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ANISOTROPIC HEISENBERG INTERFACE BETWEEN ISING BULK FERROMAGNETS: A RENORMALIZATION GROUP APPROACH

by

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ABSTRACT

We consider two semi-infinite spin 1/2 Ising media (respectively characterized by the ferromagnetic coupling constants J_1 and J_2) separated by a spin 1/2 anisotropic Heisenberg interface (characterized by a ferromagnetic coupling constant J_S, and by an anisotropy $\eta \in [0,1]$ in spin space; $\eta=1$ and $\eta=0$ respectively correspond to the Ising and isotropic Heisenberg limits). Within a real-space renormalization-group framework, we discuss the full phase diagram; this diagram exhibits, besides the paramagnetic phase, three physically different ordered phases, namely the double-bulk, single-bulk and surface ferromagnetic ones. We also analyze the various universality classes appearing in this problem, and determine, in particular, the existence of a new high-order multicritical point associated with the $J_1 = J_2$ case.

Key-words: Heisenberg; Surface magnetism; Magnetic phase diagram; Renormalization group.

I - INTRODUCTION

During the last decade, surface magnetism has raised increasing interest, both because of its applications and its intrinsic richness (see Ref [1] for a recent review). The most commonly studied problem is the *free surface one*, where the system is assumed to be a semi-infinite bulk [2-11]. However this problem can be generalized into a richer one, namely the *interface* (or *defect*) problem [12], where two semi-infinite bulks (not necessarily equal) are separated by a surface whose nature is in general different from both bulks.

In a recent paper [13] (referred hereafter as paper I) an interesting system has been discussed, namely a semi-infinite spin 1/2 Ising ferromagnet, whose free surface is a spin 1/2 anisotropic Heisenberg ferromagnet. The approach has been a real-space renormalization-group (RG) one using Migdal-Kadanoff-like-clusters (diamond-like hierarchical lattices), and the quantum nature of the surface has been taken into account within a convenient procedure recently introduced [14]. The results have been quite satisfactory, and compare well with other theories available in the literature for the pure Ising limit.

In the present work we follow along the lines of paper I, and generalize the treatment in order to cover the interface problem. We shall see that, in spite of the simplicity of the clusters, a transparent overall view of the criticality of the system emerges.

In Section II we introduce the model and the RG formalism; in Section III we present the results, concluding finally in Section IV.

II - MODEL AND FORMALISM

We consider a spin 1/2 simple cubic lattice system constituted by two semi-infinite Ising bulks, separated by a (1,0,0) interface (square lattice) with a more complex magnetic nature, namely an anisotropic Heisenberg one (see Fig. 1). The Hamiltonian is given by

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

where $<i,j>$ run over all pairs of first-neighboring sites, and the σ's are the standard Pauli matrices; (J_{ij}, η_{ij}) equals $(J_1,1)$ on one semi-infinite bulk, $(J_2, 1)$ on the other, and (J_S, η) on the separating interface ($J_1, J_2, J_S \geq 0$ and $\eta \in [0,1]$; $\eta=1$ and $\eta=0$ respectively correspond to the Ising and *isotropic* Heisenberg limits). It is convenient to introduce the following variables

$$K_r \equiv J_r/k_B T \qquad (r = 1,2,S) \qquad (2)$$

$$t_r \equiv \tanh K_r \in [0,1] \quad (r = 1,2,S) \tag{3}$$

$$\Delta \equiv \frac{J_S}{J_1} - 1 = \frac{\ln \frac{1+t_S}{1-t_S}}{\ln \frac{1+t_1}{1-t_1}} - 1 \tag{4}$$

where k_B and T respectively are the Boltzmann constant and the temperature.

It is intuitive that such a system will undergo several phase transitions. First of all, the bulks 1 and 2 will present para-ferromagnetic phase transitions at $T_c^{3D(1)} = n^{3D}J_1/k_B$ and $T_c^{3D(2)} = n^{3D}J_2/k_B$ respectively, where n^{3D} is a pure number ($n^{3D} = 4.511$ [15]). Furthermore, if Δ is sufficiently large ($\Delta > \Delta_c\,(J_2/J_1,\eta)$), the surface is expected to retain a ferromagnetic order even when both bulks have lost theirs, i.e., up to $T_c^S\,(J_S/J_1, J_2/J_1, \eta)$. In general $T_c^S \geq T_c^{2D} \equiv n^{2D}(\eta)J_S/k_B = [n^{2D}(\eta)/n^{3D}](\Delta+1)T_c^{3D(1)}$ ($\sim[n^{2D}(\eta)/n^{3D}]\Delta\, T_c^{3D(1)}$ when $\Delta \to \infty$) ; $n^{2D}(\eta)$ is a pure number that monotonously increases from 0 to 2.269... when η increases from 0 to 1 [14]; T_c^S will equal T_c^{2D} if and only if $J_1=J_2=0$ and $J_S>0$. With respect to Δ_c, a mean field argument ($4J_S+J_1+J_2 = 6J_1$, assuming $J_2 \leq J_1$) yields $\Delta_c=(1-J_2/J_1)/4$,

$\forall$ η, which we shall see is an extremely crude approximation.

