ISSN 0029 - 3865

CBPF-NF-029/86

INFLUENCE OF BOND DILUTION ON THE FREE SURFACE AND INTERFACE POTTS FERROMAGNETISM

by

Emaldo F. Sarmento[†], Eudenilson L. Albuquerque[§] and Constantino Tsallis[&§]

[&]Centro Brasileiro de Pesquisas Físicas - CBPF/CNPq
Rua Dr. Xavier Sigaud, 150
22290 - Rio de Janeiro, RJ - Brasil (Permanent address)

[†]Departamento de Física
Universidade Federal de Alagoas
57000 - Maceió, AL - Brasil

[§]Departamento de Física
Universidade Federal do Rio Grande do Norte
59000 - Natal, RN - Brasil

ABSTRACT

Within a simple real space renormalization group framework, we discuss the phase diagram of a q-sate Potts ferromagnetic system constituted by two semi-infinite bulks separated by a planar interface. Quenched bond dilution has been assumed in the bulks as well as in the interface. The system exhibits percolation-like phenomena which generalize the standard d=2 and d=3 ones. Also, competition between bulk dilution (which enhances surface magnetism) and interface dilution (which depresses surface magnetism) is observed.

Key-words: Surface magnetism; Potts model; Critical phenomena; Percolation.

I INTRODUCTION

Surface magnetism is a subject which presents great richness, from the theoretical and experimental standpoints as well as due to its important applications (catalysis, corrosion); see Refs.[1,2] for recent reviews. Situations such as the *free surface* (semi-infinite bulk) and the *interface* (surface between two semi-infinite bulks, which generalizes the free surface case) have been theoretically considered. Also several models (e.g.,spin 1/2 Ising, q-state Potts, spin 1/2 anisotropic Heisenberg, mixed ones) have been assumed. However *pure* systems (i.e., ordered, non diluted) have been almost exclusively considered. The first attempt (to the best of our knowledge) concerning the effects of (bulk) dilution is due to Ferchmin and Maciejewski[3]. Very recently, real space renormalization group (RG) work addresses this type of effects: bulk dilution for the free surface spin 1/2 Ising model[4], and surface dilution for the interface Potts model[5] within Migdal-Kadanoff RG frameworks (see [6] and references therein), and free surface dilution for the q=1,2 Potts model within a RG which uses a sophisticated cluster and yields quite accurate results[7].

In the present paper we consider, within a Migdal-Kadanoff RG approach which generalizes that presented in [6], a quite large model, namely the interface q-state Potts ferromagnet with quenched bond arbitrary dilutions in both bulks as well as in the surface between them; the results obtained in [4,5] are here recovered as particular cases. We mainly address the phase diagram, although the various critical universality classes associated with the problem emerge as well. Interesting bond-percolation-like phenomena are observed, as well as competition between bulk dilution (which enhances surface magnetic order) and surface dilution (which depresses it). In section II we introduce the model and the formalism, and in Section III we present the main results, concluding in Section IV.

II MODEL AND FORMALISM

We consider the following Potts Hamiltonian:

$$\mathcal{H} = - q \sum_{<i,j>} J_{ij} \delta_{\sigma_i,\sigma_j} \qquad (\sigma_i = 1,2,\ldots, q, \forall i) \tag{1}$$

where J_{ij} equals $J_s (J_s \geq 0)$ if *both* i and j sites belong to the (1,0,0) interface of a (first-neighbouring) simple cubic lattice, and J_{ij} equals $J_1 \geq 0 (J_2 \geq 0)$ if at least one of i and j sites belongs to the bulk-1 (bulk-2). Furthermore, the coupling constants J_{ij} are assumed to be random variables satisfying the following probability laws:

$$P_s(J_s) = (1-p_s)\delta(J_s) + p_s\delta(J_s-J_s^0) \tag{2.a}$$

$$P_r(J_r) = (1-p_r)\delta(J_r) + p_r\delta(J_r-J_r^0) \qquad (r=1,2) \qquad (2.b)$$

with $0 \leq p_s$, p_1, $p_2 \leq 1$ and J_s^0, J_1^0, $J_2^0 \geq 0$. The *pure* case corresponds to $p_s=p_1=p_2=1$, $\forall(J_s^0,J_1^0,J_2^0)$. The *free surface* case corresponds to, say, $J_2^0=0$, $\forall(p_s,p_1,p_2,J_s^0,J_1^0)$ or $p_2=0$, $\forall(p_s,p_1,J_s^0,J_1^0,J_2^0)$.

Before going on, let us introduce a convenient variable (*thermal transmissivity*[8]):

$$t_{ij} \equiv \frac{1 - e^{-qJ_{ij}/k_BT}}{1 + (q-1)\, e^{-qJ_{ij}/k_BT}} \in [0,1] \qquad (3)$$

Eqs.(2) can be rewritten as follows:

$$P_s(t_s) = (1-p_s)\delta(t_s) + p_s\delta(t_s-t_s^0) \qquad (4.a)$$

$$P_r(t_r) = (1-p_r)\delta(t_r) + p_r\delta(t_r-t_r^0) \qquad (r=1,2) \qquad (4.b)$$

To treat the model defined by Eqs.(1) and (2) we shall use the RG approach indicated in Fig.1 with the renormalized probability laws

$$P'_s(t_s) = (1-p'_s)\delta(t_s) + p'_s\delta(t_s-t_s^{0'}) \qquad (5.a)$$

$$P'_r(t_r) = (1-p'_r)\delta(t_r) + p'_r\delta(t_r-t_r^{0'}) \qquad (r=1,2) \qquad (5.b)$$

where $(p'_s, p'_1, p'_2, t_s^{0'}, t_1^{0'}, t_2^{0'})$ are parameters to be determined.

