ISSN 0029 - 3865

CBPF-NF-017/86

BOND-DILUTED INTERFACE BETWEEN SEMI-INFINITE POTTS BULKS: CRITICALITY

by

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Abstract

Within a real space renormalisation group framework, we discuss the criticality of a system constituted by two (not necessarily equal) semi-infinite ferromagnetic q-state Potts bulks separated by an interface. This interface is a bond-diluted Potts ferromagnet with a coupling constant which is in general different from those of both bulks. The phase diagram presents four physically different phases, namely the paramagnetic one, and the surface, single bulk and double bulk ferromagnetic ones. These various phases determine a multicritical surface which contains a higher order multicritical line. Particular attention is devoted to the discussion of the critical concentration p_c. Here, p_c is the concentration of the interface bonds above which surface magnetic ordering is possible even if the bulks are disordered. An interesting feature comes out which is that p_c varies continuously with J_1/J_s and J_2/J_s. The standard two-dimensional percolation concentration is recovered for $J_1=J_2=0$. From the analysis of the various fixed points obtained within the present formalism, a very rich set of critical universality classes emerges.

Key-words: Surface magnetism; Potts model; Renormalization group; Diluted magnetism.

I - INTRODUCTION

During the last decade some effort has been dedicated to the understanding of surface magnetism (see Binder 1983 for a recent review). Two main problems can be formulated, namely the free surface problem (semi-infinite bulk) and the interface or defect one (two semi-infinite bulks separated by an interface). The former has received most of the attention through various theoretical approaches such as mean field approximation (Mills 1971, 1973), series expansions (Binder and Hohenberg 1974), renormalisation group (Burkhardt and Eisenriegler 1977, Lipowsky 1982), Bethe approximation (Aguilera-Granja et al 1983), effective field theory (Sarmento et al 1984), and Monte Carlo (Binder and Landau 1984). In spite of its technical difficulties, some experimental work has also been performed (Pierce and Meier 1976, Alvarado et al 1982).

On the other hand, almost no attempts are available in the literature concerning the more general problem, namely the interface one (Lam and Zhang 1983, da Silva et al 1985).

The dilution of the surface brings out interesting features as recently shown (Kaneyoshi et al 1983), within an effective field theory, for the Ising semi-infinite ferromagnetic bulk. In the present paper we focus the general interface problem (with not necessarily equal semi-infinite bulks) for the q-state Potts simple cubic ferromagnet (q=1 and q=2 recover respectively the bond percolation and the Ising problems) assuming the (1,0,0) surface (square lattice) to be bond diluted.

The approach is a real-space renormalisation-group (RG) one, which follows along the lines of Tsallis and Sarmento 1985, where the pure (non diluted) free surface Potts problem has been investigated. Our effort is dedicated to the analysis of the phase diagram and the various critical universality classes.

In section II we introduce the model and the formalism; in section III we present the results; finally, in section IV, we conclude.

II - MODEL AND FORMALISM

We consider the following Potts Hamiltonian:

$$H = -\sum_{\langle i,j\rangle} J_{ij}\,\delta_{\sigma_i,\sigma_j} \quad (\sigma_i = 1,2,\ldots,q,\forall i) \tag{1}$$

where the sum runs over all pairs of nearest-neighbouring sites on a simple cubic lattice containing a (1,0,0) interface (see fig.1); J_{ij} equals J_1 and J_2 ($J_1 > 0$ and $J_2 > 0$) for the bulk-1 and bulk-2 respectively, and equals J_s when <u>both</u> i and j sites belong to the interface. Finally J_s is a random variable whose probability law is given by

$$P(J_s) = (1-p)\,\delta(J_s) + p\,\delta(J_s - J_0) \tag{2}$$

with $p \in [0,1]$ and $J_0 > 0$.

Let us introduce the following convenient variables (<u>thermal</u>

transmissivities, Tsallis and Levy 1981 and references therein):

$$t_r \equiv \frac{1 - e^{-qJ_r/k_BT}}{1 + (q-1)e^{-qJ_r/k_BT}} \in [0,1], \quad (r = 0,1,2,s) \tag{3}$$

as well as

$$\Delta \equiv \frac{J_o}{J_1} - 1 = \frac{\ln \dfrac{1+(q-1)t_o}{1-t_o}}{\ln \dfrac{1+(q-1)t_1}{1-t_1}} - 1 \tag{4}$$

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

To treat this problem we shall construct a RG operating in the (t_o,t_1,t_2,p)-space (or equivalently in the $(k_BT/J_1, J_2/J_1, J_o/J_1,p)$-space). Let us first of all take care of the bulk RG equations, by using (Tsallis and Sarmento 1985) the Migdal-Kadanoff-like cluster (hierarchical lattice two-terminal graph) indicated in fig (2 a). We obtain (Tsallis and Levy 1981):

$$t_1' = \frac{1 - \left[\dfrac{1-t_1^3}{1+(q-1)t_1^3}\right]^9}{1+(q-1)\left[\dfrac{1-t_1^3}{1+(q-1)t_1^3}\right]^9} \equiv f(t_1) \tag{5}$$

and

$$t_2' = f(t_2) \tag{6}$$

On the other hand, equation (2) can be rewritten as follows:

$$P(t_s) = (1-p)\ \delta\ (t_s) + p\ \delta\ (t_s - t_o) \tag{7}$$

If we associate this distribution with each one of the nine surface bonds of figure(2(b)), we obtain the following cluster distribution:

$$P_c(t_s) = (1-p^3)^3\ \delta\ (t_s - t^{(o)}) + 3p^3(1-p^3)^2\ \delta\ (t_s - t^{(1)})$$
$$+ 3p^6(1-p^3)\ \delta\ (t_s - t^{(2)}) + p^9\ \delta\ (t_s - t^{(3)}) \tag{8}$$

where

$$t^{(n)} \equiv \frac{1 - \left[\frac{1 - t_o^3}{1+(q-1)t_o^3}\right]^n \left[\frac{1 - t_1^3}{1+(q-1)t_1^3}\right]^3 \left[\frac{1 - t_2^3}{1+(q-1)t_2^3}\right]^3}{1 + (q-1)\left[\frac{1 - t_o^3}{1+(q-1)t_o^3}\right]^n \left[\frac{1 - t_1^3}{1+(q-1)t_1^3}\right]^3 \left[\frac{1 - t_2^3}{1+(q-1)\ t_2^3}\right]^3} \tag{9}$$

with n= 0,1,2,3.

In order to avoid analytically untractable parameter proliferation in the successive renormalised distributions, we approximate distribution (8) by the following <u>binary</u> one:

$$P'(t_s) = (1-p')\ \delta\ (t_s) + p'\ \delta\ (t_s - t'_o) \tag{10}$$

where p' and t'_o are to be determined.
To do so we shall preserve the first and the second momenta, i.e.,

$$<t_s>_{P'} = <t_s>_{P_c} \tag{11}$$

$$<t_s^2>_{P'} = <t_s^2>_{P_c} \tag{12}$$

hence,

$$p't'_o = (1-p^3)^3 t^{(o)} + 3p^3(1-p^3)^2 t^{(1)} + 3p^6(1-p^3)t^{(2)} + p^9 t^{(3)} \equiv F(t_o,\ t_1,\ t_2, p) \tag{13}$$

$$p't'^2_o = (1-p^3)^3[t^{(0)}]^2 + 3p^3(1-p^3)^2[t^{(1)}]^2 + 3p^6(1-p^3)[t^{(2)}]^2 + p^9[t^{(3)}]^2 \equiv G(t_o,\ t_1,\ t_2,\ p) \tag{14}$$

hence,

$$t'_o = G/F \tag{15}$$

and

$$p' = F/t'_o \tag{16}$$

Equations (5), (6), (15) and (16) close the problem as they completely determine the RG recurrence (in the (t_o,t_1,t_2,p)-space) we were looking for.

