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INFLUENCE OF THE INTERACTION ANISOTROPY ON THE APPEARENCE OF SURFACE MAGNETISM

by

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ABSTRACT

Within a simple real space renormalization group scheme, we study the phase diagram of the d=3 semi-infinite anisotropic Heisenberg ferromagnet, with surface (bulk) coupling constant J_S (J_B) and anisotropy η_S (η_B). We exhibit in particular the interesting effects of η_S and η_B on the (multicritical) ratio J_S/J_B above which surface order becomes observable even if bulk order is absent. Enhancement occurs for an Ising-like free surface ($\eta_S \simeq 1$) on top of an isotropic-Heisenberg-like bulk ($\eta_B \simeq 0$).

Key-words: Surface magnetism; Heisenberg model; Phase diagram; Universality classes.

Surface magnetism is a subject which presents interesting applications (corrosion, catalysis) as well as theoretical and experimental richness (see [1] for reviews). A semi-infinite ferromagnetic system typically presents three phases, namely the *bulk ferromagnetic* (BF; both bulk and free surface are magnetized), *surface ferromagnetic* (SF; only the free surface is magnetized), and *paramagnetic* (P; both bulk and surface are disordered) ones. The less trivial phase clearly is the SF one, and has already been experimentally observed[2]; its observation is however quite hard. We discuss here the influence of the nature of the magnetic interaction (Ising-like or isotropic-Heisenberg-like), and point out the physical regions which should enhance the appearence of the SF phase. In addition to that, clarification is provided on a theoretical point responsible for wide spread confusion in the literature and scientific meetings. We refer to the connection between facts like the Mermin and Wagner theorem[3], the *vanishing* critical temperature for the 2D isotropic Heisenberg model, and the *existence* of the SF phase; or alternatively, in what deep sense a paramagnetic bulk is expected to influence the establishment of magnetic order on the free surface.

Let us consider the following anisotropic spin 1/2 Heisenberg Hamiltonian:

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

where <i,j> run over all pairs of first-neighboring sites on a semi-infinite simple cubic bulk with a (1,0,0) free surface; (J_{ij}, η_{ij}) equals (J_s, η_s) if *both* sites belong to the surface, and equals (J_B, η_B) otherwise; $J_s, J_B \geq 0$, 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). Our present purpose is to study the criticality (phase diagram and universality classes) of this system. To do this we shall use the same type of simple (Migdal-Kadanoff-like) real-space renormalization-group (RG) framework recently introduced for the Potts (and related models) surface magnetism[4]. The RG recursive relations are indicated in Fig.1: we first solve the series array of three bonds, and then solve the parallel array which results (the method and approximations involved in such treatment of *quantum* two-rooted graphs are described in Ref.[5]). We thus obtain $(K_B', \eta_B', K_s', \eta_s')$ as explicit functions of $(K_B, \eta_B, K_s, \eta_s)$ (the K's are connected to the J's through $K \equiv J/k_BT$). The RG flow in this 4-dimensional parameter space determines the phase diagram, the P, BF and SF phases being respectively characterized by the trivial (fully stable) fixed points $(K_B, \eta_B, K_s, \eta_s) = (0,1,0,1)$, $(\infty,1,\infty,1)$ and $(0,1,\infty,1)$; it also determines, through the analysis of a variety of semi-stable or fully unstable fixed points, the relevant universality classes, which are indicated in Table I. We present in Fig.2 the RG flux in two important invariant subspaces, namely those corresponding to $\eta_B=\eta_s=1$ and to $\eta_B=\eta_s=0$. In Fig.3 we present the phase diagrams associated with typical values of (η_B, η_s).