The probability law $\bar{P}_s$ associated with the large cluster of Fig.1(a) is given by

$$\bar{P}_s(t_s) = \sum_{n_s=0}^{3} \sum_{n_1=0}^{3} \sum_{n_2=0}^{3} \binom{3}{n_s}\binom{3}{n_1}\binom{3}{n_2}$$

$$\times (1-p_s^3)^{3-n_s} p_s^{3n_s} (1-p_1^3)^{3-n_1} p_1^{3n_1} (1-p_2^3)^{3-n_2} p_2^{3n_2}$$

$$\times \delta(t_s-t^{(n_s,n_1,n_2)}) \qquad (6)$$

where

$$t^{(n_s,n_1,n_2)} \equiv \frac{1-\left[\frac{1-t_s^{0\,3}}{1+(q-1)t_s^{0\,3}}\right]^{n_s}\left[\frac{1-t_1^{0\,3}}{1+(q-1)t_1^{0\,3}}\right]^{n_1}\left[\frac{1-t_2^{0\,3}}{1+(q-1)t_2^{0\,3}}\right]^{n_2}}{1+(q-1)\left[\frac{1-t_s^{0\,3}}{1+(q-1)t_s^{0\,3}}\right]^{n_s}\left[\frac{1-t_1^{0\,3}}{1+(q-1)t_1^{0\,3}}\right]^{n_1}\left[\frac{1-t_2^{0\,3}}{1+(q-1)t_2^{0\,3}}\right]^{n_2}} \qquad (7)$$

with $n_s, n_1, n_2 = 0,1,2,3$.

Similarly, the probability law $\bar{P}_1$ associated with the large cluster of Fig.1(b) is given by

$$\bar{P}_1(t_1) = \sum_{n=0}^{9} \binom{9}{n} (1-p_1^3)^{9-n}\, p_1^{3n}\, \delta(t_1 - t_1^{(n)}) \qquad (8)$$

where

$$t_1^{(n)} \equiv \frac{1-\left[\frac{1-t_1^{0\,3}}{1+(q-1)t_1^{0\,3}}\right]^{n}}{1+(q-1)\left[\frac{1-t_1^{0\,3}}{1+(q-1)t_1^{0\,3}}\right]^{n}} \qquad (n=0,1,\ldots,9) \qquad (9)$$

The probability law $\bar{P}_2(t_2)$ associated with bulk-2 is completely analogous to $\bar{P}_1(t_1)$.

It is important to stress that the distributions $\bar{P}_s$, $\bar{P}_1$ and $\bar{P}_2$ are much more complex than the corresponding binary ones P'_s, P'_1 and P'_2. Consequently the representations indicated in Fig. 1 involve an *approximation*. This (binary) approximation could in principle be avoided by leaving the distributions free to evoluate, through successive renormalization steps, towards their fixed forms. However, it is well known that the "binary approximation" behaves quite satisfactorily in a great variety of similar systems. Consequently we shall adopt it for the present discussion. To determine the parameters p'_s, p'_1, p'_2, $t_s^{0\prime}$, $t_1^{0\prime}$ and $t_2^{0\prime}$ we impose the lower momenta to be preserved, more precisely

$$\langle t_s \rangle_{P'_s} = \langle t_s \rangle_{\bar{P}_s} \tag{10}$$

$$\langle t_s^2 \rangle_{P'_s} = \langle t_s^2 \rangle_{\bar{P}_s} \tag{11}$$

$$\langle t_r \rangle_{P'_r} = \langle t_r \rangle_{\bar{P}_r} \qquad (r=1,2) \tag{12}$$

$$\langle t_r^2 \rangle_{P'_r} = \langle t_r^2 \rangle_{\bar{P}_r} \qquad (r=1,2) \tag{13}$$

Consequently we have

$$p_s' \, t_s^{0\,'} = \sum_{n_s=0}^{3} \sum_{n_1=0}^{3} \sum_{n_2=0}^{3} \binom{3}{n_s} \binom{3}{n_1} \binom{3}{n_2}$$

$$\times \; (1-p_s^3)^{3-n_s} \; p_s^{3n_s} \; (1-p_1^3)^{3-n_1} \; p_1^{3n_1} \; (1-p_2^3)^{3-n_2} \; p_2^{3n_2}$$

$$\times \; t^{(n_s,n_1,n_2)} \equiv F_s(p_s,p_1,p_2,t_s^0,t_1^0,t_2^0) \tag{14}$$

$$p_s' \, (t_s^{0\,'})^2 = \sum_{n_s=0}^{3} \sum_{n_1=0}^{3} \sum_{n_2=0}^{3} \binom{3}{n_s} \binom{3}{n_1} \binom{3}{n_2}$$

$$\times \; (1-p_s^3)^{3-n_s} \; p_s^{3n_s} \; (1-p_1^3)^{3-n_1} \; p_1^{3n_1} \; (1-p_2^3)^{3-n_2} \; p_2^{3n_2}$$

$$\times \; [\, t^{(n_s,n_1,n_2)} \,]^2 \equiv G_s(p_s,p_1,p_2,t_s^0,t_1^0,t_2^0) \tag{15}$$

$$p_r' \, t_r^{0\,'} = \sum_{n=0}^{9} \binom{9}{n} \, (1-p_r^3)^{9-n} \, p_r^{\,3n} \, t_r^{(n)} \equiv F_r(p_r,t_r^0) \qquad (r=1,2) \tag{16}$$

$$p_r' \, (t_r^{0\prime})^2 = \sum_{n=0}^{9} \binom{9}{n} (1-p_r^3)^{9-n} \, p_r^{3n} \, [t_r^{(n)}]^2 \equiv G_r(p_r, t_r^0) \quad (r=1,2) \qquad (17)$$