III - RESULTS

The RG flow diagram for p=1 and q=2 is indicated in Fig.(3). It exhibits (for all values os q actually) the following features: i) Five different phases are respectively characterided by five fully stable fixed points, at $(t_1,t_2,t_o) = (1,0,1)$ (bulk-1 ferromagnetic phase; BF_1), (0,1,1) (bulk-2 ferromagnetic phase; BF_2), (1,1,1)(double-bulk ferromagnetic phase; BF_{12}),(0,0,1)(surface ferromagnetic phase;SF), and (0,0,0)(paramagnetic phase; P);
ii) A multicritical line is present which ends (on both sides) at the surface-single-bulk multicritical points (semi stable fixed points) SB_1 and SB_2; this line contains also (for $t_1=t_2$) a high-order multicritical point (fully unstable fixed point) noted SB_{12}; for bigger and more sophisticated clusters than the diamond-like used herein it might happen that the SB_{12} and B_{12} fixed points merge (see da Silva et al 1985 for a discussion of this point);
iii) At $t_1=t_2=0$ a semi-stable fixed point is found (noted S) which corresponds to the pure bulk- disconnected two-dimensional case; at $t_2=0$ ($t_1 = 0$) we also found the semi-stable fixed points B_1(B_2) characterising <u>simultaneous</u> magnetic ordering in the surface and in the bulk-1 (bulk-2), and B_1' (B_2') characterising bulk-1 (bulk-2) disordering while the surface still retains its order; at $t_o=t_1=1$ ($t_o=t_2=1$) we find the semi-stable fixed points C_1(C_2) corresponding to bulk-1 (bulk-2) disordering, while the surface and bulk-2 (bulk-1) remain ordered; finally, at $t_1=t_2$ we found two other semi-stable fixed points, noted B_{12} and B_{12}', respectively

characterising simultaneous interface and double-bulk ordering, and double-bulk disordering while surface order still remains; iv) various universality classes are present, which concern bulk as well as interface quantities (such as correlation lengths, magnetizations at various "depths" with respect to the interface, etc); one universality class is the standard Potts three-dimensional one (e.g., the bulk-1 and bulk-2 magnetizations are characterised by the critical exponent $\beta^{3D}(q)$, no matter the values of J_s/J_1 or J_2/J_1); another universality class is the standard Potts two-dimensional one (e.g., the interface magnetization is characterised on the P-SF critical surface, by the critical exponent $\beta^{2D}(q)$; it occurs when $\Delta > \Delta_c$, where Δ_c is the value of Δ above which interface magnetic ordering is possible even in the absence of bulk magnetisation); another two universality classes correspond to $\Delta < \Delta_c$ (e.g., the interface magnetisation is characterised, on the P-BF$_1$ and P-BF$_2$ critical surface, by the exponent $\beta_1(q)$, and, on the P-BF$_{12}$ critical line, by the exponent $\beta_1^{EB}(q)$; here EB stands for "equal bulk"); the last two universality classes correspond to $\Delta = \Delta_c$ (e.g., the interface magnetisation is characterised, on the P-SF-BF$_1$ and the P-SF-BF$_2$ multicritical lines, by the exponent $\beta^{SB}(q)$, and, through the P-SF-BF$_{12}$ super multicritical point by the exponent $\beta^{SEB}(q)$; here SB and SEB stand for 'surface-bulk' and 'surface-equal-bulk', respectively.

Let us now describe the effects of the presence of random impurities (in the interface) on the thermal critical behaviour of the system. From equations (5), (6), (16) and (17) we find that the critical behaviour of the system depends on whether q is greater or less than a q*, where $q^* \cong 3.64$ in the present approximation. We refer the reader to figs. (4a) and (4b) where we illustrate this situation by showing the RG flow diagrams associated with $p < 1$ in the $(t_0 - t_1 - p)$ - space (with $t_2=0$), for q=3 ($q<q^*$) and q=4 ($q>q^*$), respectively. It exhibits the following features:

i) for $q < q^*$, a semi-stable fixed point is found, namely $(t_1,t_0,p) = (0,1,\ 0.682)$ which corresponds to the diluted bulk-disconnected two-dimensional case, that is, the percolation point (noted SP). It should be noted here, that the direction of the flow is from the SP point to the pure S point. Hence, the critical behaviour of the system is <u>stable with respect to randomness</u>. Also, as t_1 increases from $t_1=0$, the critical concentration continuously decreases from its maximum value $p_c=0.682$ down to $p_c= 0.614$ (for q=3) where t_1 attains its critical value t_1^c;

ii) for $q > q^*$, an additional semi-stable fixed point is found, namely $(t_1, t_0, p) = (0,0.640,0.9)$ for q=4, referred to as the random point (noted SR), which emerges from the pure one S characterising a crossover between pure and diluted behaviour. Notice that now the flow line is reversed and goes from the S point to the random one SR. Hence, the critical behaviour of the system has become <u>unstable with respect to randomness</u>.

The switching of universality class which occurs at $q=q^*$ (pure system universality class for $q < q^*$, and random system universality class for $q > q^*$) is consistent with the Harris 1974 criterion for Bravais lattices, as well as with similar though more complex phenomena (Costa and Tsallis 1984) ocurring for hierarchical lattices.

In fig (5) we illustrate the phase boundaries in the $(T-J_0/J_1)$ -space associated with both free surface (figs.(5a-b)) and interface cases figs.(5c-d)); the critical lines between the P and SF phases are shown for various values of q (fig.(5a)) and p (figs.(5b-d)). Typical phase boundaries and a few representative flows are shown in fig.(6), for q=2, in the (t_0-t_1)-space for both free surface (fig.(6a)) and interface cases (fig.(6b)); the critical lines scparating the P and SF phases are indicated for several values of the concentration p. The interesting behaviour of the critical concentration p_c (above which surface magnetic ordering is possible even if the bulks are disordered) as a function of the bulk coupling constant is shown in fig.(7), for several values of q , for the free surface (fig.(7a)) as well as for the interface case (fig.(7b)). Note that, when $J_1=J_2=0$, one recovers the standard two-dimensional bond-percolation concentration. The fact that p_c varies continuously with J_1/J_S and J_2/J_1 shows that the (free or interface) surface may sustain long range order for concentrations <u>lower</u> than the ordinary two-dimensional percolation concentration (this is due to surface correlations through the bulks).

Finally, in fig.(8) we illustrate the behaviour of Δ_c as a function of q and p, for the free-surface model (figs.(8a),(8b)) as well as for the interface model (figs.(8b),(8d)). In all the cases, the qualitative behaviour is roughly the same and Δ_c diverges as $q \to 0$ and as $p \to p_c$. In particular for the pure Ising free surface model, we find Δ_c(pure) ≃ 0.74.. This value may be compared with 0.6 obtained from high-temperature series expansion up to eighth order (Binder and Hohenberg 1974), with 0.5, the Monte Carlo result (Binder and Landau 1984), and with 0.30 obtained from a variational approach (Plascak 1984). The usual mean-field approximation yields Δ_c=0.25.

IV - CONCLUSION

This paper discusses the criticality of a system constituted by two semi-infinite ferromagnetic q-state Potts bulks (with exchange interactions J_1 and J_2) separated by a bond-diluted Potts interface (with exchange interaction J_s). Using renormalisation-group methods based on Migdal-Kadanoff-like clusters (diamond-like hierarchical lattices), we estimate the phase diagrams (for various values of q), which exhibit a very rich set of universality classes as described in the last section. A study of the q-evolution of the critical behaviour of the system , reveals interesting features. The increase of the number of states of the model corresponds to a decrease of the critical value $\Delta_c(p)$. Furthermore, as q is increased over a limiting value q*, we find that the impurities drive the pure system to a new critical behaviour, i.e. to a new set of critical exponents. This type of behaviour is consistent with the Harris criterion. Another interesting feature that appears, is the fact that the presence of a disordered bulk reinforces the "effective" surface percolation. More specifically, the interface critical concentration $p_c(J_1=J_2 \neq 0)$ is higher than the free surface critical concentration $p_c(J_1 \neq 0,\ J_2 = 0)$, which in turn is higher than the pure surface percolation critical point. Furthermore p_c varies <u>continuously</u> with J_1 and J_2.

All the results that we have presented in this work are valid in the second order phase transition region, that is, $q<q_c(2) = 4$ for $d = 2$ and $q < q_c(3) \simeq 3$ for $d = 3$. However, as the transitions in the range $q_c < q < 4$ display small latent heat, one can retain these results as a rough approximation over the entire range $0<q<4$.

The present approach provides, in spite of its simplicity, a clear overall picture of the criticality of a quite complex system. From a quantitative point of view, we have obtained results which are only roughly satisfactory whenever comparison is possible. An exception to this general trend is the values for Δ_c which seem to be quite accurate. Errors in our results stem from two sources: the use of small and simple clusters and the use of the binary approximation for the renormalised distributions. It seems that the errors coming from the binary approximation are small in comparison with the errors originated by the use of small RG-cells (Stinchcombe and Watson 1976, Yeomans and Stinchcombe 1978). Therefore, to improve significantly the results obtained here from a quantitative point of view, one must use more sophisticated clusters. We are presently working along this line.

FIGURE CAPTIONS

Fig.1 - Cell of two semi-infinite simple cubic lattices separated by an interface with coupling constants J_1 (full bonds ____), J_2 (dotted bonds ...), and J_s (dashed bonds ---).