To discuss the criticality associated with Hamiltonian (1) we shall proceed as follows. The RG equation for the bulk 1 will be given by the recursion indicated in Fig. 2(a)[11]; therefore[16]

$$\frac{1-t_1'}{1+t_1'} = \left(\frac{1-t_1^3}{1+t_1^3}\right)^9 \tag{5}$$

where $t_1' \equiv \tanh K_1'$. Eq. (5), together with Eq. (3), immediately provides the *explicit* recursion

$$K_1' = f(K_1) \tag{6}$$

Analogously we have

$$K_2' = f(K_2) \tag{7}$$

To obtain (K_S', η') as function of (K_S, η, K_1, K_2) the operations are considerably more complex (but follow closely those indicated in paper I) and are indicated in Fig. 2(b). We first consider a two-terminal graph made by a linear chain of four spins and three (K_S, η)-bonds, and note (K_3^s, η_3^s) the equivalent parameters of a single bond graph (s stands for "series"); these parameters have already been calculated in paper I (see also

Ref. [14]), and therefore the functions $K_3^S(K_S,\eta)$ and $\eta_3^S(K_S,\eta)$ are explicitely known. We then consider the same linear chain graph but now made of three $(K_1,1)$-bonds; we note $(K_3^{(1)},1)$ the equivalent parameters, and obtain[16]

$$K_3^{(1)} = \text{arctanh}\ [(\tanh K_1)^3] \tag{8}$$

Analogously

$$K_3^{(2)} = \text{arctanh}\ [(\tanh K_2)^3] \tag{9}$$

Finally the parameters (K_S', η') we are looking for are given by

$$K_S' = 3[K_3^S(K_S,\eta) + K_3^{(1)}(K_1) + K_3^{(2)}(K_2)] \tag{10}$$

$$\eta' = \frac{3[K_3^S(K_S,\eta)\eta_3^S(K_S,\eta) + K_3^{(1)}(K_1) + K_3^{(2)}(K_2)]}{K_S'} \tag{11}$$

where we have used the parallel-array composition law (which for the present quantum subgraph of Fig. 2(b) represents an approximation: see paper I).

Eqs. (6), (7), (10) and (11) (together with Eqs. (8) and (9)) completely close the problem, as they determine the RG flow in the (K_1,K_2,K_S,η) space (or, equivalently, in the (t_1,t_2,t_S,η) space).

III - RESULTS

The present RG admits a few interesting *invariant subspaces* in the (t_1,t_2,t_S,η) space, such as the *Ising* limit ($\eta=1$) , the *isotropic Heisenberg* limit ($\eta=0$), the *pure surface* case ($t_1=t_2=0$), the *free surface* case ($t_2=0$, or equivalently $t_1=0$) and the *equal bulk* case ($t_1=t_2$), as well as the $t_S=1$, $t_1=1$ and $t_2=1$ planes.

The flow diagram associated with $\eta=1$ is indicated in Fig. 3. It exhibits:

i) Five fully stable fixed points, namely (t_1,t_2,t_S) = (0,0,0) (corresponding to the *paramagnetic* (P) phase), (1,0,1) (*bulk-1 ferromagnetic* (BF_1) phase), (0,1,1,) (*bulk-2 ferromagnetic* (BF_2) phase), (1,1,1) (*bulk-1-2 ferromagnetic* (BF_{12}) phase), and (0,0,1) (*surface ferromagnetic* (SF) phase);

ii) the following semi-stable fixed points: $(t_B,0,1)$ (with $t_B \simeq 0.3401$), $(0,t_B,1)$, $(t_B,t_B,1)$, $(1,t_B,1)$, $(t_B,1,1)$, $(t_B,0,t_{S1})$ (with $t_{S1} \simeq 0.1229$), $(0,t_B,t_{S1})$, (t_B,t_B,t_{S12}) (with $t_{S12} \simeq 0.3401$), $(0,0,t_S^S)$ (with $t_S^S \simeq 0.6180$; S point), $(t_B,0,t_{SB1})$ (with $t_{SB1} \simeq 0.5475$; SB_1 multicicritical point), $(0,t_B,t_{SB1})$ (SB_2 multicritical point);

iii) the fully unstable fixed point (t_B,t_B,t_{SB12}) (with $t_{SB12} \simeq 0.3720$), hereafter refered as the SB_{12} *super multicritical point*;