And finally

$$p_s' = F_s^2/G_s \qquad (18)$$

$$t_s^{0\prime} = G_s/F_s \qquad (19)$$

$$p_r' = F_r^2/G_r \qquad (r=1,2) \qquad (20)$$

$$t_r^{0\prime} = G_r/F_r \qquad (r=1,2) \qquad (21)$$

Equations (18-21) completely determine the RG recursive relations in the 6-dimensional parameter-space $(p_s, p_1, p_2, t_s^0, t_1^0, t_2^0)$ (or equivalently in the $(k_BT/J_1^0,\ J_s^0/J_1^0,\ J_2^0/J_1^0,\ p_s, p_1, p_2)$ space). The RG flow diagram in this space fully determines the complex phase diagram (hypersurfaces in a 6-dimensional space) as well as the corresponding critical universality classes. In the next section we present convenient cuts of this phase diagram and its evolution with q.

III RESULTS

We have chosen as a prototype the *free surface* (i.e., $p_2=0$ and/or $J_2^o=0$) *pure* (i.e., $p_s=p_1=1$) *Ising model* (i.e., q=2): its RG flux diagram is indicated in Fig.2. It exhibits three phases, namely the *bulk ferromagnetic* (BF; both bulk and surface are magnetically ordered), *surface ferromagnetic* (SF; the surface *only* is magnetically ordered) and *paramagnetic* (P; magnetically fully disordered system) ones. The P-SF critical line belongs to the d=2 universality class (characterized by the $t_1=0$ semi-stable fixed point); the SF-BF critical line belongs to the d=3 universality class (characterized by the $t_s^o=1$ semi-stable fixed point); the P-BF critical line belongs, for the surface magnetization, to a non trivial universality class (characterized by the $0<t_s^o$, $t_1^o<1$ semi-stable fixed point) which differs from both d=2 and d=3 ones; all three critical lines join in multicritical point which constitutes by itself a new universality class (characterized by the unique fully unstable fixed point). This RG flux diagram evoluates smoothly with q. The influence of *bulk dilution* is to shift the "vertical" asymptote to the right, therefore *enhancing* the SF phase; for $p_1=p_c^{3D}$ (d=3 bond percolation threshold) the asymptote attains the $t_1^o=1$ axis. The influence of *surface dilution* is to shift the "horizontal" asymptote to upper values of t_s^o, therefore *depressing* the SF phase; for $p_s=p_c^{2D}$ (d=2 bond percolation threshold) the $t_1^o=0$ point of the "horizontal" asymptote attains the $t_s^o=1$ axis. Simultaneous bulk and surface dilutions move *both* asymptotes, thus appearing *competition* concerning the SF phase. For q high enough, surface and bulk dilution yield new non trivial critical fixed points, thus driving the system into new (*random*) universality classes. This fact is consistent with the Harris criterion[9]; however the main purpose of the present work being the phase diagram, we will not study the details of this type of crossover.

The effect of surface dilution (with $p_1=1$) in the T vs. J_s^o/J_1^o representation is illustrated in Fig.3 (T_c^{3D} denotes the d=3 Ising critical temperature). Note that the SF phase exists even *below* the d=2 percolation threshold (i.e., for $p<p_c^{2D}$), a new percolation-like threshold now appearing. This effect can be referred as "bulk-assisted surface percolation".

The effect of bulk dilution (with $p_s=1$) in the T vs. J_s^o/J_1^o representation is illustrated in Fig.4. The effect of *simultaneous* surface and bulk dilutions is illustrated in Fig.5. The influence of p_s and p_1 on the phase diagram in conveniently synthetized by looking at the way they monitorize the location J_s^*/J_1^o of the multicritical point: these are depicted in Figs.6a,b,c.

We have represented in Fig.7 the q-evolution of the pure case ($p_s=p_1=1$) phase diagram. The q-dependence of J_s^*/J_1^o appears in Fig.9 (on the $J_2^o/J_1^o=0$ plane).

Let us now turn our attention onto the *interface* case (both J_1^o and J_2^o non vanishing). A typical phase diagram is indicated in Fig.8, where BF_{12} means that *both* bulks as well as the interface are magnetized, and BF_1 refers to the fact that only bulk-1 (and of course the interface) is magnetized, bulk-2 now being paramagnetic. The location of the multicritical point is indicated in Fig.9 for the pure case.

IV CONCLUSION

The quenched bond-diluted double-bulk Potts ferromagnet is a quite complex system, whose phase diagram is almost completely unknown. At the T=0 limit it recovers the standard d=2 and d=3 percolation thresholds (see Refs.[10-12] for the simple cubic with (1,0,0) interface values). Within a simple real space renormalization group scheme we have calculated it (and also obtained some information on its various universality classes). We believe the results are qualitatively reliable (the checks are satisfactory whenever possible), although quantitatively somehow rough. This is so whenever we are dealing with second-order phase transitions (i.e., $q \leq q_c \simeq 3$), the framework not being appropriate for the description of first-order phase transitions. The q-evolution of the phase diagram has been followed, and various interesting phenomena have been exhibited. Among them we must quote the competitive trends of bulk dilution, which enhances surface magnetism, and surface dilution, which depresses it (see Figs.6a,b,c). We would be very happy if the present work could act as a guide to the choice of convenient real systems, and stimulate further (and quantitatively more precise) theoretical and experimental work on surface magnetism in diluted and/or mixed magnetic substances.