Fig.2 - Renormalisation group cell transformation: (a) for the bulks (transmissivities t_1 and t_2); (b) for the interface (transmissivity t_s). Here, ○ denotes the terminals and ● denotes the internal modes, which are decimated.

Fig.3 - Flow diagram of the two-state Potts bulks and (pure) interface in the t_1-t_2-t_0- space, showing fixed points and typical flow lines. ■ denotes trivial (stable) fixed points, ● denotes critical (semi-stable) fixed points, and ⊙ denotes the multicritical (unstable) fixed point. Five phases are possible: bulk-1 ferromagnetic phase (BF_1), bulk-2 ferromagnetic phase (BF_2), double bulk ferromagnetic phase (BF_{12}), surface ferromagnetic phase (SF), and paramagnetic phase (P).

Fig.4 - Flow diagrams in the t_1-t_0- (1-p) - space, for the free-surface problem (t_2=0);

(a) the critical curve t_o^c (p) is shown for $q = 3 < q^*$. It flows from the percolation point SP=(0,1,0.318) to the pure point S = (0,0.616,0), indicating that the system is stable with respect to randomness.

(b) $q=4 > q^*$, and the presence of the random point SR indicates that the system is unstable with respect to randomness.

Fig.5 - Phase boundaries in the $(T - J_0/J_1)$ - space, using the renormalised variable T_c/T_c^{3D}, (here T_c^{3D} denotes the ordinary three-dimensional transition temperature) illustrating critical lines between the P and SF phases for:

(a) typical values of q, for the pure free-surface model $(p=1,\ J_2=0)$.

(b) typical values of p for the two-state free surface model $(q=2,\ J_2=0)$.

(c) typical values of p for the two-state interface (different-bulk) model $(q=2,\ J_2=J_1/2)$

(d) typical values of p for the two-state interface (equal-bulk) model $(q=2,\ J_2=J_1)$.

Fig.6 - Phase boundaries in the $t_0 - t_1$ - space illustrating critical lines between the P and SF phases for various values of concentration p for:

(a) free-surface model, $t_2=0$

(b) interface (equal-bulk)model, $t_1 = t_2$

Fig.7 - Dependence of the critical concentration p_c upon the bulk interaction strength for several values of q for the:

(a) free surface model, $J_2 = 0$.

(b) interface model

Fig.8 - Dependence of Δ_c upon:

(a) q, for selected values of concentration p, for the free-surface model ($J_2=0$).

(b) q, for selected values of p, for the interface model (equal-bulk) model ($J_1=J_2$).

(c) p , for selected values of q for the free-surface model ($J_2=0$).

(d) p, for selected values of q, for the interface (equal-bulk) model ($J_1=J_2$).

