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SURFACE MAGNETIC ORDER AND EFFECTS OF THE NATÚRE OF THE INTERACTIONS*

by

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We discuss, within a real-space renormalization-group, interesting thermal effects (surface singularity at the bulk transition; Ising-Heisenberg crossover) concerning the free surface of a semi-infinite d=3 spin 1/2 anisotropic Heisenberg ferromagnet. Comparison with the Mermin-Wagner theorem and with experimental work is done.

Key-words: Surface magnetism; Renormalization-group; Semi-infinite d=3 ferromagnet; Ising-Heisenberg crossover; Mermin-Wagner theorem; Surface singularity.

PACS index: 75.30 Pd; 68.35 Rh; 05.50+q; 75.40 Cx.

1 INTRODUCTION

Surface magnetism is nowadays an active field of research. This is due both to its theoretical richness and to its important applications (corrosion, catalysis, information storage). See Ref.[1] for a general review, and Refs.[2] and [3] for reviews of respectively real-space and reciprocal - space renormalization-group (RG) approaches.

The theoretical prototype for surface magnetism is the spin 1/2 Ising ferromagnet in simple cubic lattice with a (0,0,1) free surface, J_S and J_B respectively being the surface and bulk coupling constants. The corresponding phase diagram is indicated in Fig.1: three distinct phases, namely the *bulk ferromagnetic* (BF; both bulk and free surface are magnetized), the *surface ferromagnetic* (SF; only the free surface is magnetized) and the *paramagnetic* (P; both bulk and surface are disordered) ones, join at a multicritical point (located at $\Delta \equiv J_S/J_B - 1 = \Delta_c$).

In the present work we discuss, within a real-space RG framework, two interesting effects, namely (i) the influence of the symmetry of the magnetic interaction and its connection with the Mermin-Wagner theorem, and (ii) the singularity which the surface magnetization thermal behavior exhibits at the bulk critical point for $\Delta > \Delta_c$ (*extraordinary* transition). In Section 2 we introduce the model and the RG formalism; in Sections 3 and 4 we discuss the influence of the interaction symmetry and the surface singularity respectively. We finally conclude in Section 5.

2 MODEL AND RG FORMALISM

We consider the spin 1/2 *anisotropic* Heisenberg dimensionless Hamiltonian

$$-\beta H = \sum_{\langle i,j\rangle} K_{ij} [(1-\eta_{ij})(\sigma_i^x\sigma_j^x+\sigma_i^y\sigma_j^y)+\sigma_i^z\sigma_j^z] \qquad (1)$$

where $\beta \equiv 1/k_B T$ and $\langle i,j\rangle$ run over all pairs of first-neighboring sites on a semi-infinite simple cubic lattice with a (0,0,1) free surface ; (K_{ij},η_{ij}) equals (K_S,η_S) if both sites belong to the surface and equals (K_B,η_B) otherwise ($K_S \equiv J_S/k_B T$ and $K_B \equiv J_B/k_B T$); J_S, $J_B \geq 0$ and $0 \leq \eta_S,\eta_B \leq 1$ ($\eta_{ij}= 1$ recovers the standard Ising interaction and $\eta_{ij}=0$ recovers the *isotropic* Heisenberg interaction); σ_i^x, σ_i^y and σ_i^z are the spin 1/2 Pauli matrix.

To obtain the phase diagram in the (K_B,K_S,η_B,η_S) space (or equivalently in the ($k_BT/J_B,J_S/J_B,\eta_B,\eta_S$) space) within the RG approach we have to establish the recurrence relations

$$K_B' = f(K_B,\eta_B) \qquad (2.a)$$

$$K_S' = g(K_B,K_S,\eta_B,\eta_S) \qquad (2.b)$$

$$\eta_B' = h(K_B,\eta_B) \qquad (2.c)$$

$$\eta_S' = k(K_B,K_S,\eta_B,\eta_S) \qquad (2.d)$$

Notice that the bulk affects the surface but the opposite is not true, since the surface is subextensive with respect to the bulk.

Also we expect the Ising particular case (i.e., $\eta_B = \eta_S = 1$) to be a subspace which remmains *invariant* under renormalization since it presents a fully developed axial symmetry. For this to occur it suffices that $h(K_B,1) = k(K_B,K_S,1,1) = 1$ for all (K_B,K_S). The recurrence equations then become

$$K_B' = f(K_B,1) \qquad (3.a)$$

$$K_S' = g(K_B,K_S,1,1) \qquad (3.b)$$

We finally expect that the isotropic Heisenberg particular case (i.e., $\eta_B = \eta_S = 0$) also remains *invariant* under renormalization, since nothing disturbs the perfect isotropy of the interactions. For this to occurs it suffices that $h(K_B,0) = k(K_B,K_S,0,0) = 0$ for all (K_B,K_S). The recurrence equations then become