iv) six different universality classes, namely the *three-dimensional* (3D) one, associated with the bulks quantities (e.g., whatever be the values of J_2/J_1 and J_S/J_1, the deep magnetization in bulk-1 vanishes as $(T_C^{3D(1)}-T)^{\beta^{3D}}$; analogously the deep magnetization in bulk-2 vanishes as $(T_c^{3D(2)}-T)^{\beta^{3D}}$), the *free surface* one, associated with the interface quantities for $J_2/J_1 \gtrless 1$ and $\Delta < \Delta_c$ (e.g., the interface magnetization vanishes as $(T_c^{3D(1)}-T)^{\beta_1}$ if $J_2 < J_1$, and as $(T_c^{3D(2)}-T)^{\beta_1}$ if $J_2 > J_1$), the *equal bulk interface* one, associated with the interface quantities for $J_2/J_1=1$ and $\Delta < \Delta_c$ (e.g., the interface magnetization vanishes as $(T_C^{3D(1)}-T)^{\beta_1^{EB}}$), the *surface-bulk multicritical* one, associated with the interface quantities for $J_2/J_1 \gtrless 1$ and $\Delta=\Delta_c$ (e.g., the interface magnetization vanishes as $(T_c^{3D(1)}-T)^{\beta^{SB}}$ if $J_2 < J_1$, and as $(T_c^{3D(2)}-T)^{\beta^{SB}}$ if $J_2 > J_1$), the *surface-equal-bulk super multicritical* one, associated with the interface quantities for $J_2/J_1=1$ and $\Delta = \Delta_c$ (e.g., the interface magnetization vanishes as $(T_c^{3D(1)}-T)^{\beta^{SEB}}$), and the *two-dimensional* (2D) one, associated with the interface quantities for $J_2/J_1 \gtrless 1$ and $\Delta > \Delta_c$ (e.g., the interface magnetization vanishes as $(T_c^S-T)^{\beta^{2D}}$).

If $J_1 \neq 0$ and/or $J_2 \neq 0$, the universality classes corresponding to $0 \leq \eta < 1$ are the same as those for $\eta = 1$, because the single (double) Ising bulk connected to the interface, drives the whole system into the Ising symmetry, i.e., $\eta = 1$. A different situation occurs if $J_1=J_2=\eta=0$: in this case the interface becomes a pure two-dimensional isotropic Heisenberg system, thus exhibiting the corresponding universality class, which is different from all six universality classes mentioned above. All these facts have been numerically verified within the present RG.

In Fig. 4 we have represented, in the (t_1, t_S) space, the phase diagrams corresponding to both free surface (Fig. 4(a)) and interface (Fig. 4(b)) cases; the critical line between the P and SF phases has been indicated for typical values of η. Typical phase diagrams have also been represented, in Fig.5, in the (T, Δ) space. Finally, in Fig. 6, we have indicated Δ_c (value of Δ above which the surface magnetic order can subsist even in the absence of bulk order) as function of η and J_2/J_1. For $\eta = 1$ and $J_2/J_1=0$ we obtain $\Delta_c \simeq 0.736$, which compares reasonably well with the series result 0.6 ± 0.1[3] and with the Monte Carlo one 0.50 ± 0.03[10] (the mean field approximation result is 0.25).

IV - CONCLUSION

We have considered an anisotropic Heisenberg interface between two not necessarily equal semi-infinite Ising simple cubic bulks. The criticality of this system has been discussed within a real-space renormalization-group which uses quite simple

Migdal-Kadanoff-like clusters (diamond-like hierarchical lattices); as far as we know, this is the first-time such a discussion is performed. Great richness has been exhibited in both the phase diagram (four physically different phases are present, namely the paramagnetic, the double-bulk, the single-bulk and the surface ferromagnetic ones) and with respect to the universality classes (seven different classes are present, namely the two-dimensional isotropic Heisenberg one, as well as six Ising-type: the standard two-and three-dimensional ones, the free-surface and equal-bulk-interface critical ones, the surface-bulk multicritical one, and the surface-equal-bulk super multicritical one). It is worth stressing the appearance, when the bulks are equal among them, of a high order multicritical point.

We have given special attention to the calculation, as function of the spin anisotropy η and the ratio J_2/J_1 (relative strength of the coupling constants in both bulks), of the value of the ratio J_S/J_1 (relative strength of the surface and bulk-1 coupling constants) above which surface magnetic order can exist even if it has disappeared from both bulks (see Fig. 6).For the particular free surface ($J_2/J_1=0$) Ising ($\eta=1$) case, we have obtained, for the just mentioned critical value of the ratio J_S/J_1, 1.736, to be compared with the series value 1.6 ± 0.1[3] and the Monte Carlo value 1.50 ± 0.03[10], the mean field approximation value being 1.25. For the interface equal bulk ($J_1=J_1$) Ising ($\eta=1$) case we have obtained 1.130 for this ratio; we are not aware of any other numerical proposal excepting that of the mean field approximation which yields 1.

CAPTION FOR FIGURES

Fig. 1 - Two semi-infinite simple cubic bulks separated by a square-lattice interface (dashed bonds).

Fig. 2 - RG transformation for the bulk (a) and the interface (b). The types of bonds coincide with those of Fig.1. o (●) denotes terminal (internal) nodes.