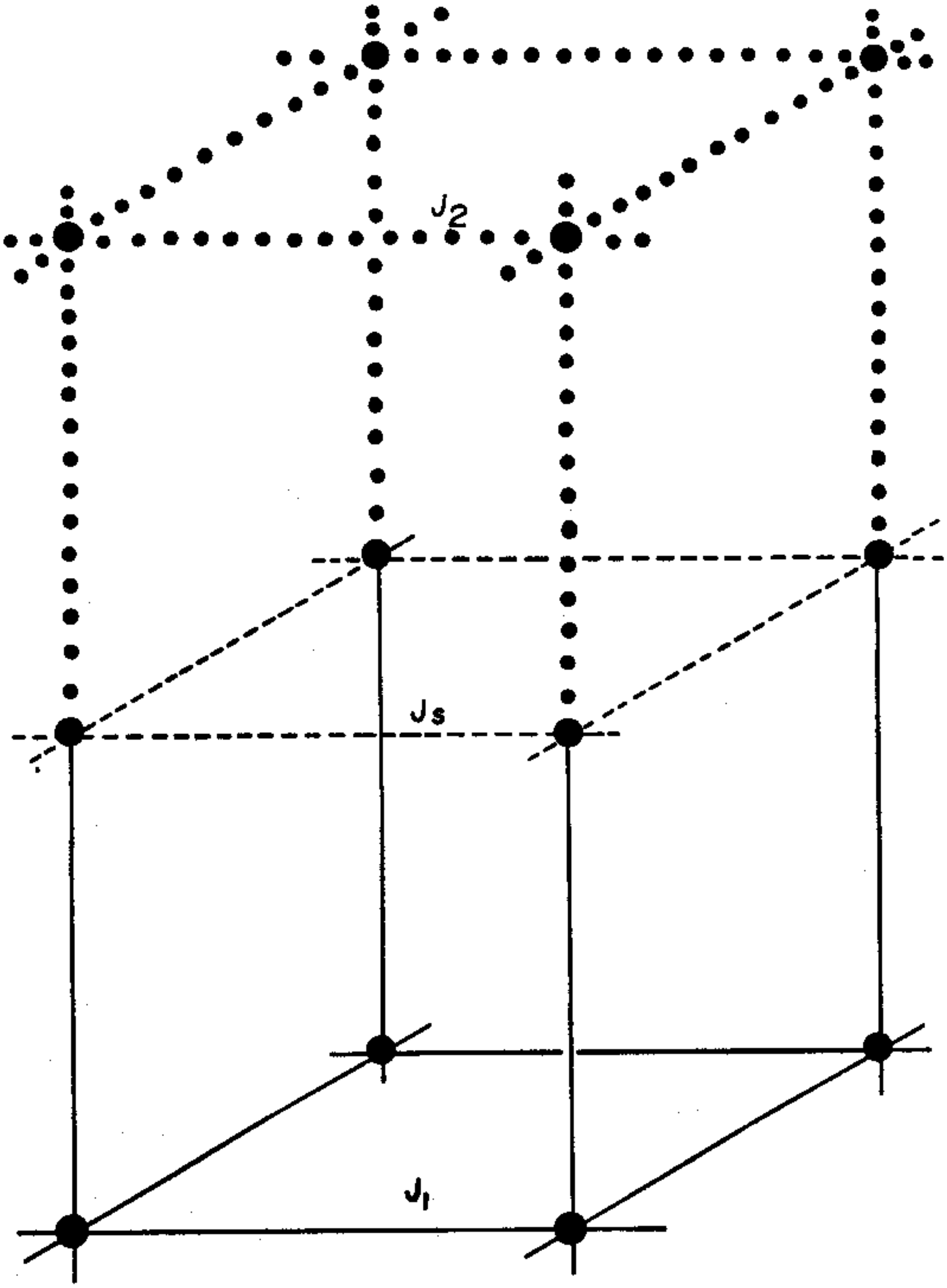


FIG. 1

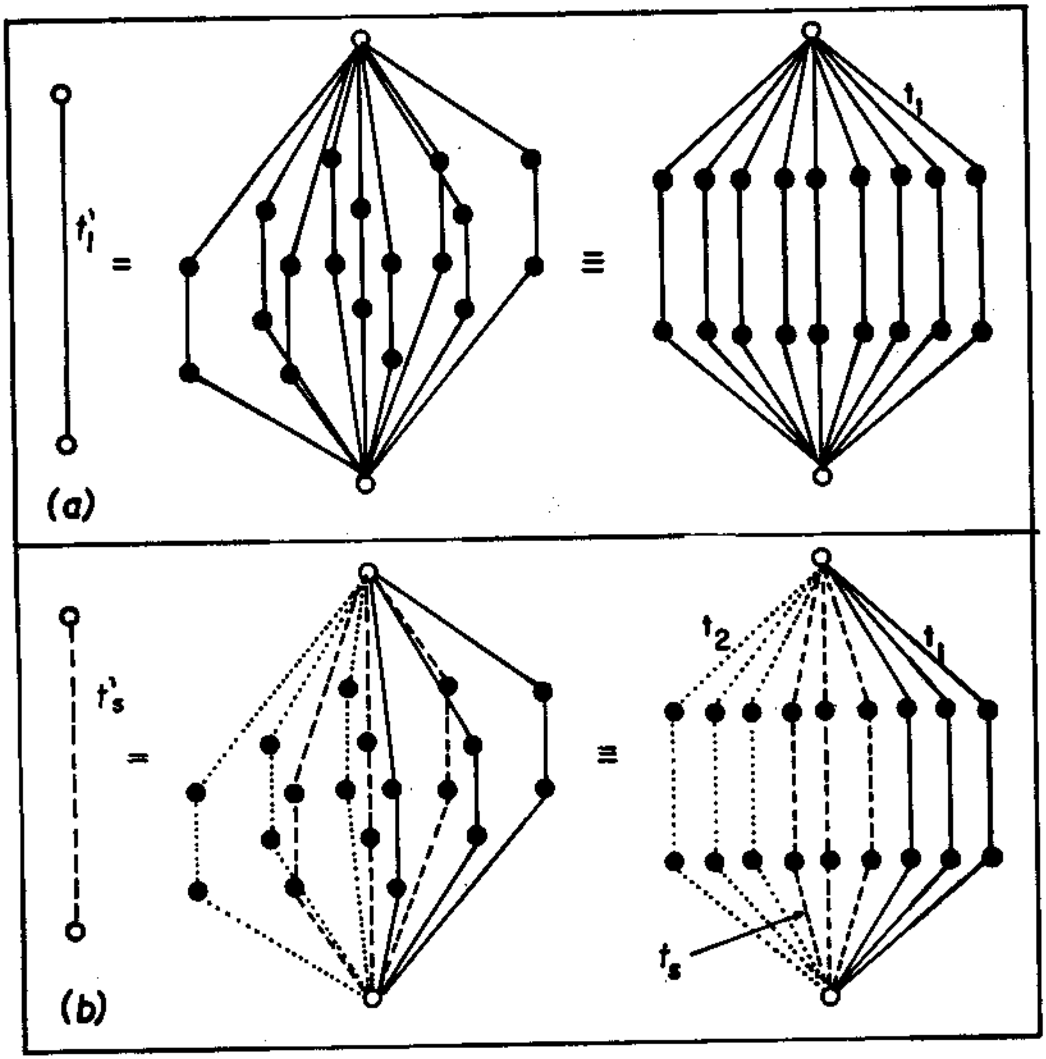


FIG. 2

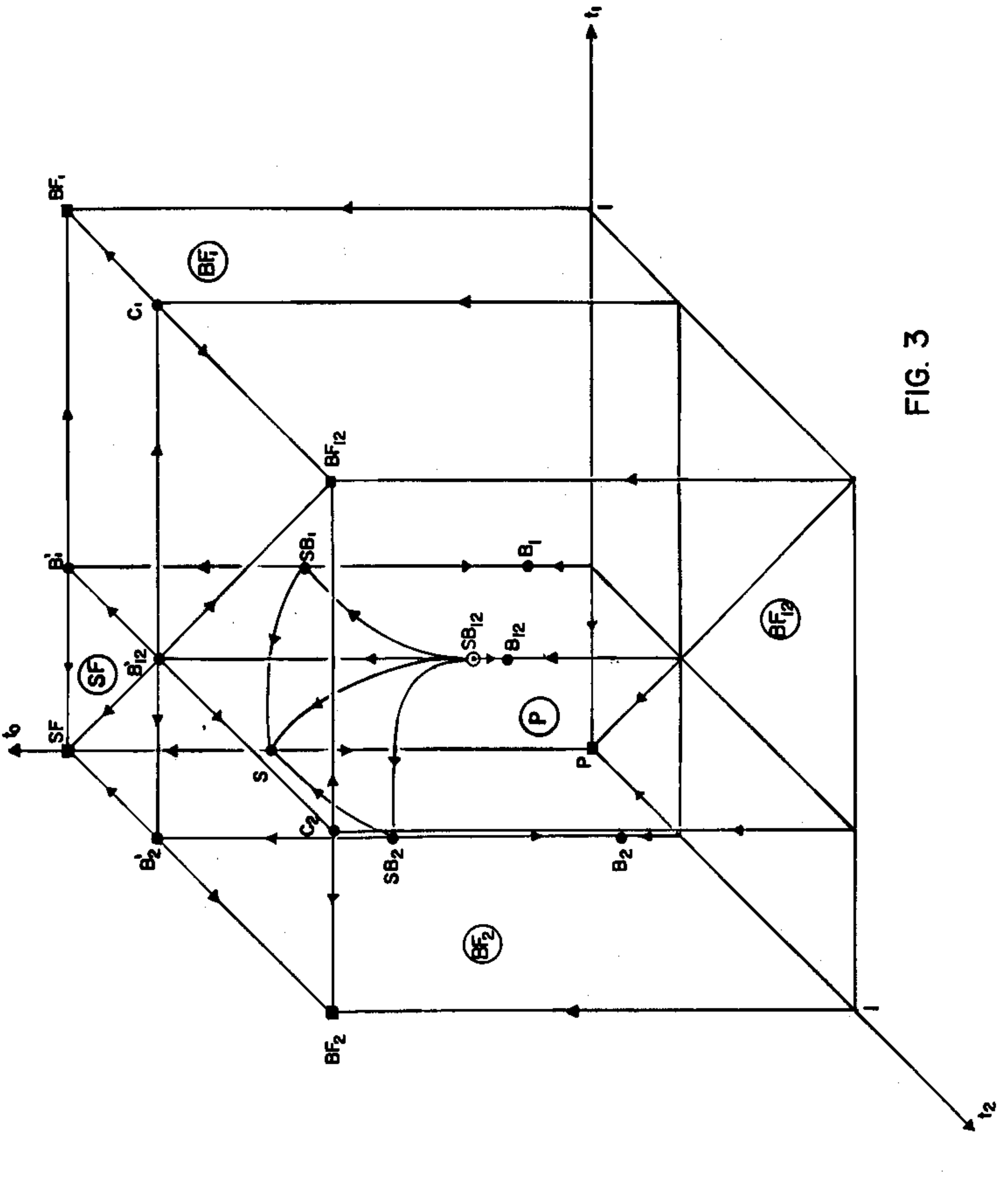


FIG. 3

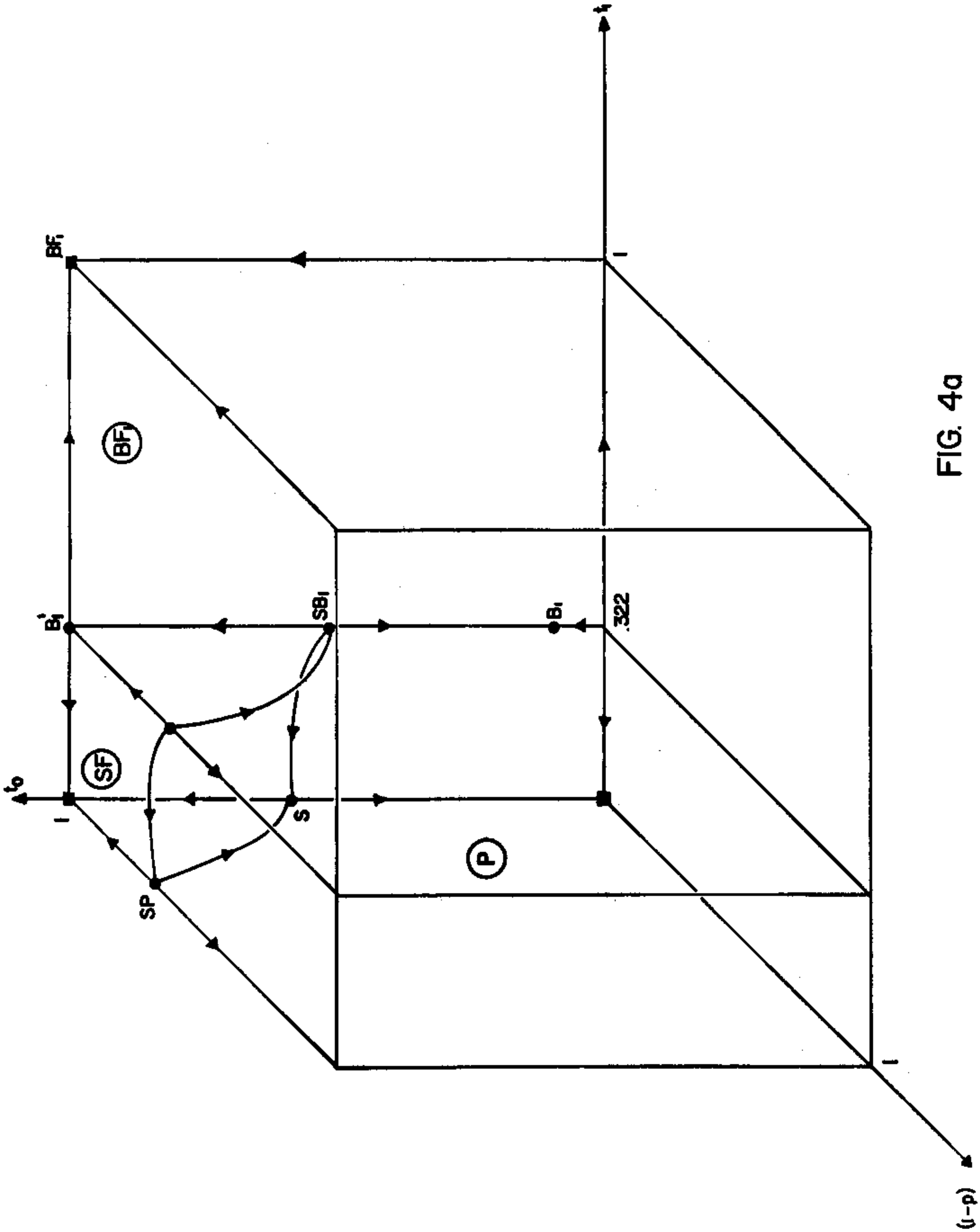


FIG. 4a