$$K_B' = f(K_B,0) \qquad (4.a)$$

$$K_S' = g(K_B,K_S,0,0) \qquad (4.b)$$

Both the above invariances(i.e., $\eta_{ij}=1$ and $\eta_{ij}=0$) can be *simultaneously* satisfied if we establish the RG Eqs.(2) following Ref.[4]. The method essentially consists in preserving, through renormalization, the correlations between the *roots* (or *terminal sites*) of conveniently chosen two-rooted finite graphs. In other words, $\mathrm{Tr}_{\text{internal sites}}\, e^{-\beta H}$ is to be preserved under renormalization. If the model is classical(which happens here if $\eta_{ij}= 1$), this method provides the exact answer [5] for the hierarchical lattice associated with the particular graph that has been chosen. There is no unique manner for determining the best choices for graphs: this partially relies on a kind of "culinary art". Two-rooted graphs very well fitted to the simple cubic lattice have been introduced in Ref.[6]. Here we shall rather follow Ref.[7] and adopt the simpler two-rooted graphs, Migdal-Kadanoff-like, indicated in Fig.2. By so doing we partially loose the information corresponding to the particular site connections existing in the simple cubic lattice and its (0,0,1) free surface, but the results are expected to remain qualitatively (even quantitativelly occasionally) correct: this has in fact been so for the Ising particular case ($\eta_{ij}=1$).

Let us now focus a problem of further complexity, namely the calculation, for all temperatures, of the bulk magnetization M_B as well as of the surface one

M_S. To perform this calculation we adopt the simple RG procedure introduced in Ref.[8] and follow along the lines of Ref.[9]. Excepting for appropriate scaling factors, M_B and M_S respectively coincide with μ_B and μ_S, the dimensionless elementary magnetic dipoles respectively associated with the bulk and the surface sites (see [8,9] for details). The RG equations for μ_B and μ_S are established by imposing that the bulk and surface total magnetic moments (*extensive* quantities) must be preserved through renormalization. The equations have the following forms:

$$\mu_B' = l(K_B, \eta_B)\mu_B \tag{5.a}$$

$$\mu_S' = m(K_B, K_S, \eta_B, \eta_S)\mu_S \tag{5.b}$$

Together with Eqs.2 they close the RG procedure. For $\eta_B = \eta_S = 1$ they become

$$\mu_B' = l(K_B, 1)\mu_B \tag{6.a}$$

$$\mu_S' = m(K_B, K_S, 1, 1)\mu_S \tag{6.b}$$

and, for $\eta_B = \eta_S = 0$, they become

$$\mu_B' = l(K_B, 0)\mu_B \tag{7.a}$$

$$\mu_S' = m(K_B, K_S, 0, 0)\mu_S \tag{7.b}$$

Eqs.(6) (Eqs.(7)) are to be used together with Eqs.(3) (Eqs.(4)) to study the Ising (isotropic Heisenberg) particular case.

3 INFLUENCE OF THE NATURE OF THE INTERACTIONS

The Mermin-Wagner theorem [10] essentially states that no spontaneous magnetization at finite temperatures can exist if the three following conditions are simultaneously satisfied:

(i) the system only involves short-range interactions;

(ii) the system is two dimensional;

(iii) the symmetry breakdown corresponds to interactions which are associated with a *continuous* group of symmetries.

The question we want to focus is whether the SF can exist if $\eta_S = 0$, *no matter the value of* η_B. There is a relatively widespread confusion concerning this central point. A (fallacious) argument is frequently raised as follows: 'condition (i) is obviosly satisfied; the surface is a two dimensional system hence condition (ii) also is satisfied; finally $\eta_S = 0$, therefore condition (iii) also is satisfied; consequently the SF cannot exist and this for any value of η_B. In fact this is not true : it is *only if* η_B vanishes as well that the SF cannot exist. One easy way out of the paradox is to say that the theorem does not apply because condition (ii) is not satisfied, the system strictly being a d=3 one (semi-infinite bulk). And this is of course correct. However we believe, on physical grounds, that the

surface magnetization vanishes, for $\Delta > \Delta_c$, *exponentially* while entering deep into the bulk. This exponential behavior leads to a system which can, in practice, be considered as a $\infty \times \infty \times$ finite one, i.e., a d=2 one, and consequently condition (ii) can, in practice, be considered as satisfied. Consistently, only remains condition (iii) as the one whose satisfaction would lead us out of the fallacy. And it is indeed so, because to satisfy (iii) *all* the relevants interactions have to satisfy it, which is not the case. Indeed the *finite* width of the active surface includes much more layers than the unique free surface layer (for which $\eta_S = 0$).
Summarizing, the SF phase is expected to exist if at least one of η_S and η_B is non vanishing. It must disappear only if *both* η_S and η_B vanish since then the Mermin-Wagner theorem, in practice, applies. In Figs.3 and 4 we reproduce the RG results [7] which are consistent whith the above considerations.
Let us discuss a last point. For the SF phase to disappear in the $(\eta_S, \eta_B) \to (0,0)$ limit, it is not *necessary* that Δ_c diverges: it could well remain *finite* and even so the SF phase disappear through the collapse of the P - SF critical line on the SF - BF critical line. It is not necessary that Δ_c

diverges, *but it does* (as shown in Fig.5).

4 SURFACE MAGNETIZATION

The thermal behaviors of M_B and M_S have been calculated within the present RG approach only for the $\eta_B = \eta_S = 1$ model. The results [9] are presented in Fig. 6 .