CAPTION FOR FIGURES

Fig. 1 - RG transformation (the large clusters are renormalized into the small ones); O and ● respectively denote terminal and internal sites. (a) interface RG transformation; (b) bulk-1 RG transformation (that of bulk-2 is completely analogous).

Fig. 2 - Pure ($p_s=p_1=1$) Ising model ($q=2$) for the free surface case ($p_2=0$ and/or $t_2^o=0$): RG flux diagram. ■ , ● and O respectively denote the trivial (fully stable), critical (semi-stable) and multicritical (fully unstable) fixed points. P, BF and SF respectively denote the paramagnetic, bulk ferromagnetic and surface ferromagnetic phases. t_s^o and t_1^o are transmissivities.

Fig. 3 - $q=2$, $p_1=1$ phase diagram for $p_2=0$ and/or $J_2^o=0$, and typical values of p_s.

Fig. 4 - $q=2$, $p_s=1$ phase diagram for $p_2=0$ and/or $J_2^o=0$, and typical values of p_1.

Fig. 5 - $q=2$ phase diagram for $p_2=0$ and/or $J_2^o=0$ and typical values of $p_s=p_1$.

Fig. 6 - Concentration-dependence of J_s^*/J_1^o (location of the mul-

ticritical point) for the q=2, p_2=0 and/or J_2^o=0 model. a) p_s=1; b) p_1=1; c) p_s=p_1

Fig. 7 - q-evolution of the pure (p_s=p_1=1) model for the free surface case.

Fig. 8 - q=2, p_1=p_2=p_s=1 diagram for the double-bulk J_2^o/J_1^o=1/2 case.

Fig. 9 - q-evolution of the location of the multicritical point as a function of J_2^o/J_1^o for the double-bulk p_1=p_2=p_s=1 model.