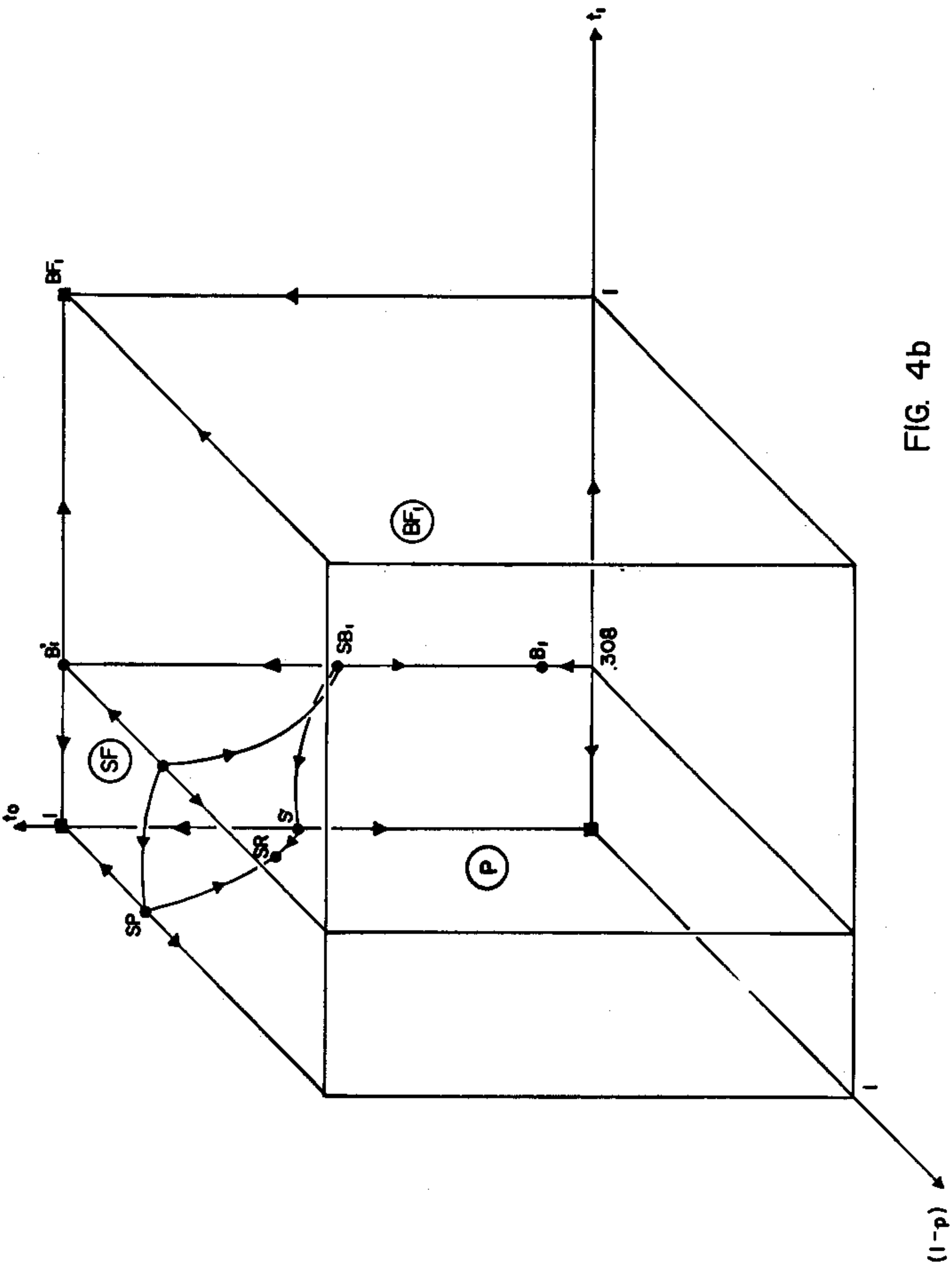


FIG. 4b

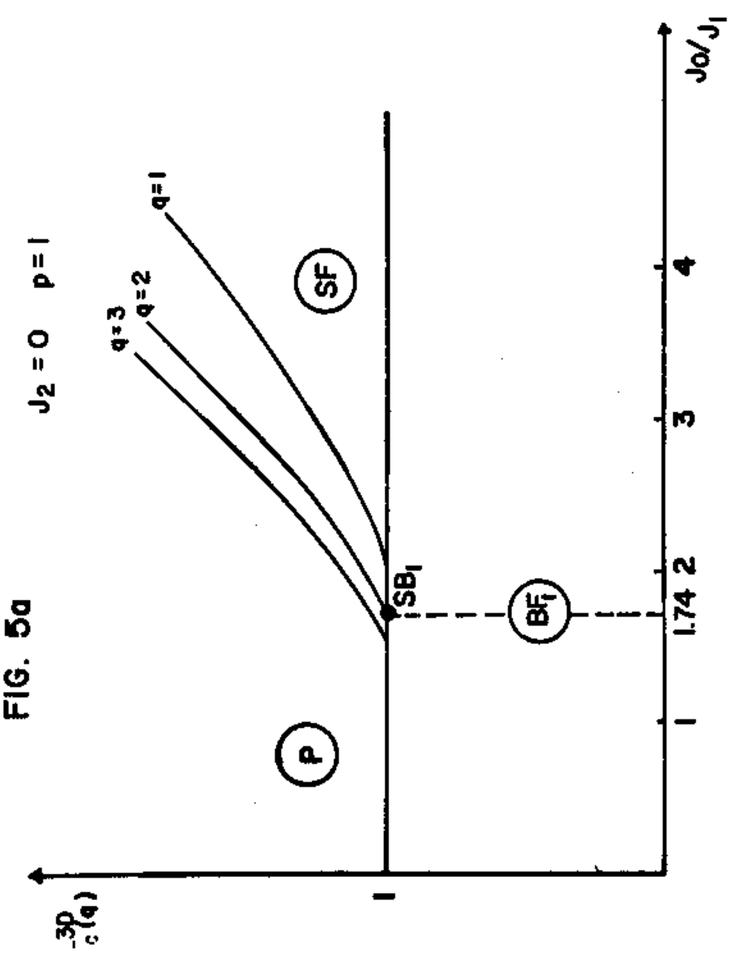


FIG. 5a

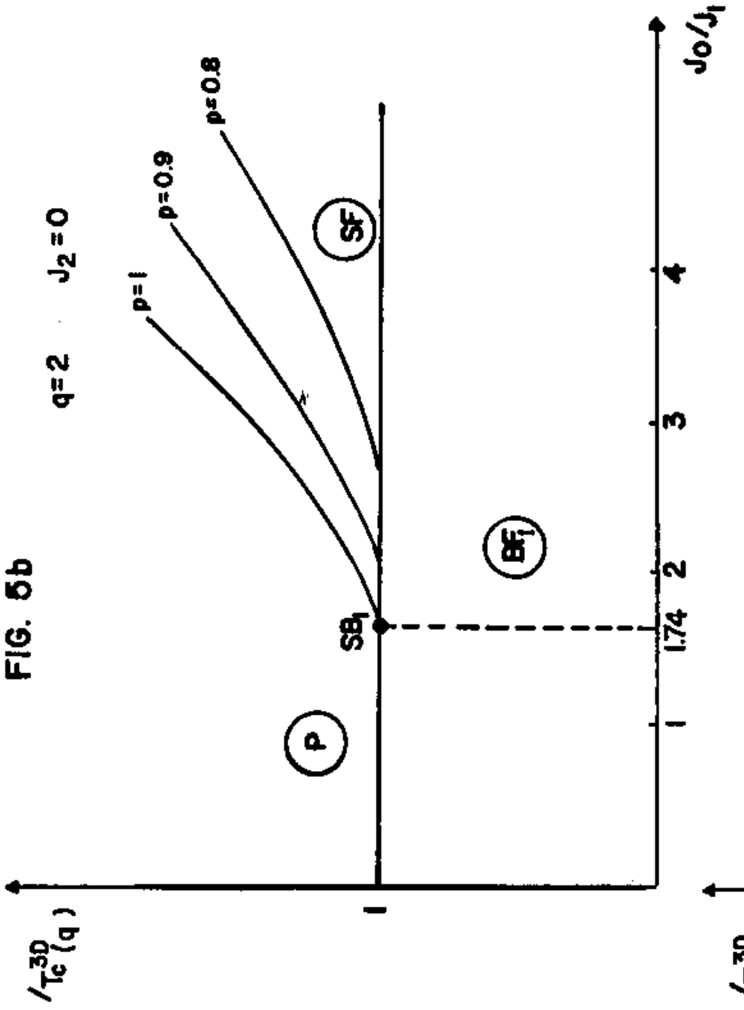


FIG. 5b

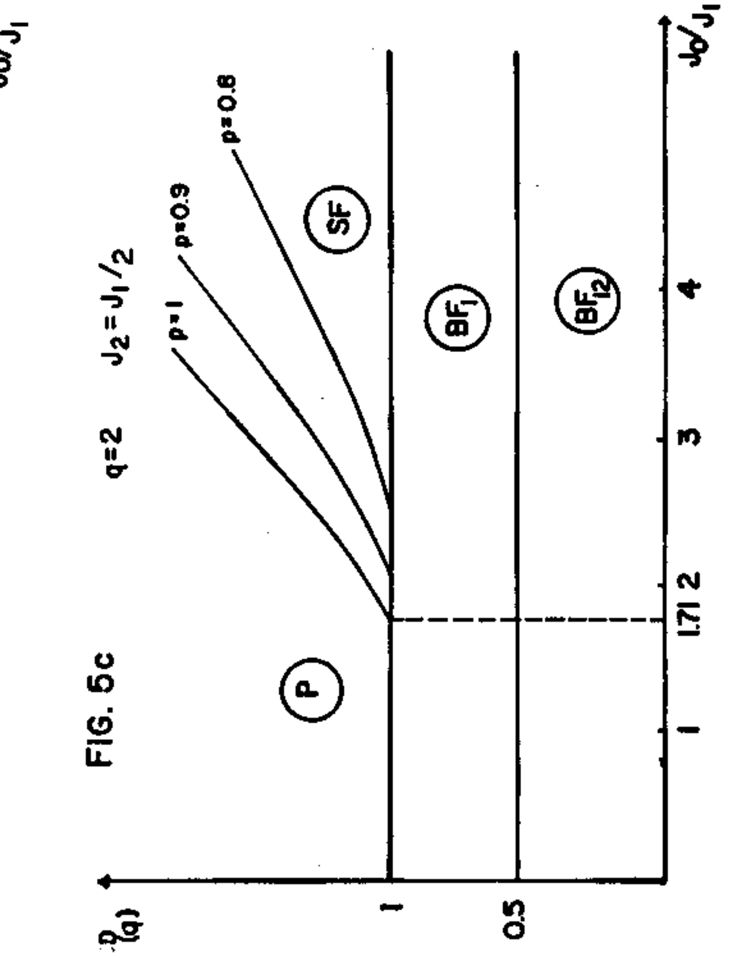


FIG. 5c