It is well known that

$$M_B \propto (T_c^{3D} - T)^{\beta^{3D}} \quad (8)$$

and

$$M_S \propto \begin{cases} (T_c^{3D} - T)^{\beta^{ord}} & \text{if } \Delta < \Delta_c \quad (9.a) \\ (T_c^{3D} - T)^{\beta^{sp}} & \text{if } \Delta = \Delta_c \quad (9.b) \\ (T_c^{S}(J_S/J_B) - T)^{\beta^{2D}} & \text{if } \Delta > \Delta_c \quad (9.c) \end{cases}$$

in the neighborhood of the temperatures where M_B and M_S vanish. All these facts are consistently recovered within the present RG approach. What we want to discuss here is a more subtle point, namely the singularity which might exist in $M_S(T)$ at the bulk critical point T_c^{3D} if $\Delta > \Delta_c$. We expect, in this case,

$$M_s(T)-M_s(T_c^{3D}) \sim \begin{cases} A_-(1-T/T_c^{3D})^{x_-} & \text{for } T \leq T_c^{3D} \quad (10.a) \\ -A_+(T/T_c^{3D}-1)^{x_+} & \text{for } T \geq T_c^{3D} \quad (10.b) \end{cases}$$

The central questions we address here are what the values of A_-/A_+, x_+ and x_- are. The present RG numerical results [9] are consistent with $x_+ = x_- = 1$ and $A_-/A_+ \neq 1$, i.e., a *discontinuous* temperature derivative of M_s (A_+ and A_- depend on J_s/J_B, but the ratio A_-/A_+ roughly remains equal to 4). This result is in clear variance with Mean Field calculations [11] since they yield $A_-/A_+ = 1$, i.e., a *continuous* temperature derivative of M_s.

On experimental grounds, surface magnetism in Gd has been studied [12,13]. We focus here the recent experiment by Rau and Robert [13]. Their data are consistent with $A_-/A_+=1$, in agreement with Mean Field calculations but in disagreement with the present RG ones. One possible explanation could be the fact that Gd seems to be close to the *isotropic* Heisenberg model, whereas the present calculation has been done for the Ising model. The theoretical treatment of the dependence of A_-/A_+ on (η_B, η_s)

would enlighten this point, but this is still to be done. However, if even in the limit $\eta_B = \eta_S = 0$ A_-/A_+ remains different from unity, then the understanding of Rau and Robert results should be searched elsewhere.

Since the bulk order acts on the surface as an external magnetic field, one could expect for $A_-/A_+ < 1$. It is however $A_-/A_+ > 1$ which actually occurs. We believe this must be due to surface-bulk correlation phenomena : a kind of feed-back effect related to the fact that the bulk is magnetically more susceptible for $T \gtrsim T_c^{3D}$ than for $T \lesssim T_c^{3D}$. Equivalently, for $T \gtrsim T_c^{3D}$ the bulk acquires a relatively important magnetization induced by the surface magnetization; this bulk magnetization in turn enhances M_S.

Let us finally mention that we observe in Fig.6 a slight, but surprising, non monotonicity in the M_S vs. T curves as function of J_S/J_B for $J_S/J_B \ll 1$.

5 CONCLUSION

The main results of the present RG treatment of surface magnetism in a semi-infinite ferromagnetic bulk can be summarized as follows :

(i) The surface ferromagnetic (SF) phase exists as long as either the surface or the bulk (or both) interactions are Ising-like. It disappears in the simultaneous surface and bulk isotropic Heisenberg case, and it does so through the divergence of Δ_c. The entire behavior is consistent with the Mermin-Wagner theorem ;

(ii) At the bulk critical point and for $\Delta > \Delta_c$, the temperature derivative of the surface magnetization is *discontinuous* for the Ising model. This could be considered as consistent with the surface tension experiments [14] on liquid ^{4}He, but clearly disagrees with the recent experiments [13] on Gd (possibly isotropic Heisenberg like). In order to clarify this question, the study of the influence of the nature of the magnetic interactions on the surface magnetization temperature derivative would be very welcome.

CAPTION FOR FIGURES

Fig.1 - Phase diagram for the spin 1/2 Ising ferromagnet in the semi-infinite simple cubic lattice with a (0,0,1) free surface.

Fig.2 - RG cluster transformation for the bulk (a) and its free surface (b); ● and o respectively denote internal and terminal sites.

Fig. 3 - RG flow diagrams in the invariant subspaces (a) $\eta_B = \eta_S = 1$ and (b) $\eta_B = \eta_S = 0$; ■ , ● and o respectively denote trivial (fully stable), critical (semi-stable) and multicritical (fully unstable) fixed points ; dashed lines are indicative ; BF, SF and P respectively denote the bulk ferromagnetic, surface ferromagnetic and paramagnetic phases.

Fig.4 - η_S- evolution of the phase diagram for Ising bulk (a) and isotropic Heisenberg bulk (b); ● denotes the multicritical point.

Fig.5 - (η_B, η_S)- dependence of the location Δ_c of the multicritical point appearing in Fig.4. Notice, in the $\eta_S = 0$ plane, a slight minimum.