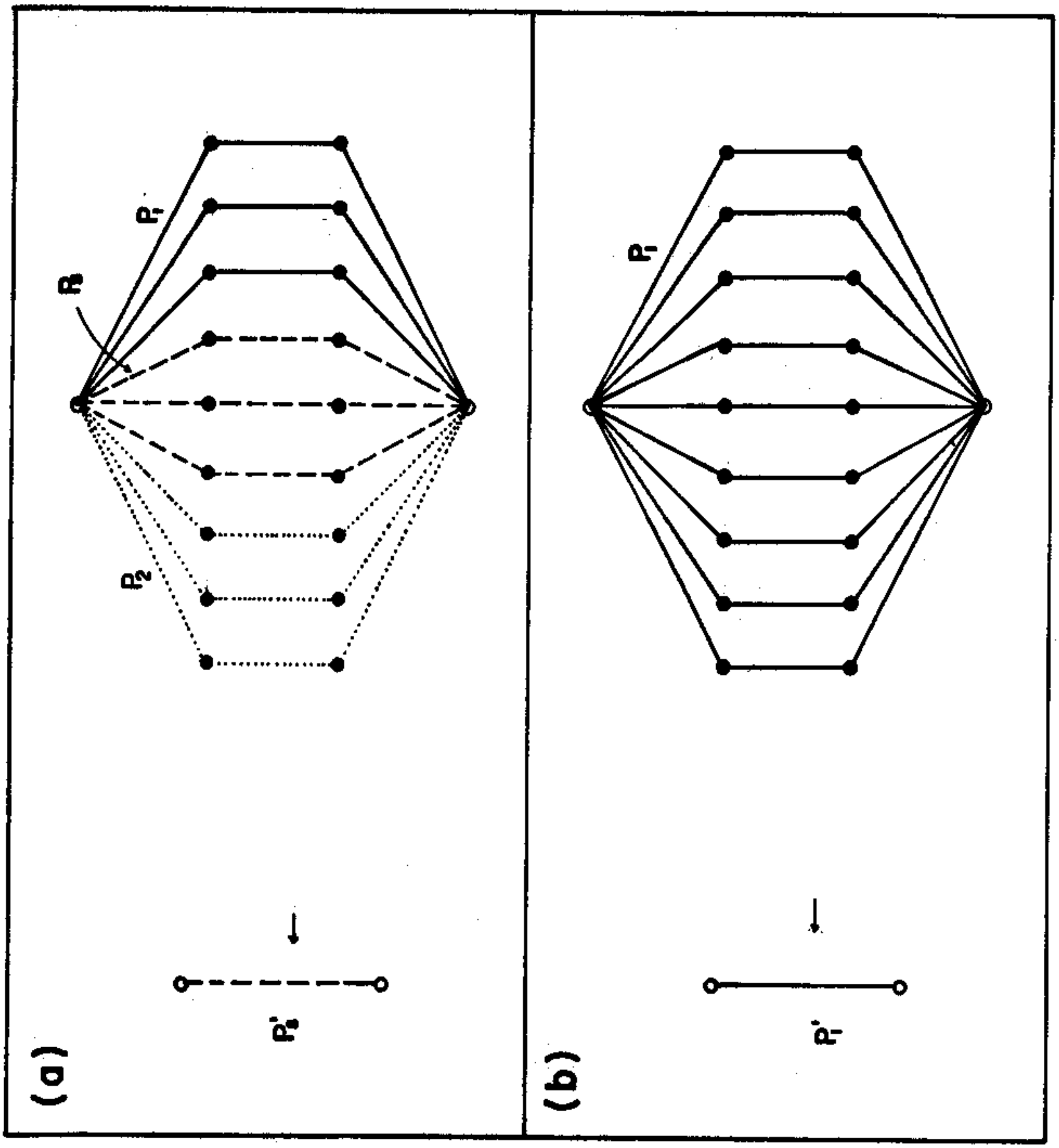

FIG. 1

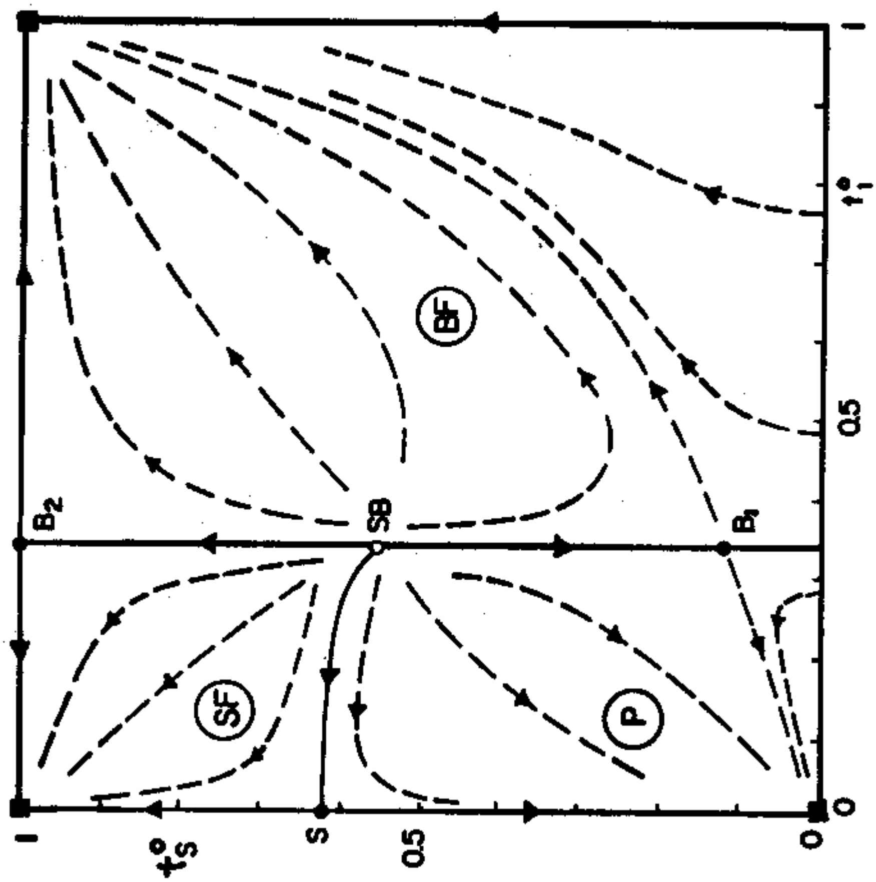

FIG. 2

