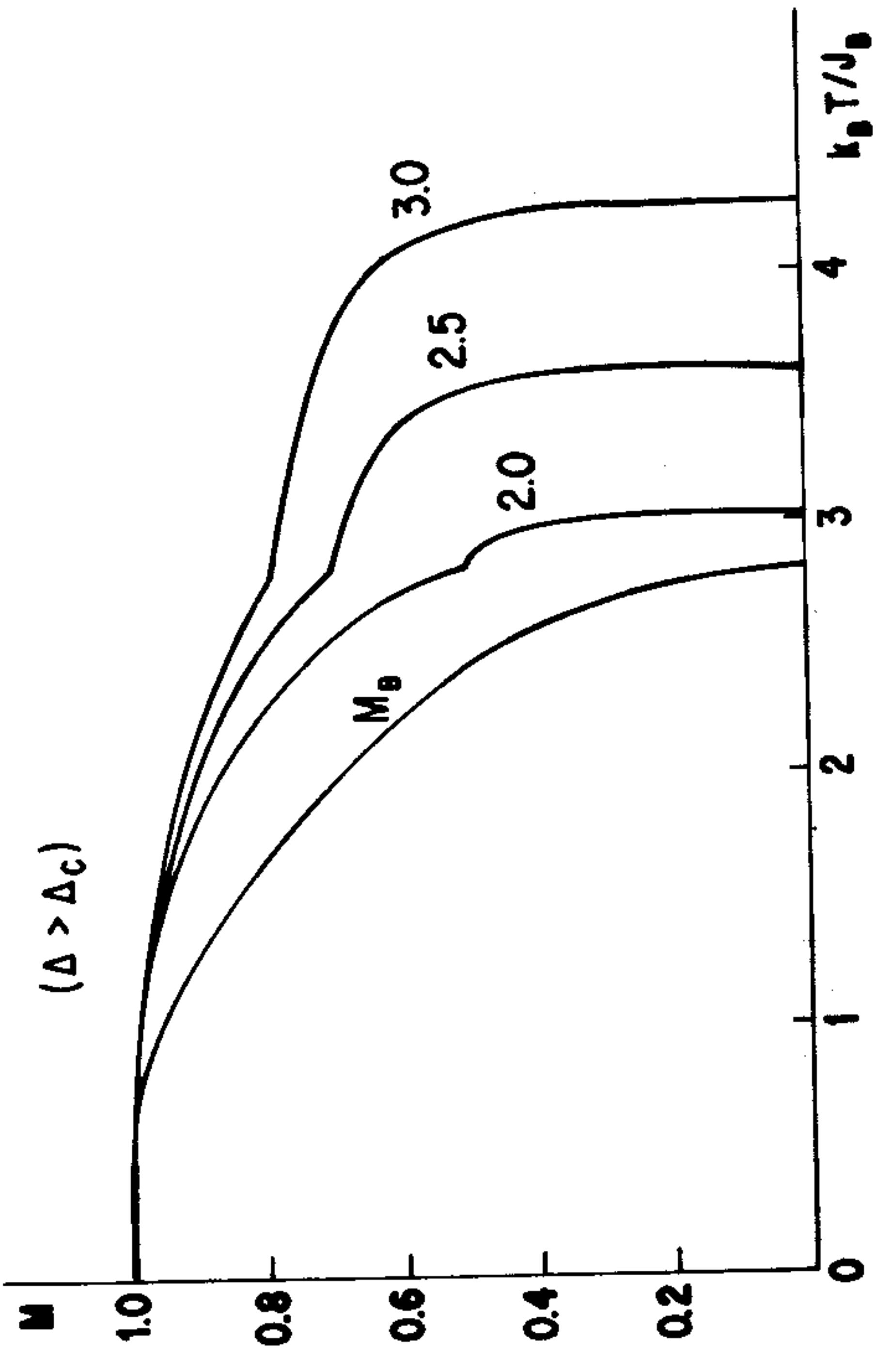


FIG.5

(a) G_1' configuration	weight	m
	$e^{K_B'}$	$2\mu_B'$
	$e^{-K_B'}$	0

TABLE 1

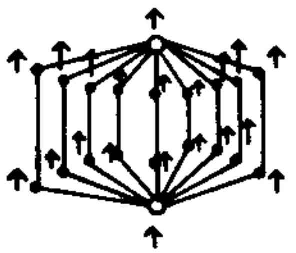
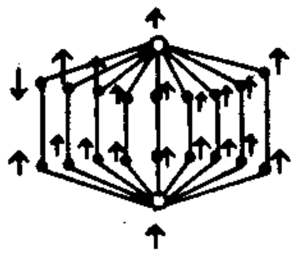
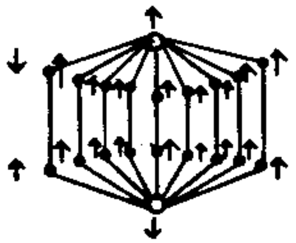
(b) G_1 configuration	weight	m
	e^{27K_B}	$54\mu_B$
	e^{23K_B}	$50\mu_B$
	e^{5K_B}	$32\mu_B$

TABLE 1

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

TABLE 2

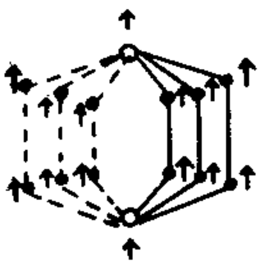
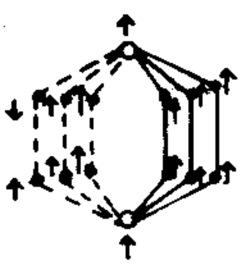
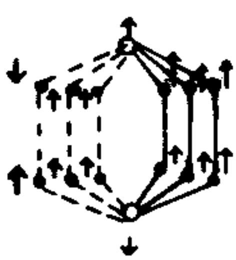
(b) G_2 configuration	weight	m
	$e^{9K_B+9K_S}$	$(18+18\,K_S/K_B)\,\mu_S$
	$e^{9K_B+5K_S}$	$(18+14K_S/K_B)\,\mu_S$
	$e^{3K_B-K_S}$	$(12+8\,K_S/K_B)\,\mu_S$

TABLE 2

BULK MAGNETIZATION		
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[21]	2.30617 (Series[20])	—

SURFACE MAGNETIZATION			
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 TRANSION			
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[20])	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

TABLE 3

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