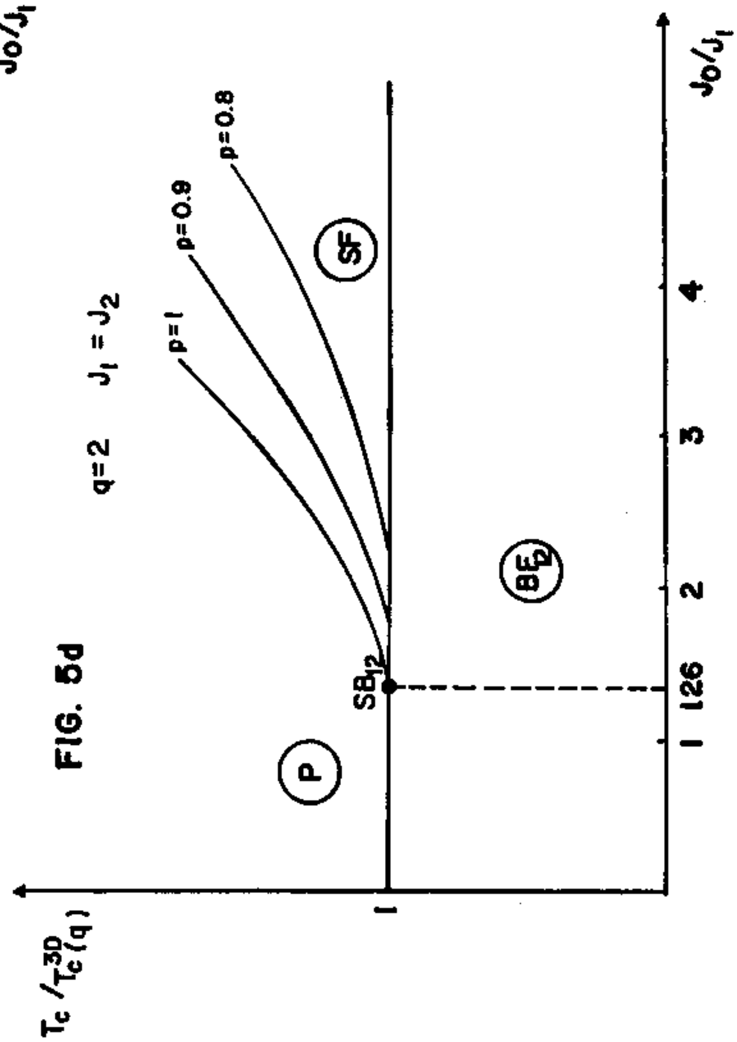


FIG. 5d

FIG. 6a

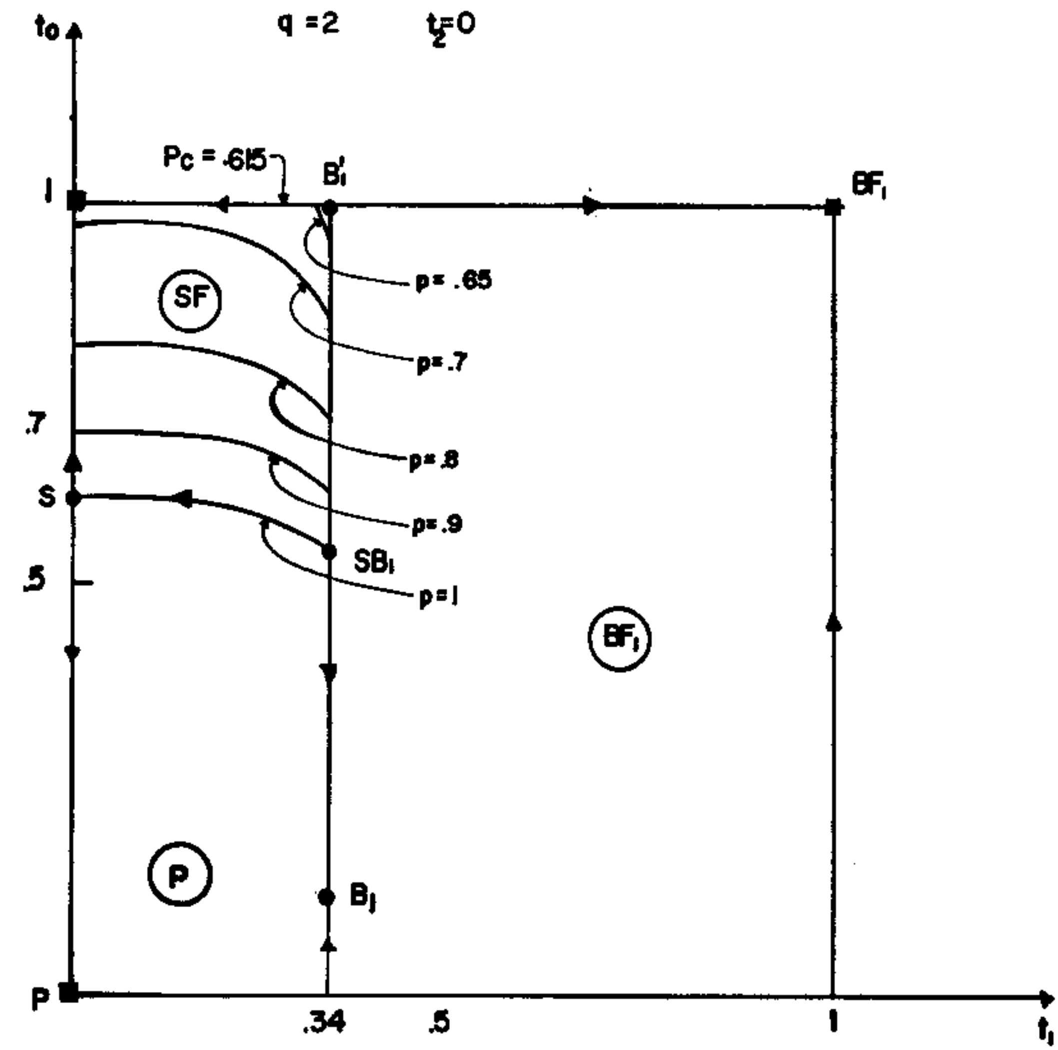

q = 2
t_2=0
t_0
P_c = .615
B_1'
BF_1
I
SF
p= .65
p= .7
p= .8
p= .9
p= 1
.7
S
SB_1
.5
BF_1
P
B_1
P
.34
.5
1
t_1