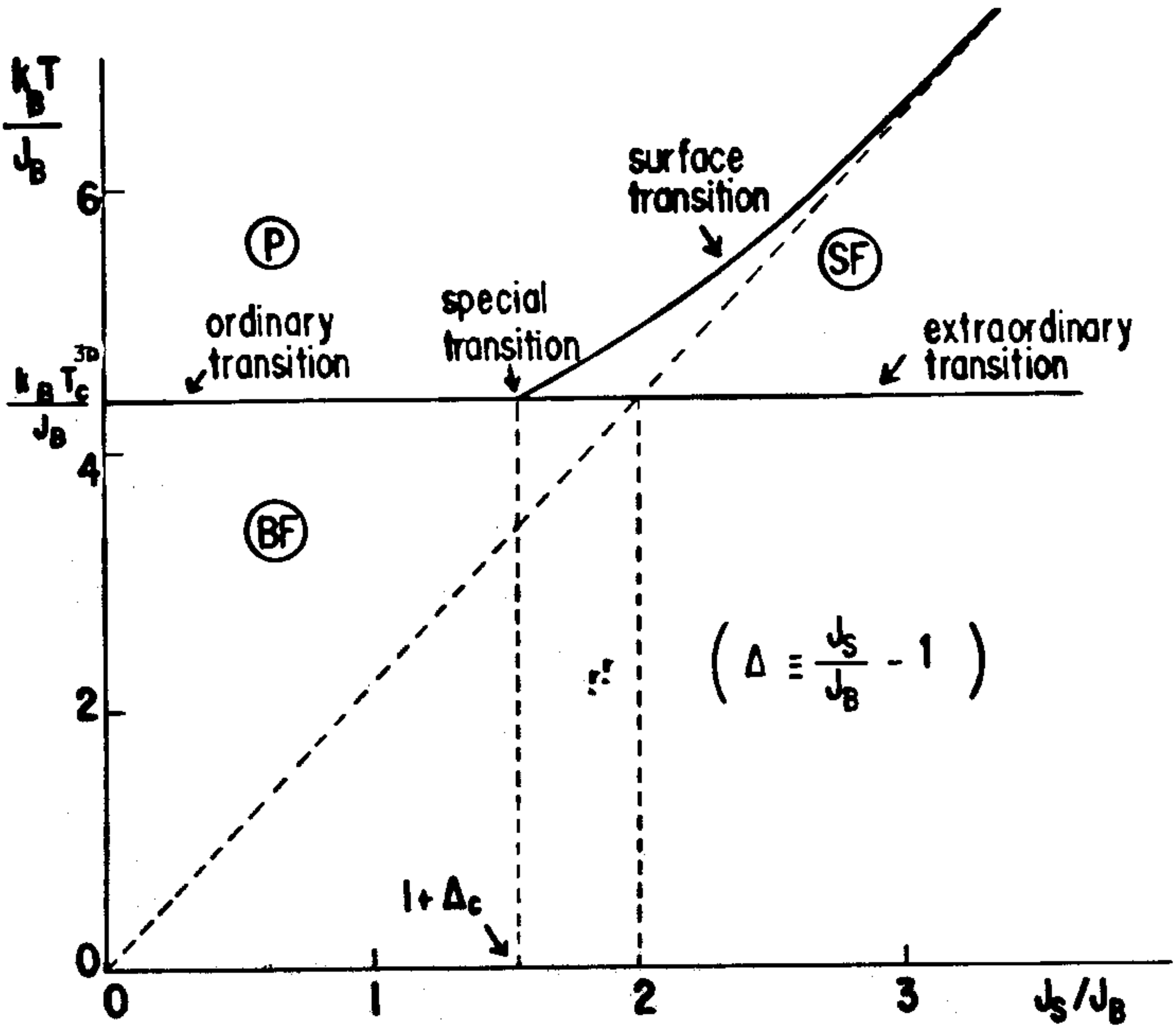
k_BT/J_B
6
4
2
0
$k_BT_c^{3D}/J_B$
P
BF
SF
ordinary transition
special transition
surface transition
extraordinary transition
$1+\Delta_c$
$\left(\Delta \equiv \frac{J_S}{J_B} - 1\right)$
0
1
2
3
J_S/J_B