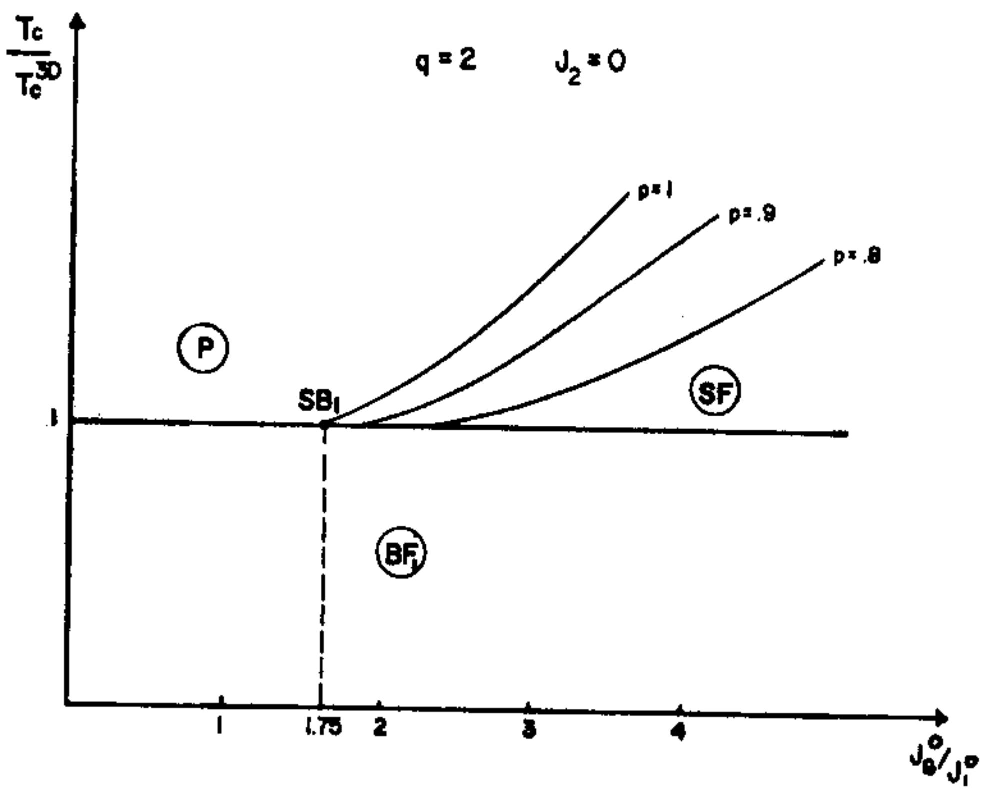

FIG. 3

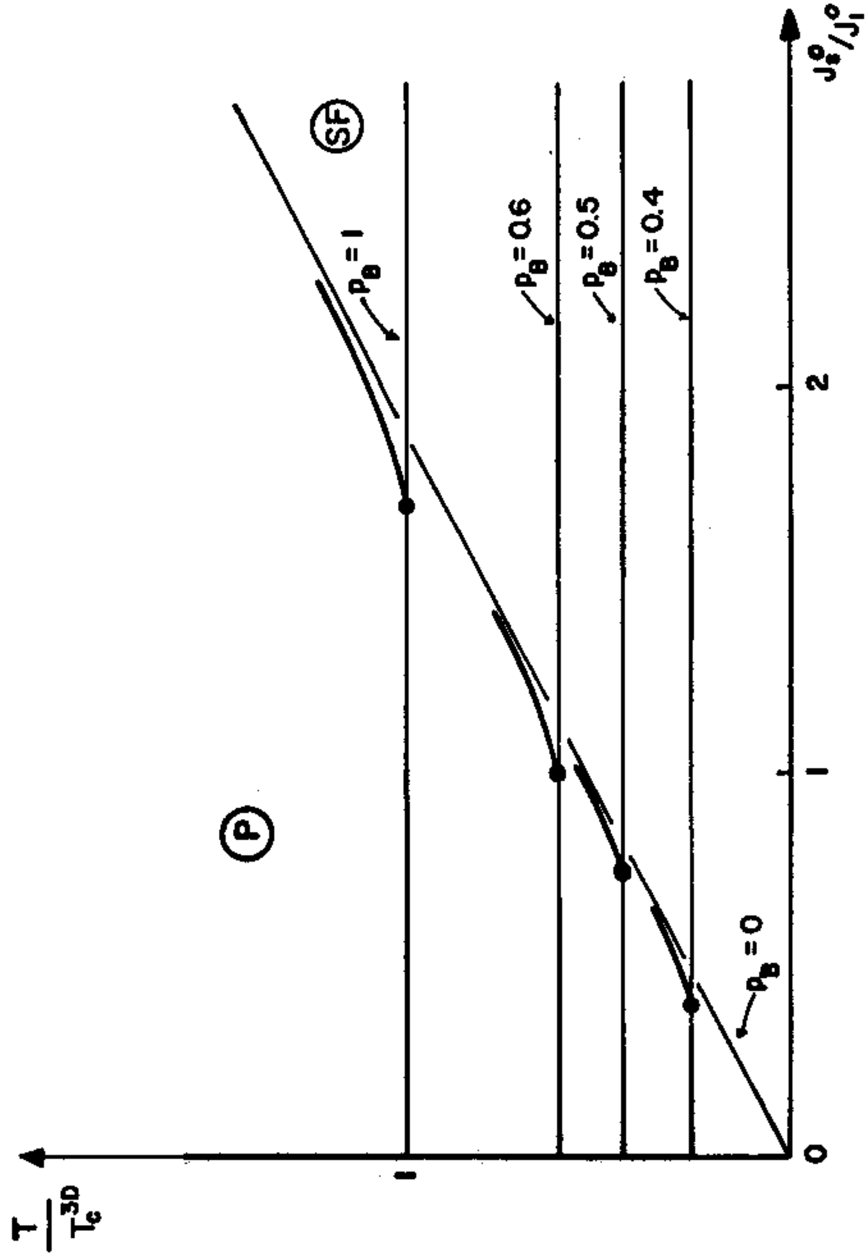

FIG. 4