FIG. 6b

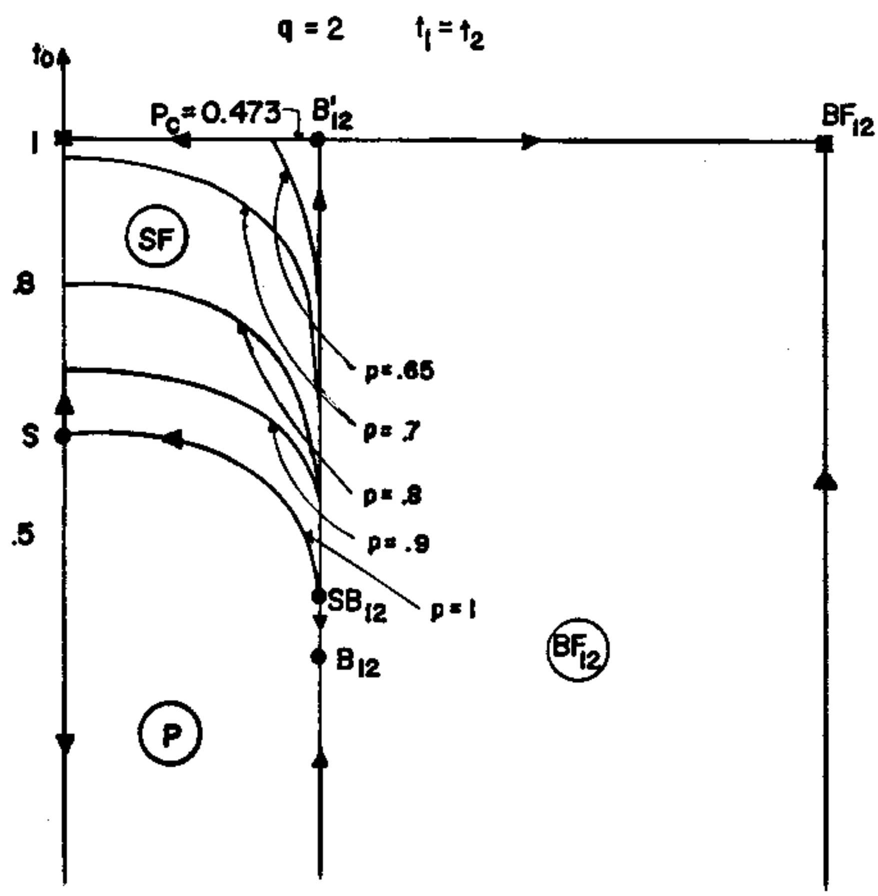

q = 2
$t_1 = t_2$
t_0
P_c= 0.473
B_{12}'
BF_{12}
I
SF
.8
p= .65
p= .7
p= .8
p= .9
p= 1
S
.5
SB_{12}
B_{12}
BF_{12}
P

FIG. 7b

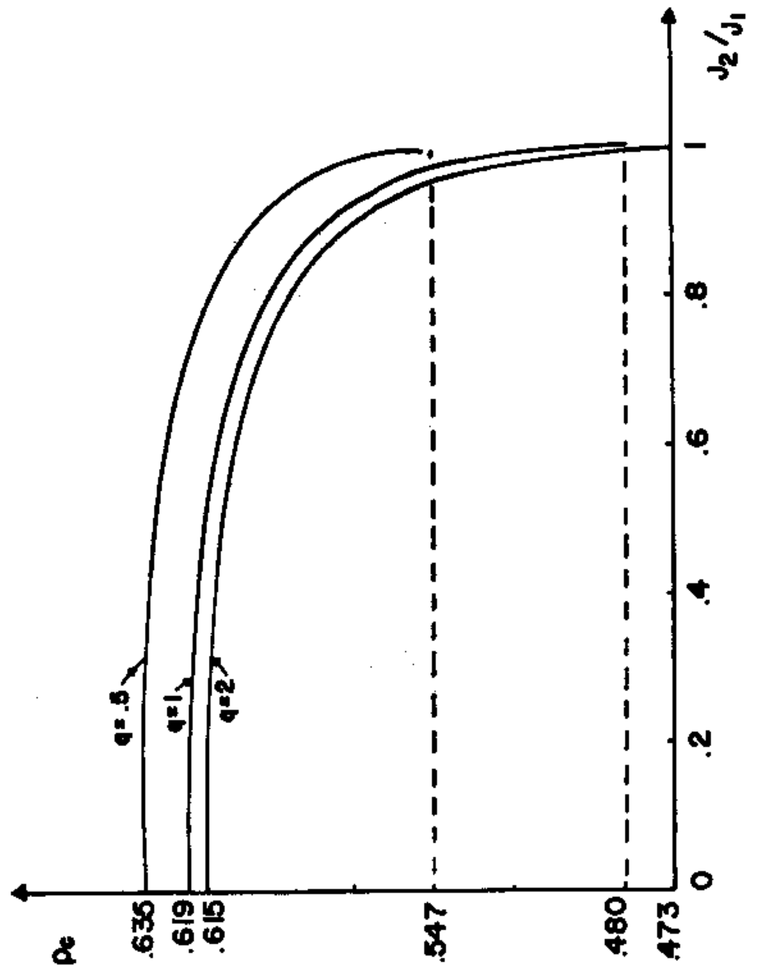
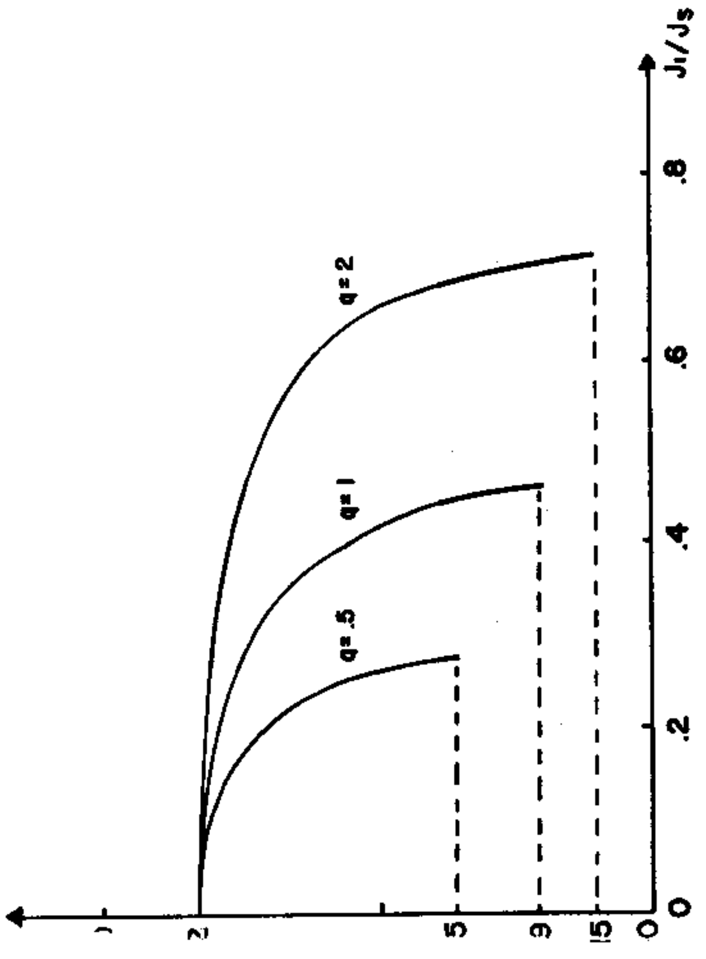