Fig.3 - $\eta = 1$ RG flow diagram in the (t_1, t_2, t_S) space. The paramagnetic (P), bulk-1 ferromagnetic (BF_1), bulk-2 ferromagnetic (BF_2), bulk-1-2 ferromagnetic (BF_{12}) and surface ferromagnetic (SF) phases are indicated. ■ (●) denotes fully stable (unstable or semi-stable) fixed points.

Fig. 4 - Phase diagrams, in the (t_1, t_S) space, for typical values of η: (a) free surface case, (b) equal bulk case.

Fig. 5 - $T - \Delta$ cuts of the phase diagram for typical values of η and J_2/J_1: (a) free surface case, (b) intermediate case, (c) equal bulk case.

Fig. 6 - Δ_c as a function of η and J_2/J_1: (a) for typical values of J_2/J_1, (b) for typical values of η.

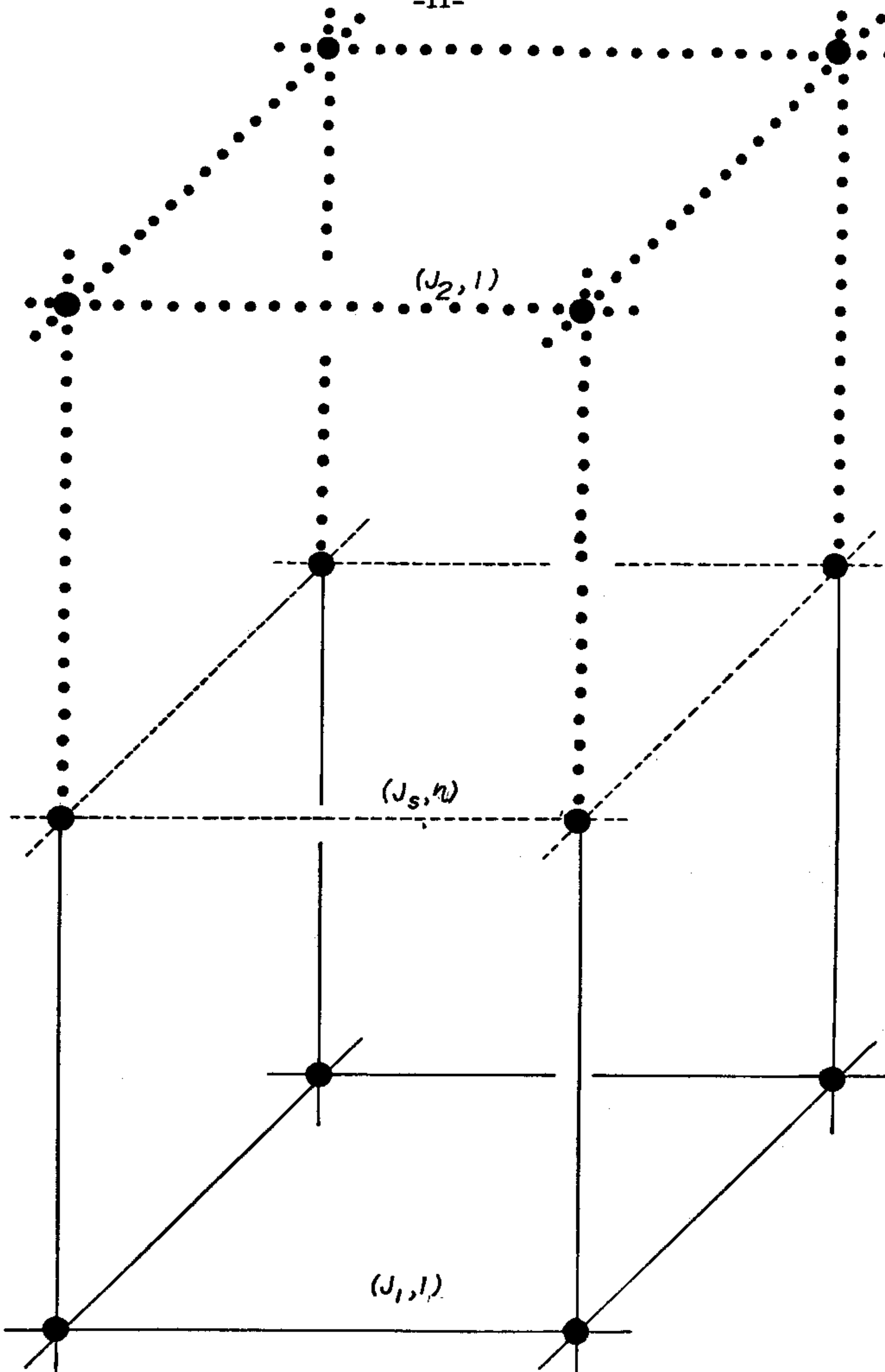


FIG. 1

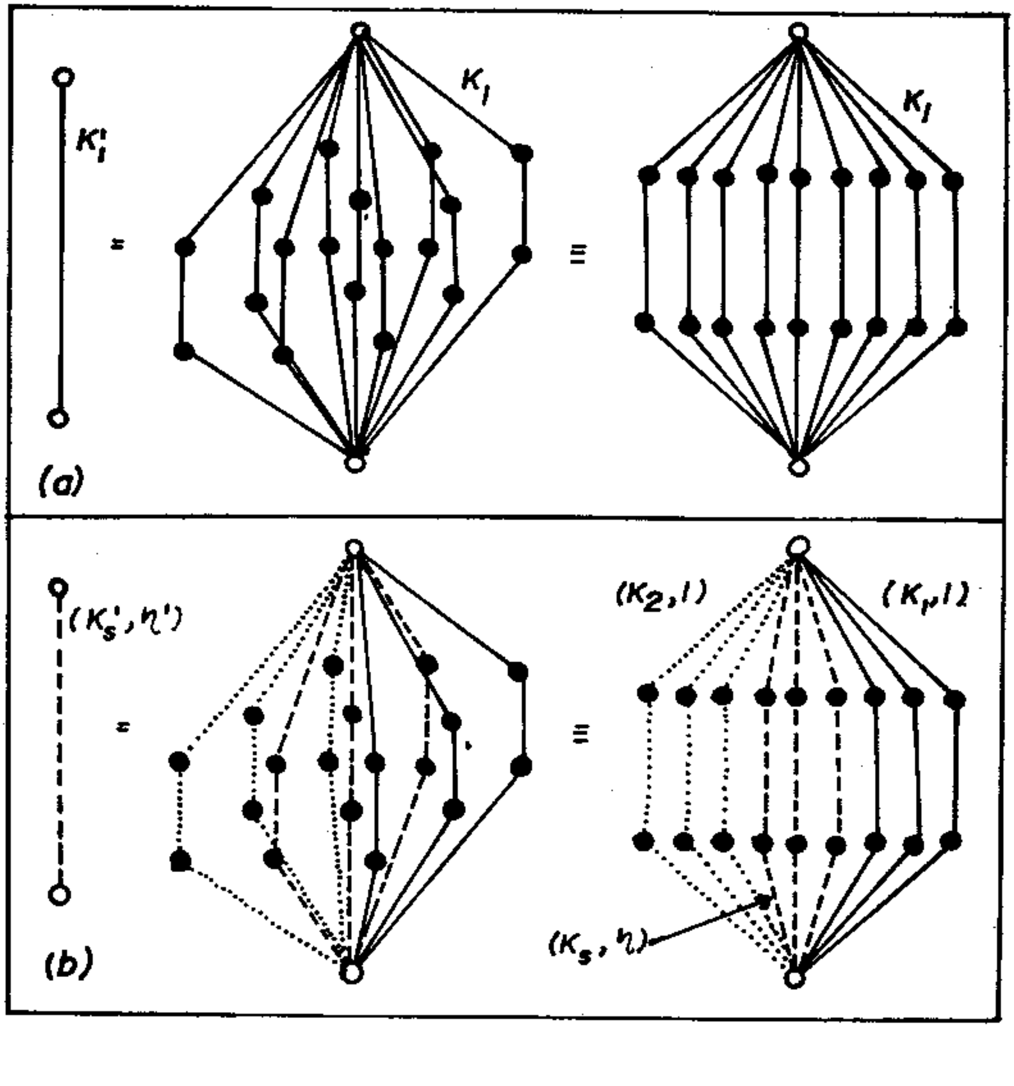


FIG. 2

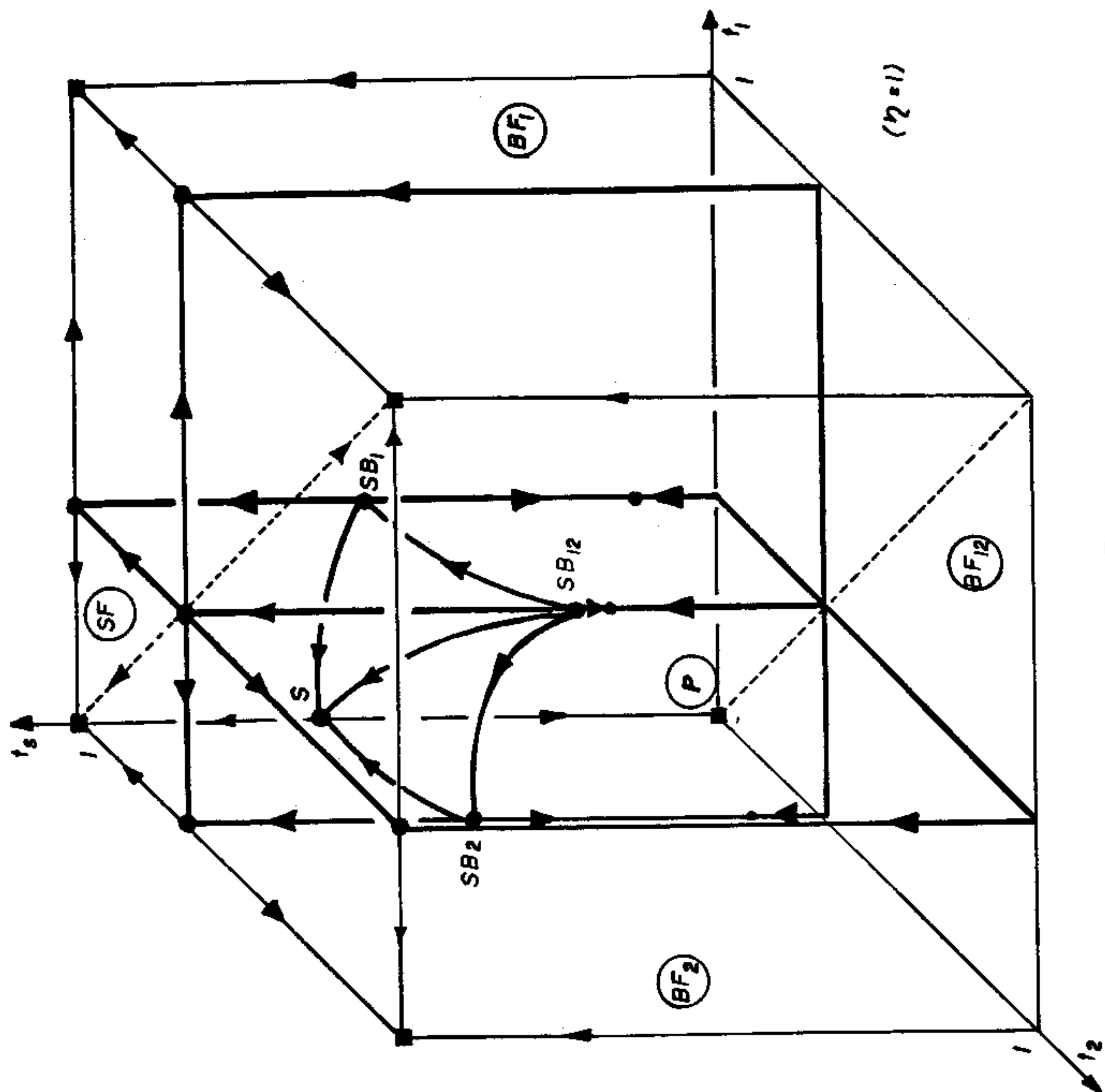


FIG. 3

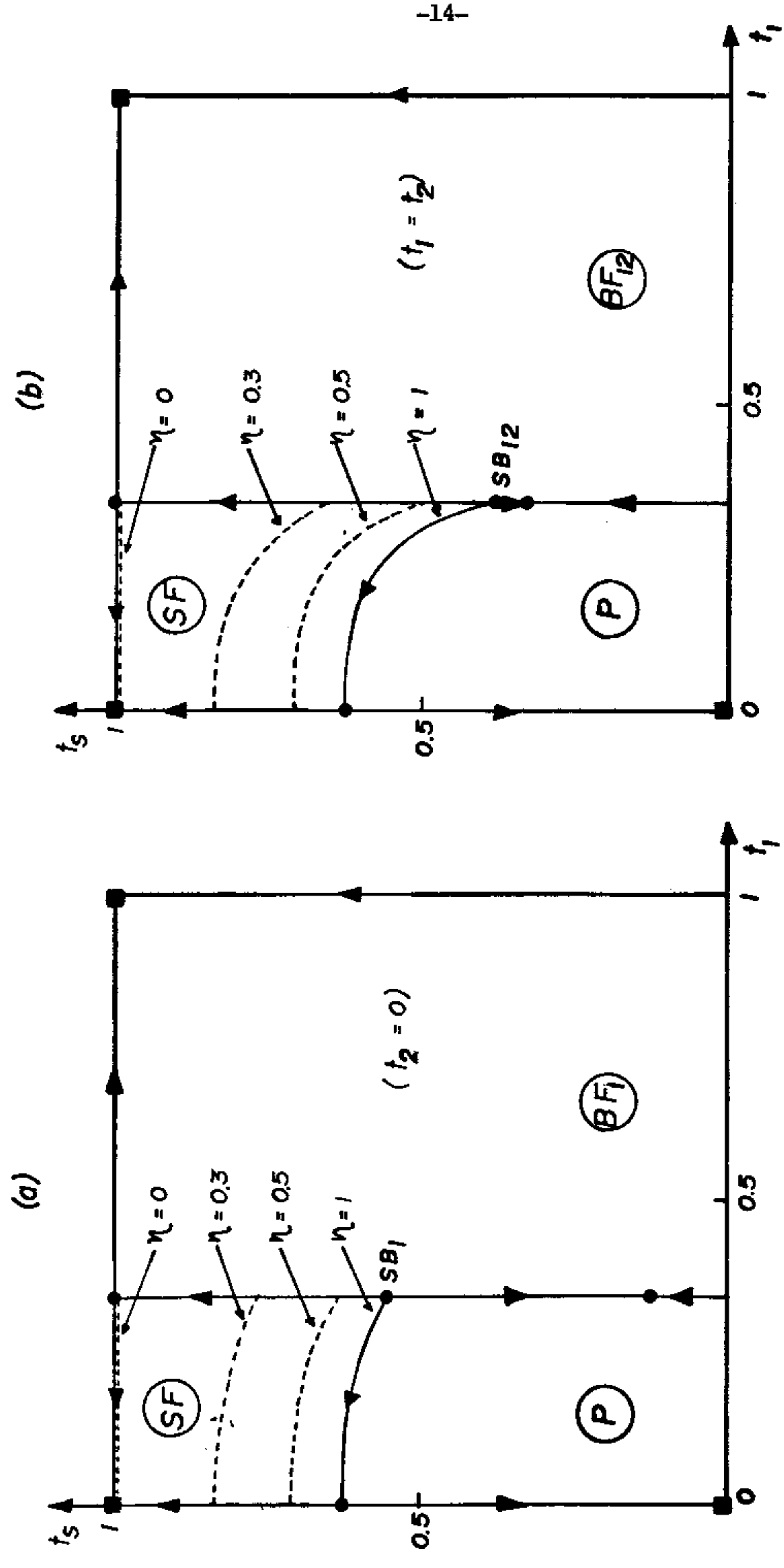
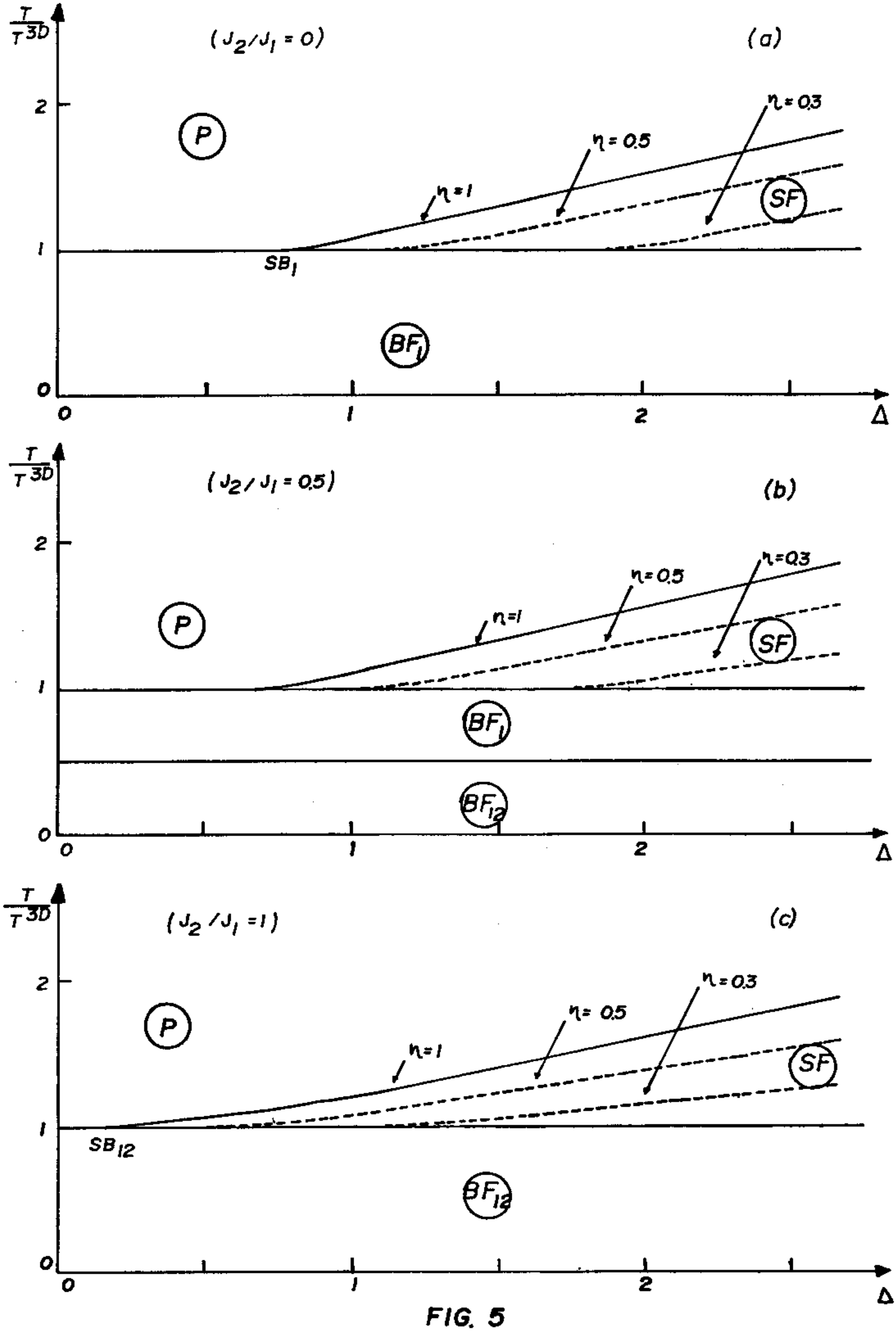