Finaly, we present in Fig.4 the location of the multicritical point where all three P-BF, P-SF and BF-SF critical lines join, i.e. the value Δ_c above which the SF phase appears ($\Delta \equiv J_S/J_B - 1$). This is a very instructive figure: (i) For $\eta_B = \eta_S = 1$, Δ_c equals 0.74 (to be compared with the series value 0.6 ± 0.1 [6], the Monte Carlo value 0.5 ± 0.03 [7], and a sophisticated cluster RG extrapolated value 0.569 [8]; (ii) We note, at the $\eta_S = 0$ plane, the existence of a slight *minimum* resulting from a delicate balance between the trends, for decreasing η_B, to decrease the bulk critical temperature and to decrease the bulk-assisted surface critical temperature; (iii) We note, at the $\eta_S = 1$ plane, that Δ_c monotonously *decreases* for decreasing η_B, which means that the influence of the decreasing bulk critical temperature is "all the way long" *stronger* than the influence of the decreasing bulk-enhanced surface critical temperature; this is an important result as it implies that substances with Ising-like surface on top of isotropic-Heisenberg-like bulks are privileged for *experimental observation* of the SF phase; (iv) At the $\eta_B = 0$ plane, Δ_c monotonously increases for decreasing η_S and diverges for $\eta_S = 0$, therefore *no finite critical value of* η_S *exists* for the SF phase to be possible, contrarily to what was suggested by a RPA analysis [9] (in this type of analysis a *paramagnetic bulk* is somehow assimilated, because of its vanishing magnetization, to a *disconnected bulk*, and consequently it badly takes into account the important bulk-assisted correlations between the free surface spins); (v) We note that Δ_c *diverges only in the* $\eta_B = \eta_S = 0$ *corner* (and not, for instance, for all values of η_B if $\eta_S = 0$), and consistently only there the SF phase (i.e., non vanishing free surface magnetization simultaneously with vanishing bulk magnetization) cannot exist; this is fully consistent with the Mermin and

Wagner theorem which only holds (hence forbbidens finite spontaneous magnetization at any finite temperature) if (a) the system involves no long range interactions (hypothesis satisfied by our model), (b) the system is two-dimensional (hypothesis satisfied by our model in the sense that it can be considered a $\infty \times \infty \times$ *finite* system due to the *exponentially* decaying profile of the magnetization while going deep into the bulk), and (c) the system presents a symmetry break-down corresponding to magnetic interactions which are, *all of them*, associated with *continuous* group of symmetries (hypothesis satisfied by our model *if and only if both* η_B *and* η_s *vanish*); in other words, an Ising-like bulk prevents, *even if it is magnetically disordered*, condition (c) of the theorem to be satisfied, and therefore it does not apply.

We aknowledge useful discussions with L.R.da Silva.

CAPTION FOR FIGURES AND TABLE

Fig.1 - RG cluster transformation for the bulk (a) and its free surface (b); ● and O respectively denote internal and terminal sites.

Fig.2 - RG flow diagrams in the invariante subspaces $\eta_B=\eta_s=1$ (a) and $\eta_B=\eta_s=0$ (b); ■, ● 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.3 - η_s-evolution of the phase diagram for Ising bulk (a) and isotropic Heisenberg bulk (b); ● denotes the multicritical point.

Fig.4 - (η_B,η_s) dependence of the location Δ_c of the multicritical point appearing in Fig.3.

Table I - Universality classes corresponding to the *free surface* critical quantities (e.g., magnetization); the bulk universality classes are the 3D (isotropic) Heisenberg and 3D Ising ones if $\eta_B=0$ and $0<\eta_B\leq 1$ respectively. P-SF, P-BF and SF-BF refer to critical lines; P-SF-BF refers to the multicritical point. * refers to the fact that a soft singularity is expected, at $T=T_c^{3D}$, in the surface magnetization, even if the present formalism does not characterizes it. I-IX denote non trivial universality classes which do not correspond (presumably) to any usual two-and three-dimensional model.