Fig. 1

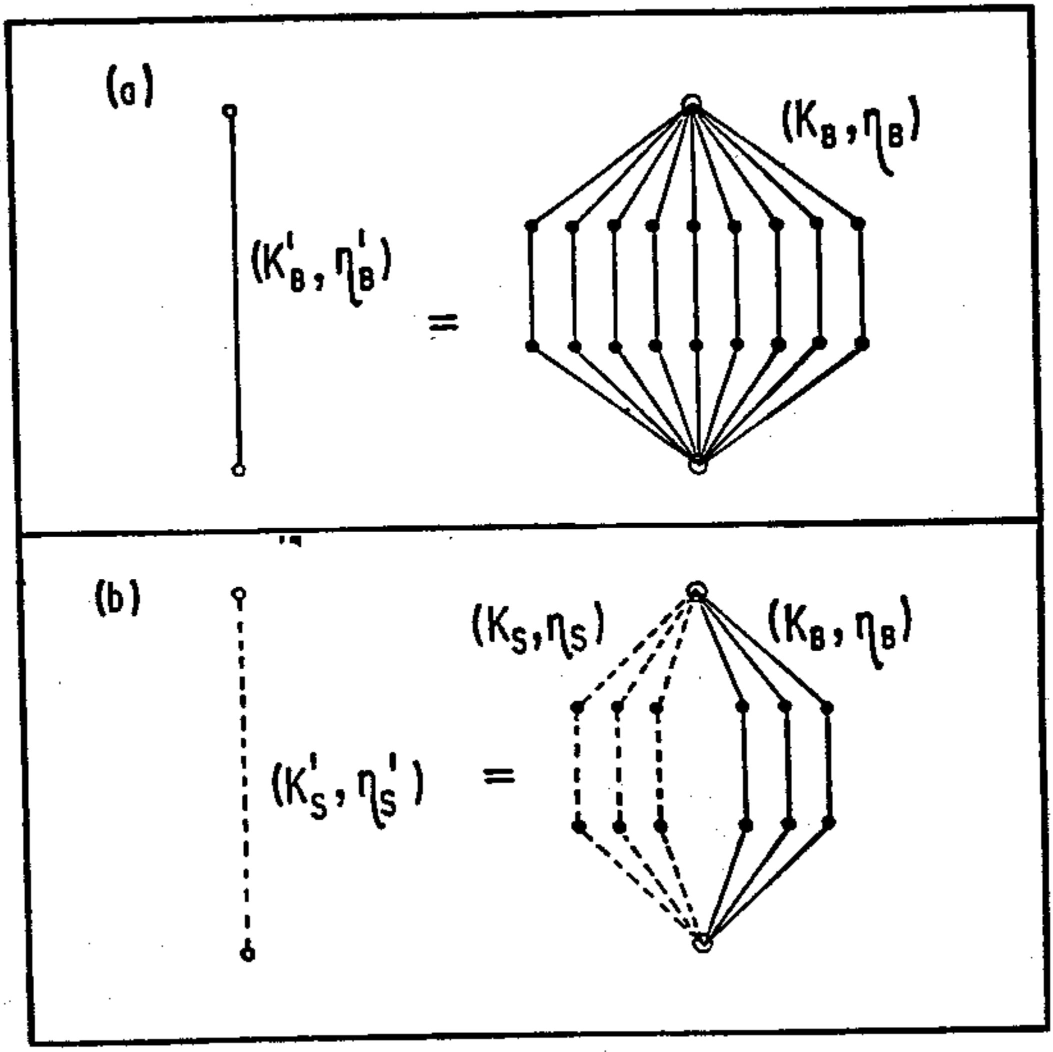

Fig. 2

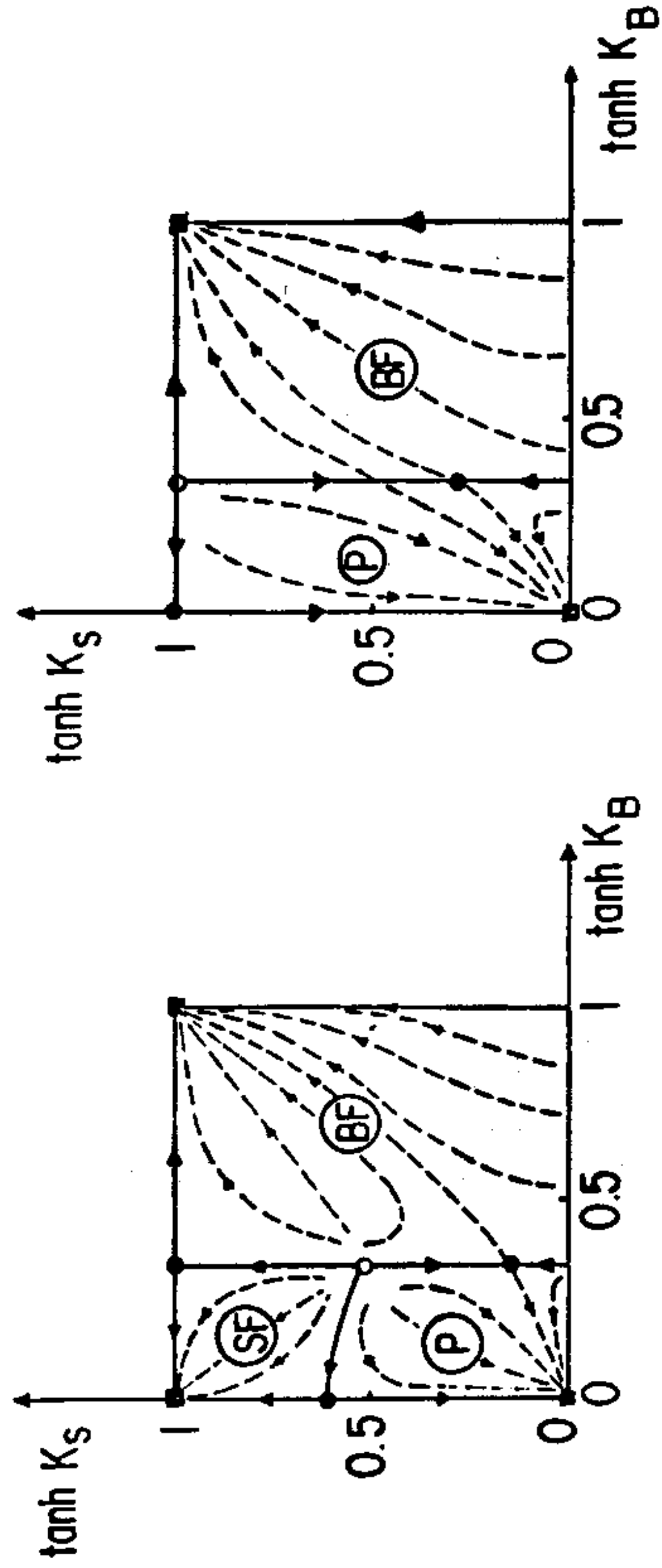

Fig. 3

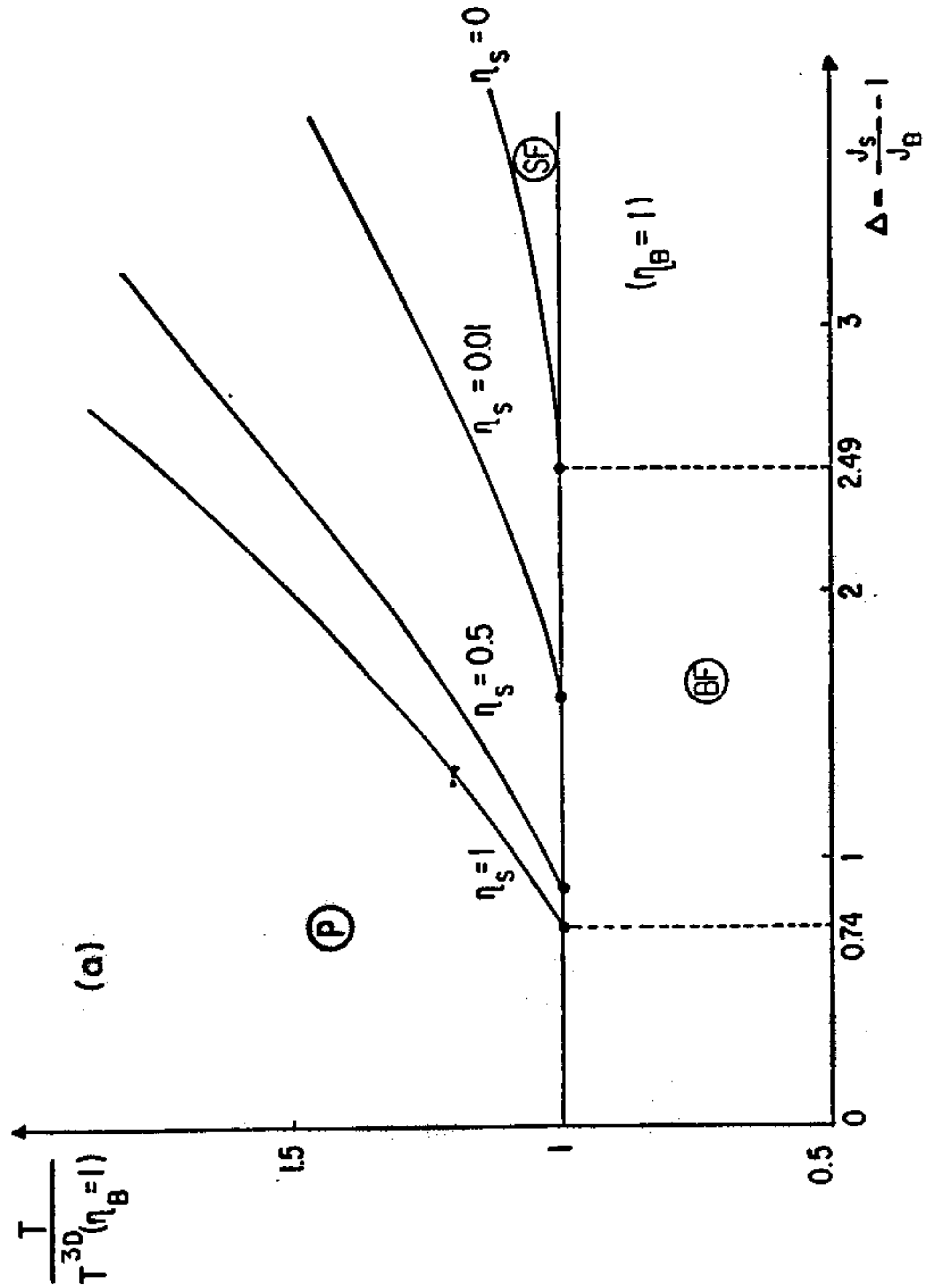
(a)
P
BF
SF
$\eta_s = 0$
$\eta_s = 0.01$
$\eta_s = 0.5$
$\eta_s = 1$
$(\eta_B = 1)$
$\frac{T}{T^{3D}(\eta_B = 1)}$
$\Delta = \frac{J_S}{J_B} - 1$
0.5
1
1.5
0
0.74
1
2
2.49
3