(a)
(b)
$\eta = 0$
$\eta = 0.3$
$\eta = 0.5$
$\eta = 1$
SB_1
SB_{12}
SF
P
BF_1
BF_{12}
$(t_2 = 0)$
$(t_1 = t_2)$
t_s
t_1
0
0.5
1

FIG. 4



T/T^3D
(J2/J1 = 0)
(a)
2
1
0
P
η = 0.3
η = 0.5
η = 1
SF
SB1
BF1
0
1
2
Δ
(J2/J1 = 0.5)
(b)
η = 0.3
η = 0.5
η = 1
P
SF
BF1
BF12
(J2/J1 = 1)
(c)
η = 0.3
η = 0.5
η = 1
P
SF
SB12
BF12

FIG. 5

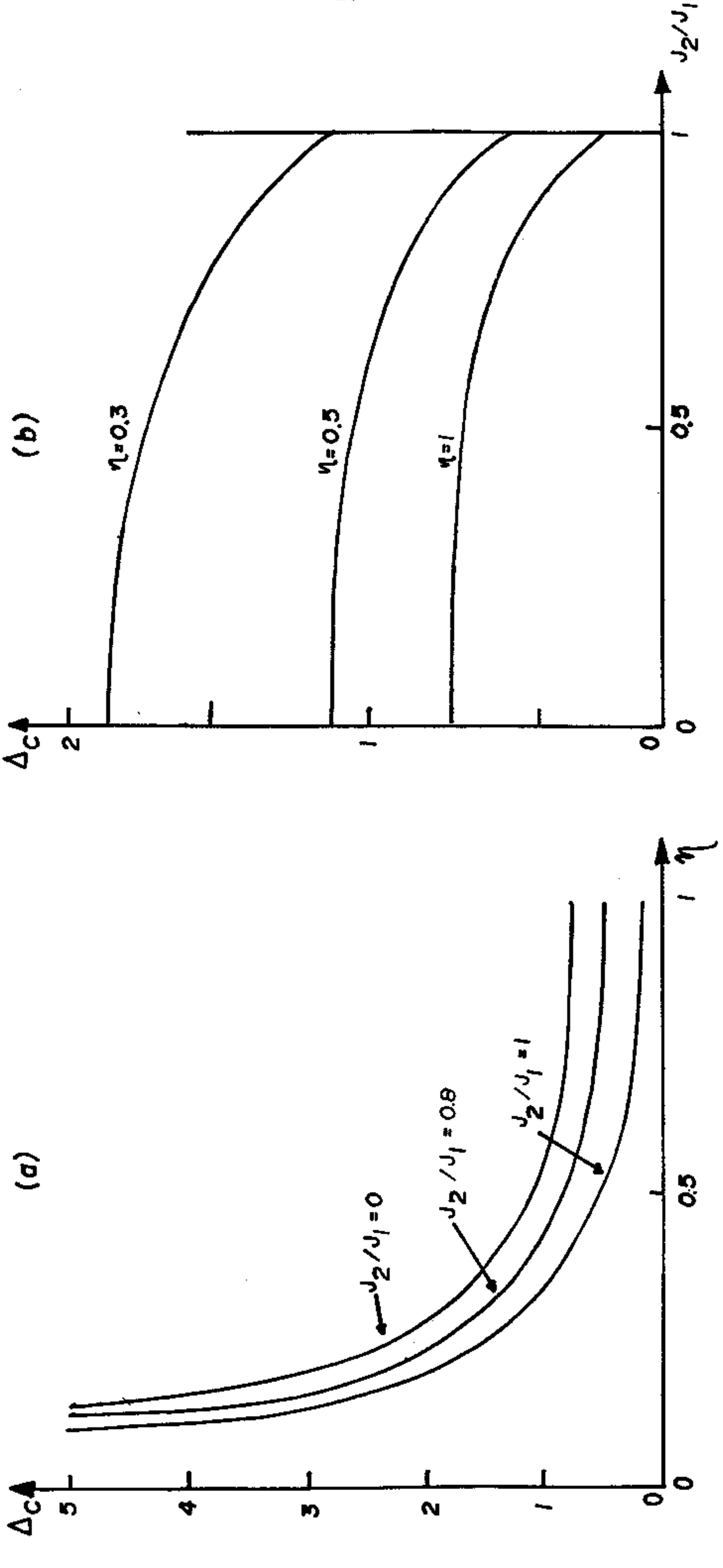

(a)
Δ_c
5
4
3
2
1
0
0
0.5
1
η
$J_2/J_1=0$
$J_2/J_1=0.8$
$J_2/J_1=1$
(b)
Δ_c
2
1
0
0
0.5
1
J_2/J_1
$\eta=0.3$
$\eta=0.5$
$\eta=1$

FIG. 6

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