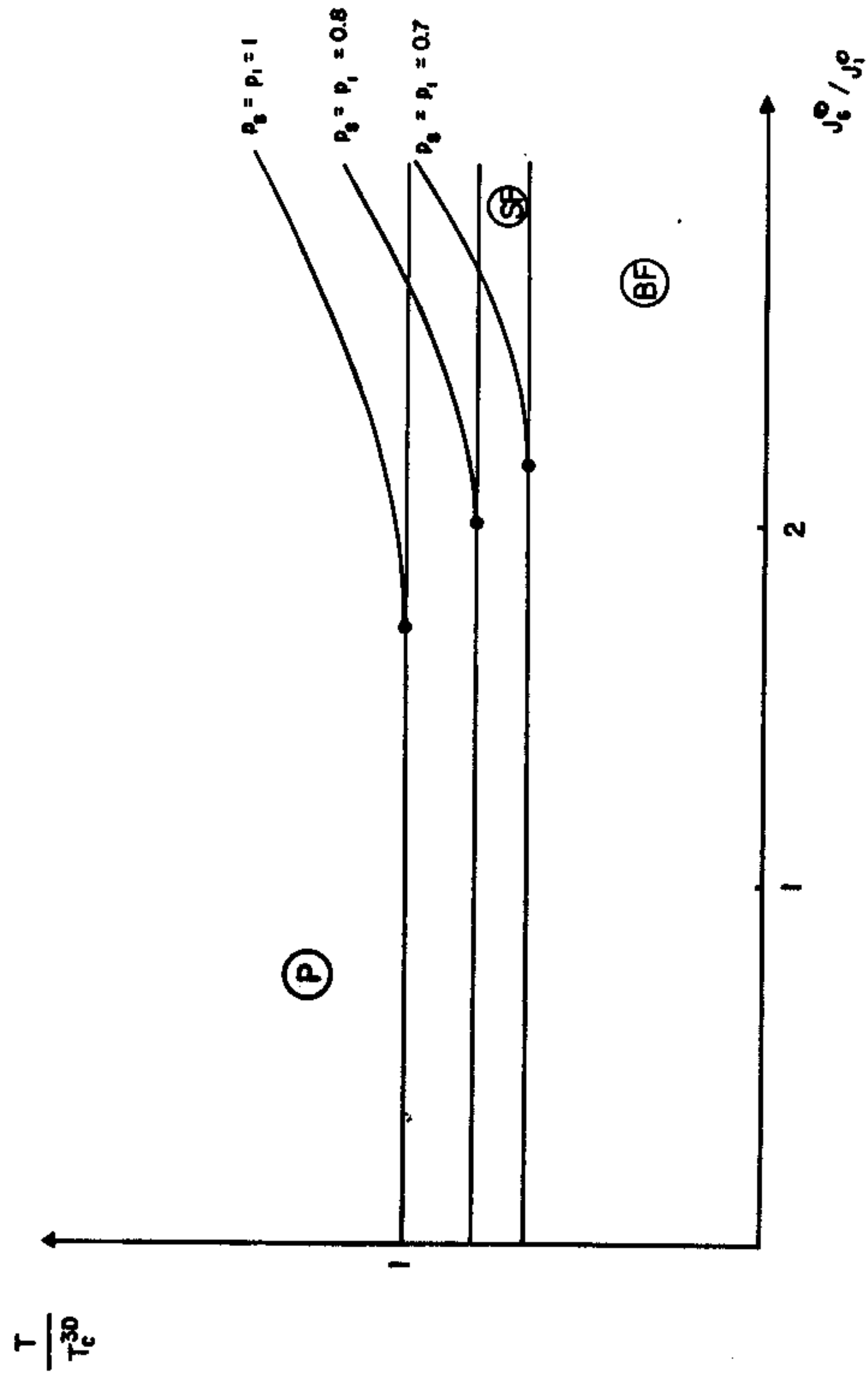

FIG. 5

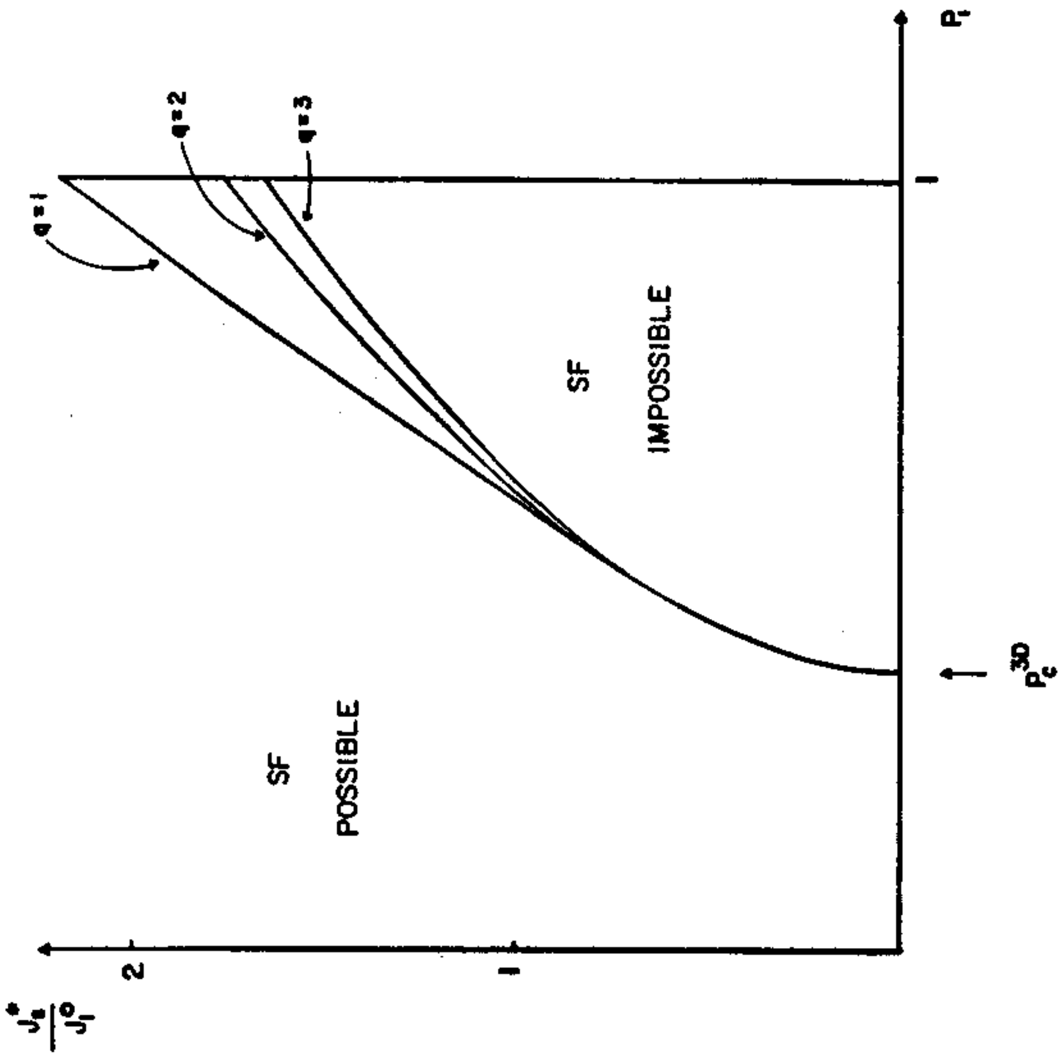

FIG. 6 (a)