Fig. 4

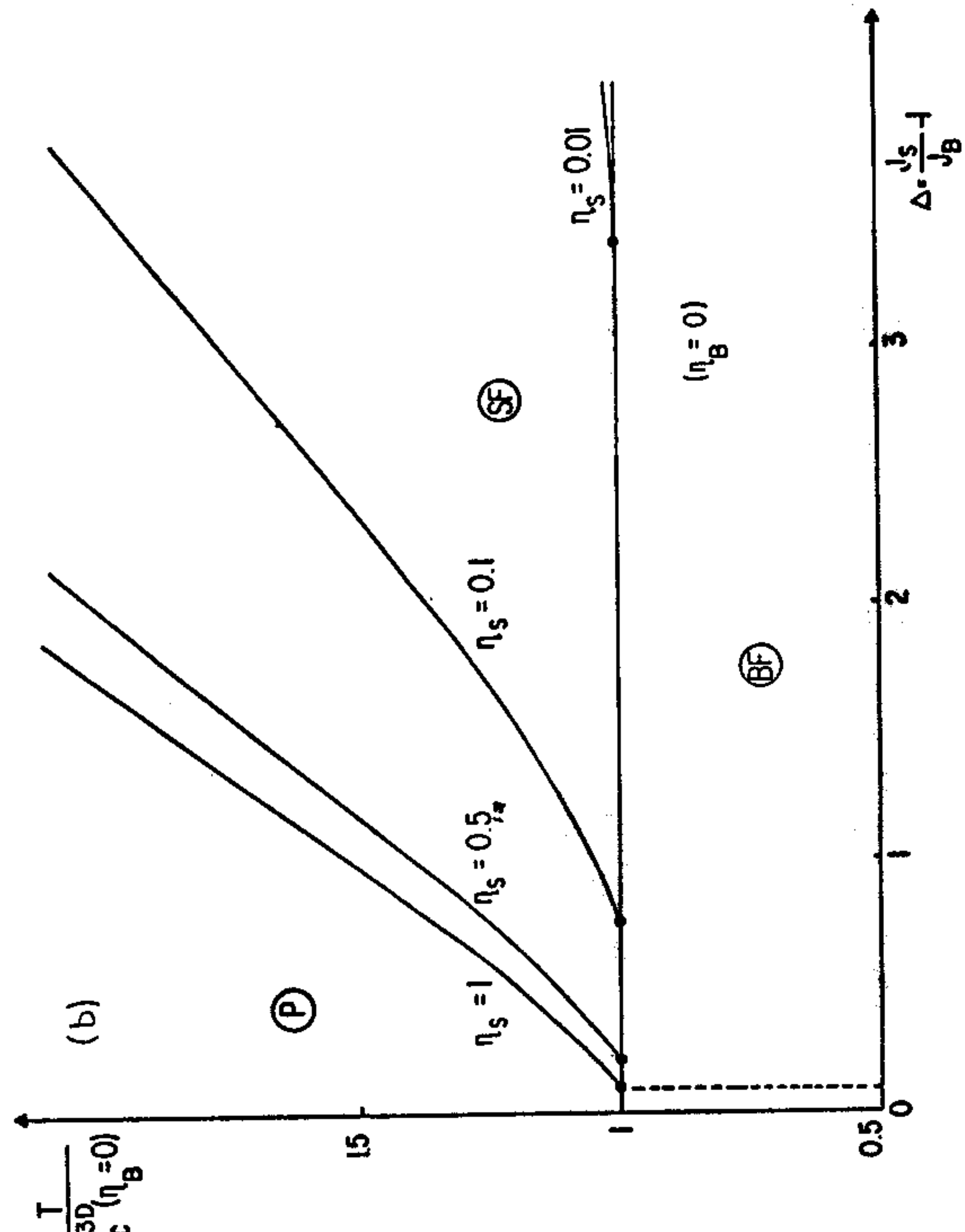

Fig. 4

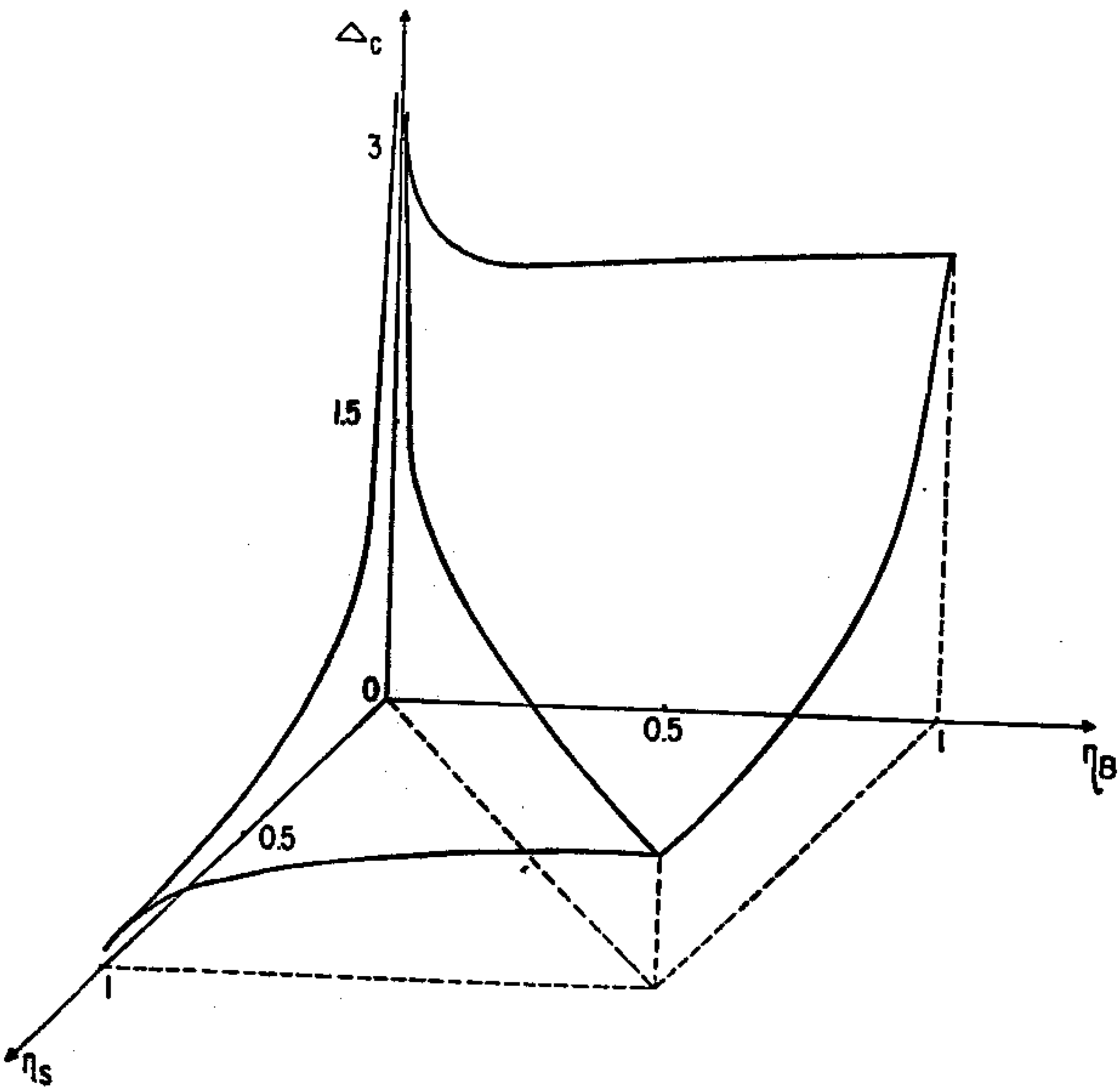

Fig. 5