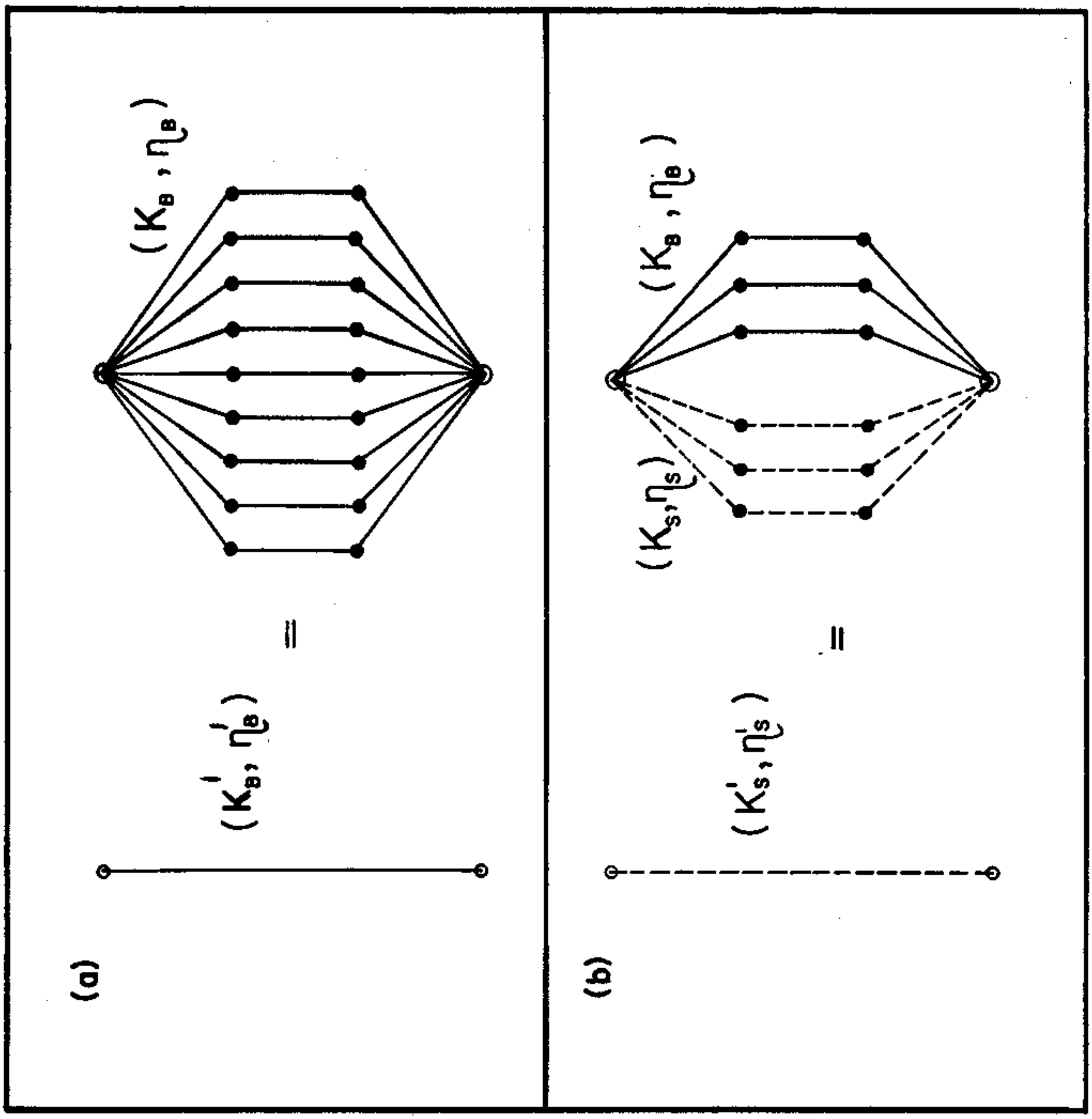

Fig. 1

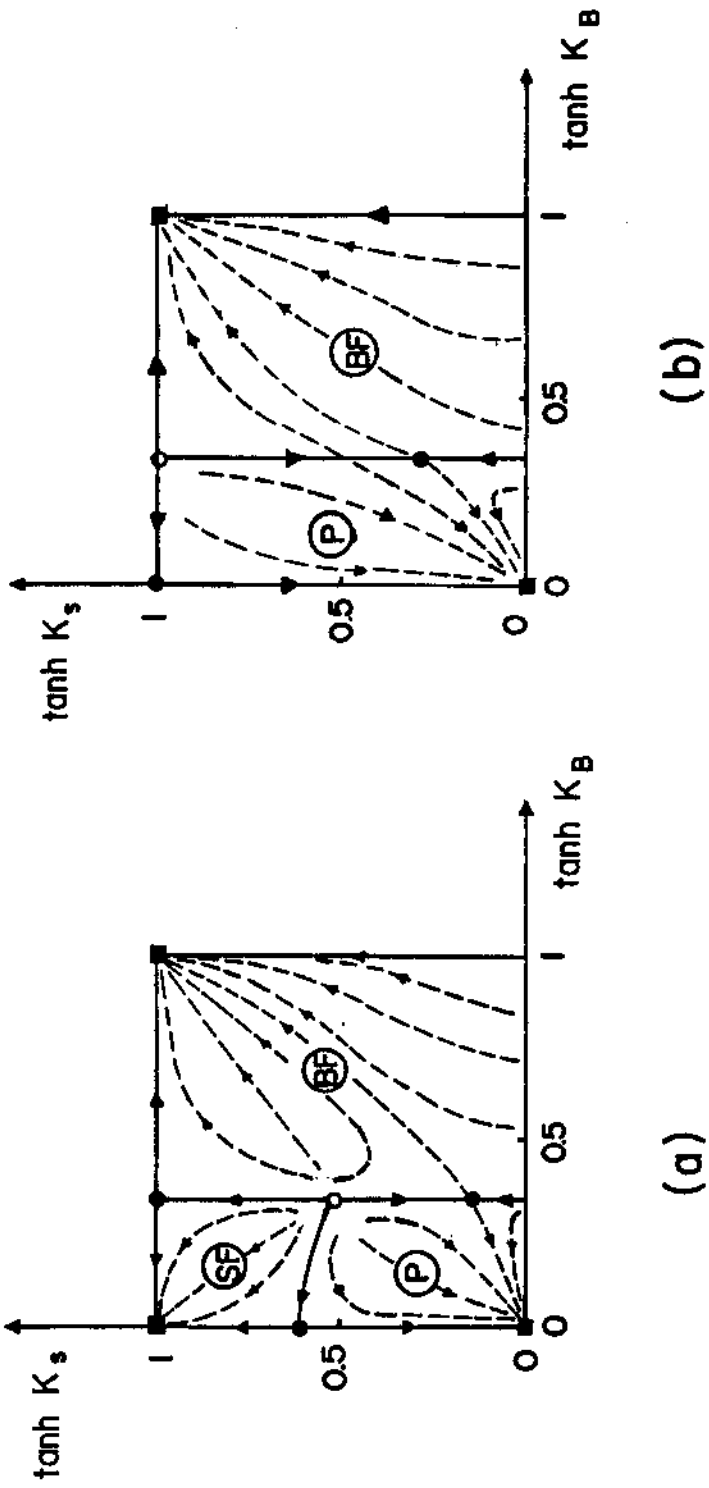

Fig. 2