ρ_e
.636
.619
.615
.547
.480
.473
q=.5
q=1
q=2
0
.2
.4
.6
.8
1
J_2/J_1

FIG. 7a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q=1
q=2
0
.2
.4
.6
.8
J_1/J_s

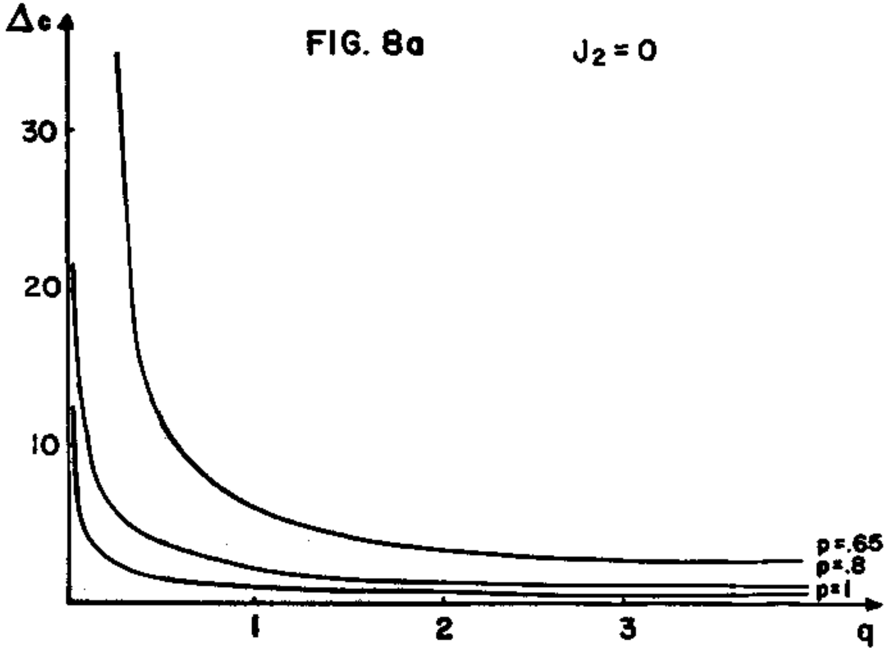

FIG. 8a

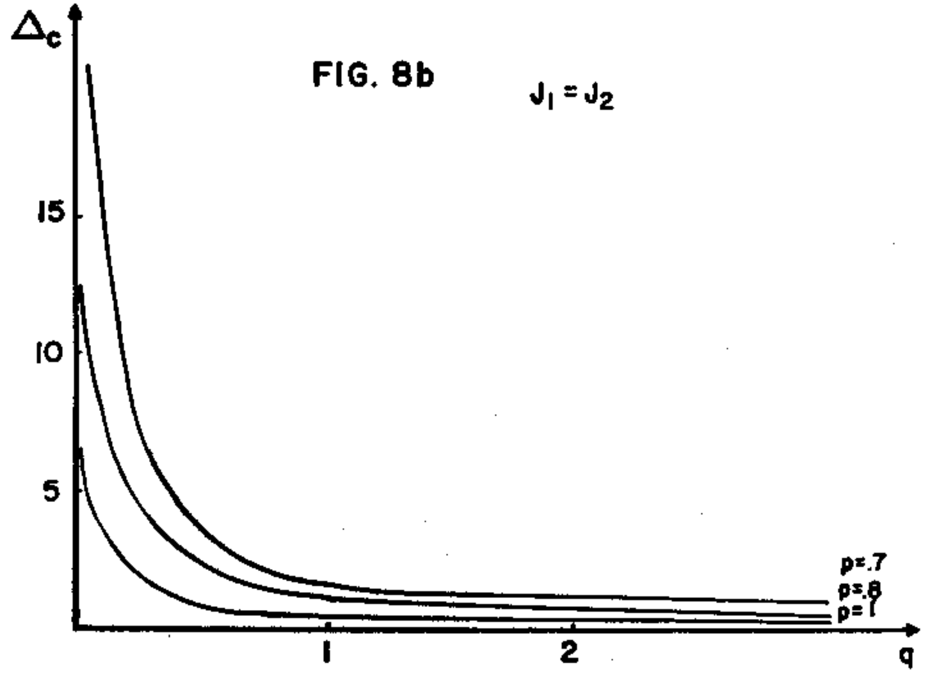

FIG. 8b

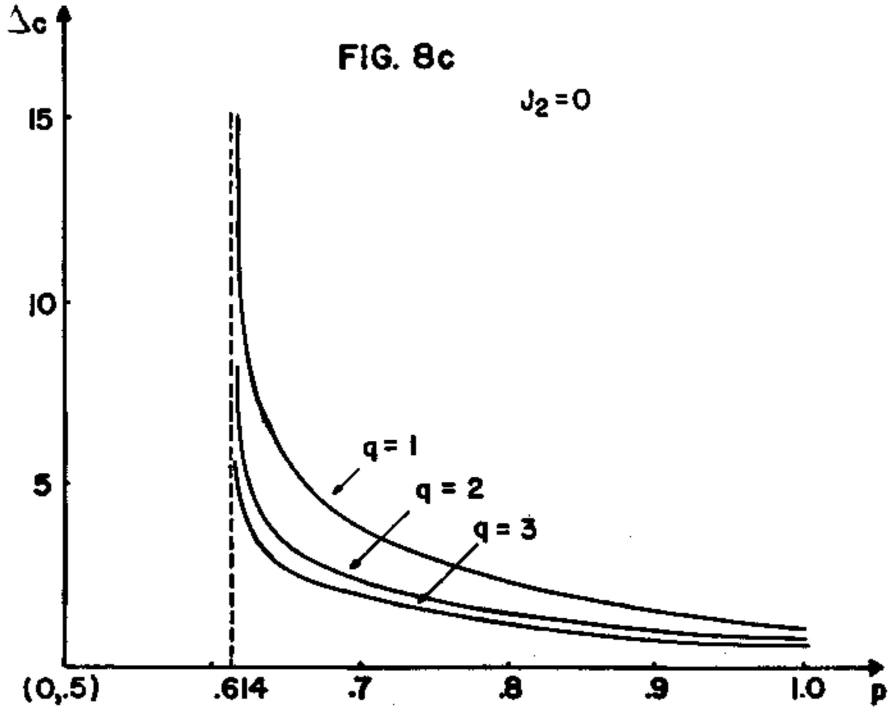

FIG. 8c

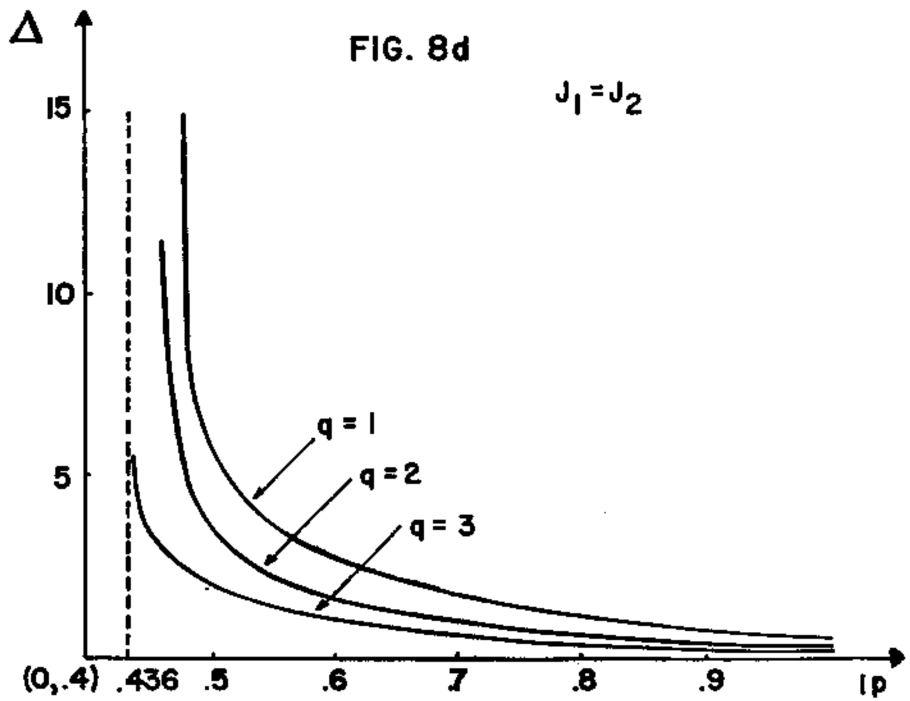

FIG. 8d

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