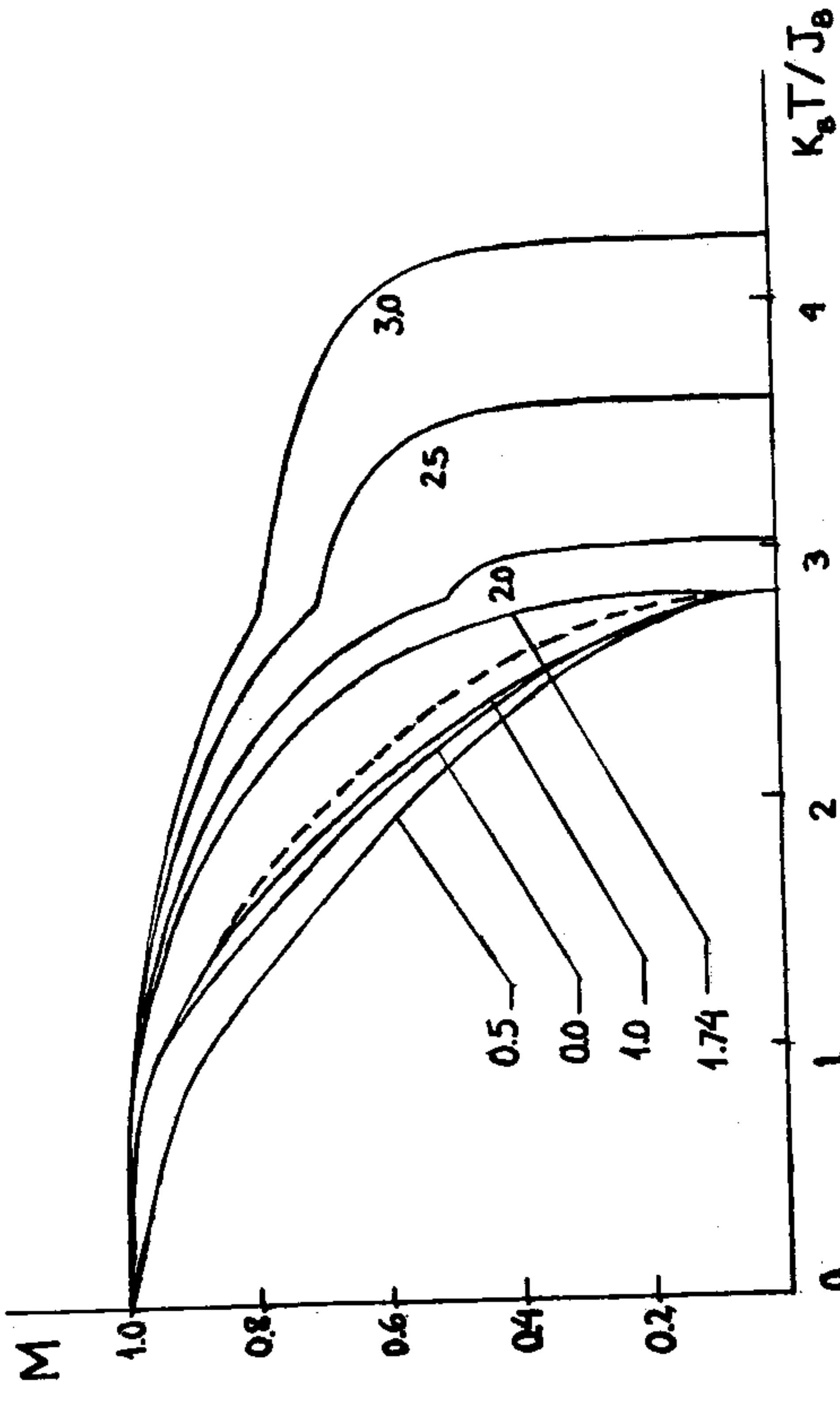

Fig. 6

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