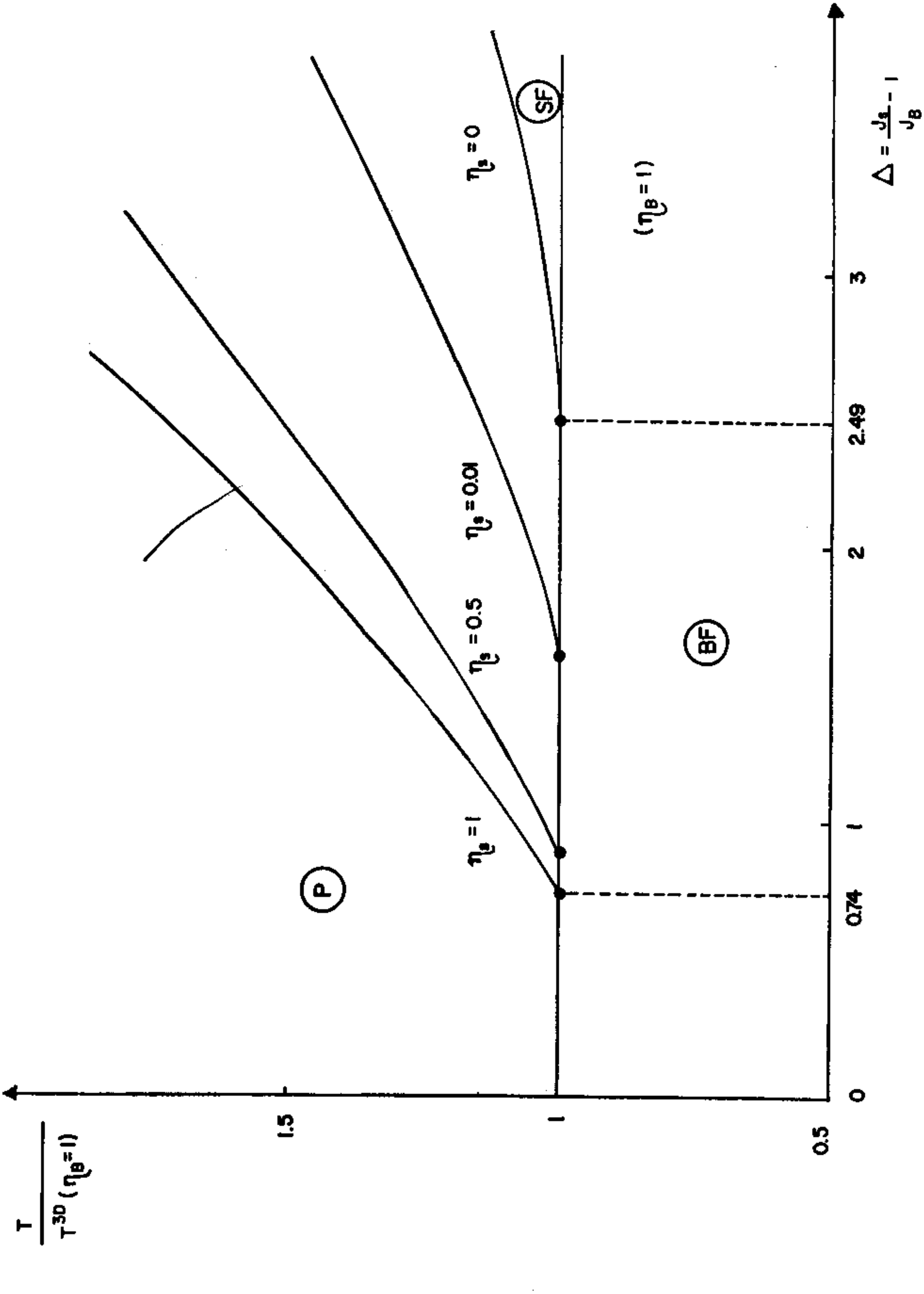
$\frac{T}{T^{3D}(\eta_B=1)}$
1.5
1
0.5
0
0.74
1
2
2.49
3
$\Delta = \frac{J_s}{J_B} - 1$
P
BF
SF
$\eta_s = 1$
$\eta_s = 0.5$
$\eta_s = 0.01$
$\eta_s = 0$
$(\eta_B = 1)$

Fig.3-(a)

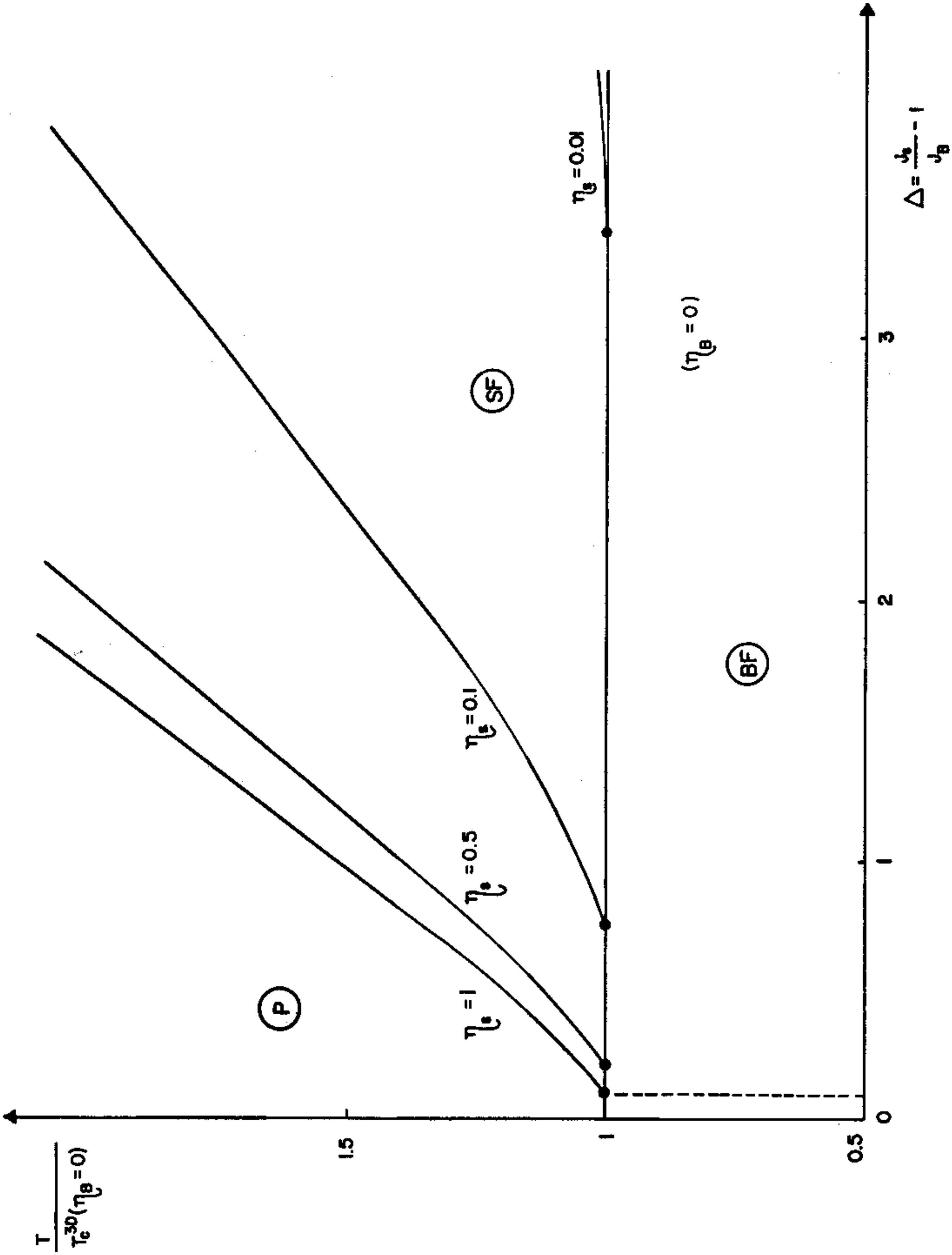

Fig. 3- (b)

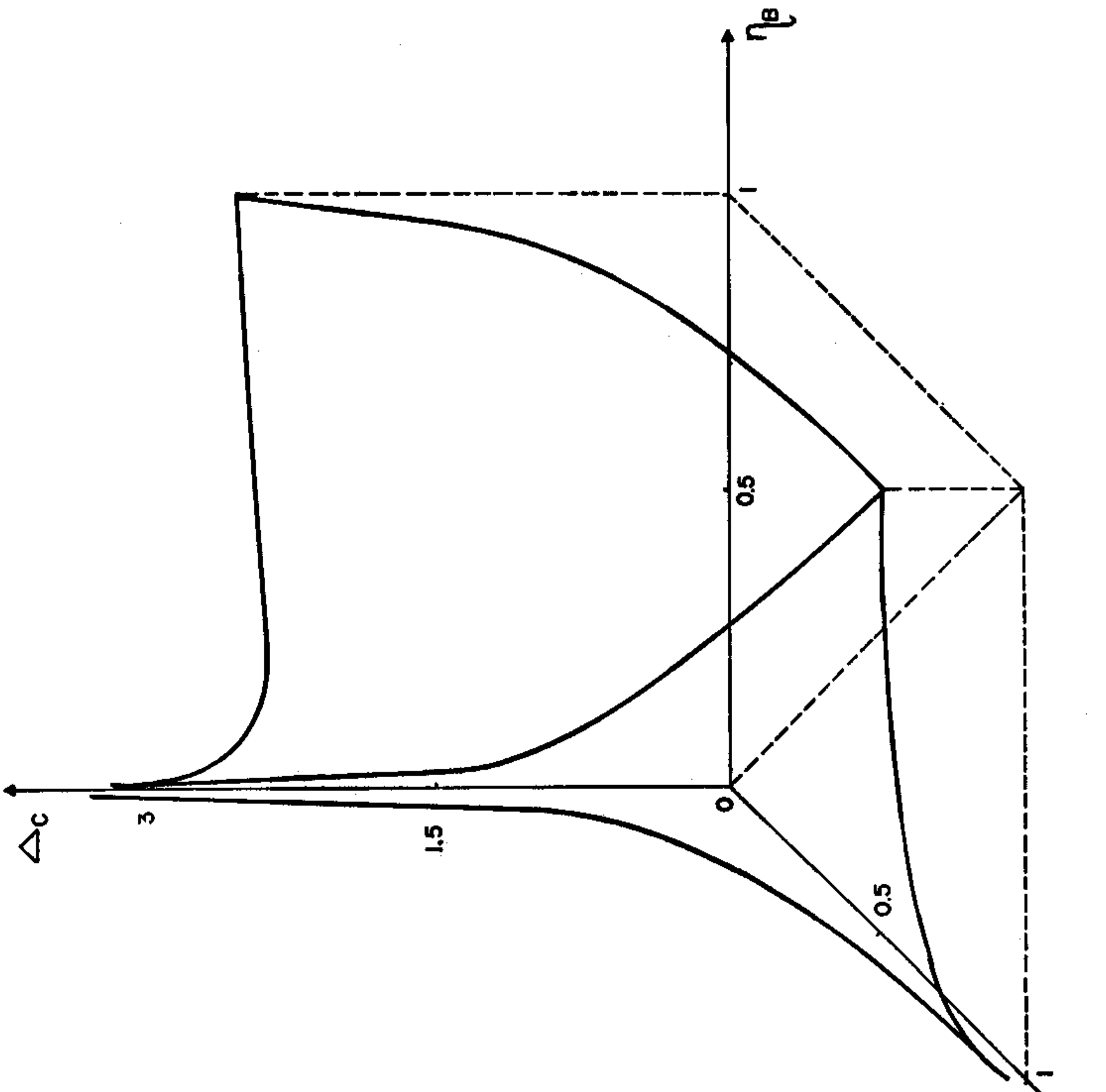

Fig. 4

TABLE I

	$\eta_S = 0$	$0 < \eta_S \leqslant 1$
$\eta_B = 0$	P-SF : 2D HEISENBERG P-BF : I SF-BF : II * P-SF-BF : III	P-SF : 2D ISING P-BF : IV SF-BF : V * P-SF-BF : VI
$0 < \eta_B \leqslant 1$	P-SF : 2D ISING P-BF : VII SF-BF : VIII * P-SF-BF : IX	P-SF : 2D ISING P-BF : VII SF-BF : VIII * P-SF-BF : IX

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