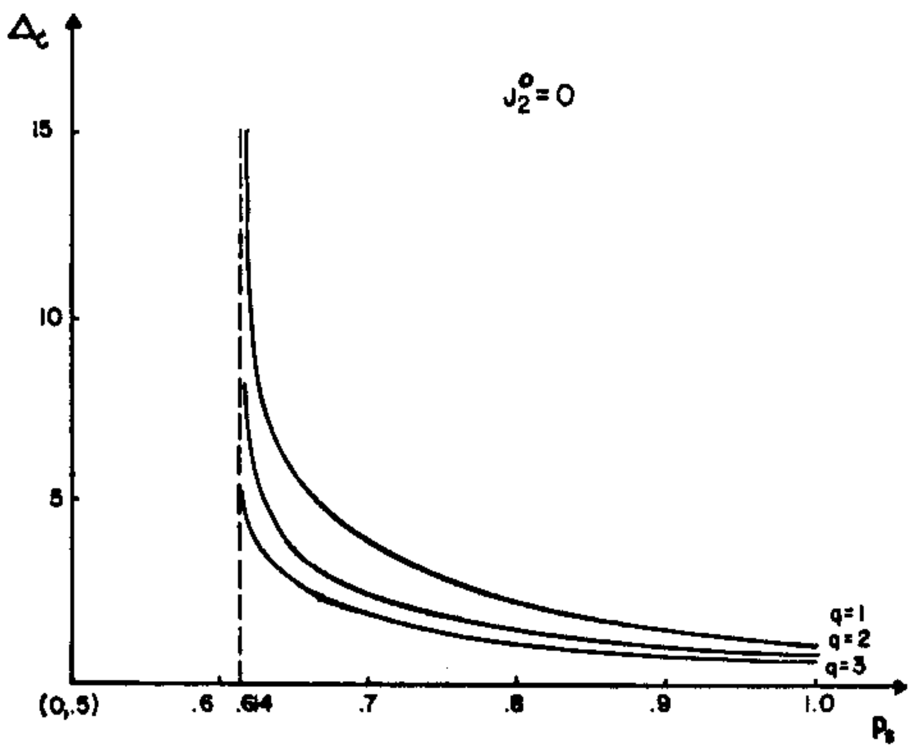

FIG. 6 (b)

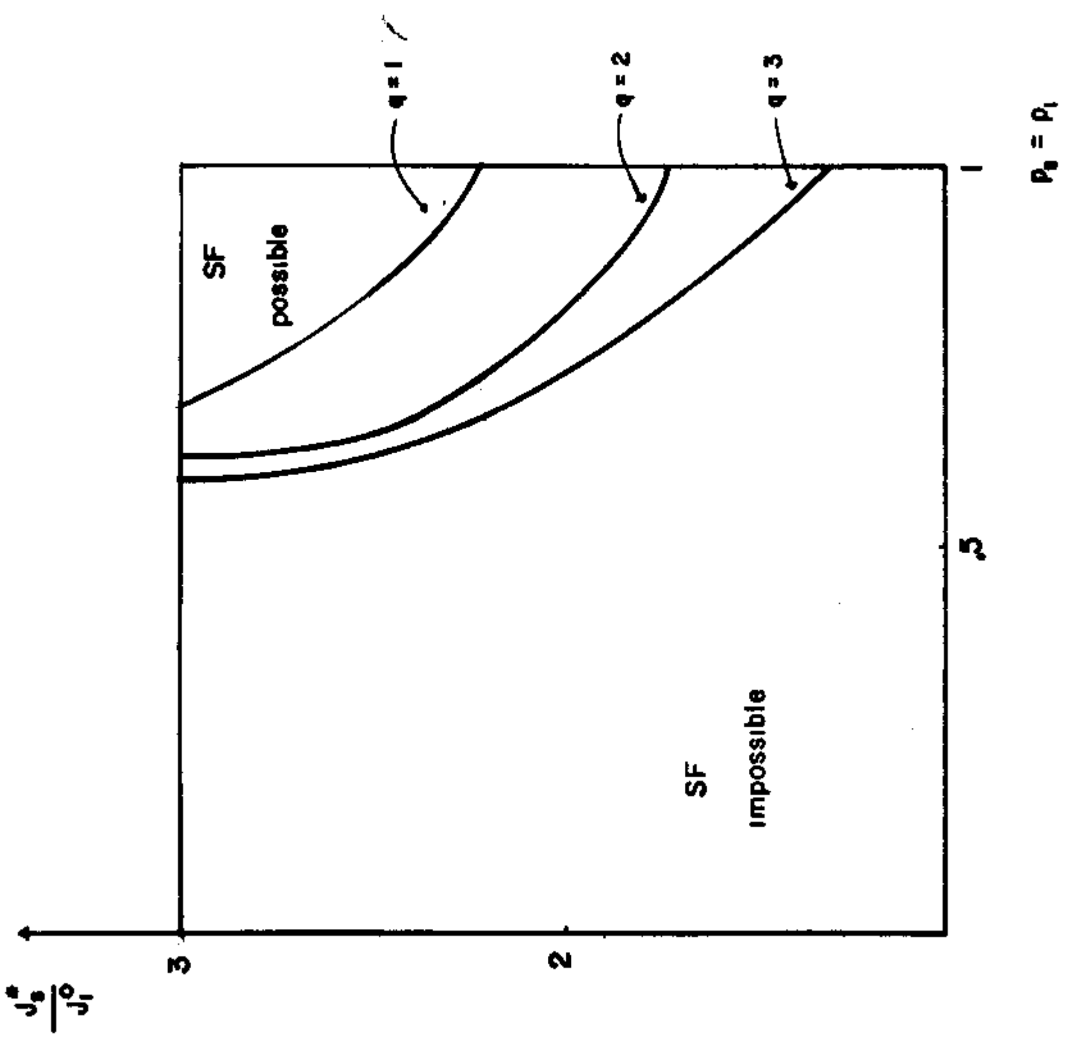

FIG. 6(c)

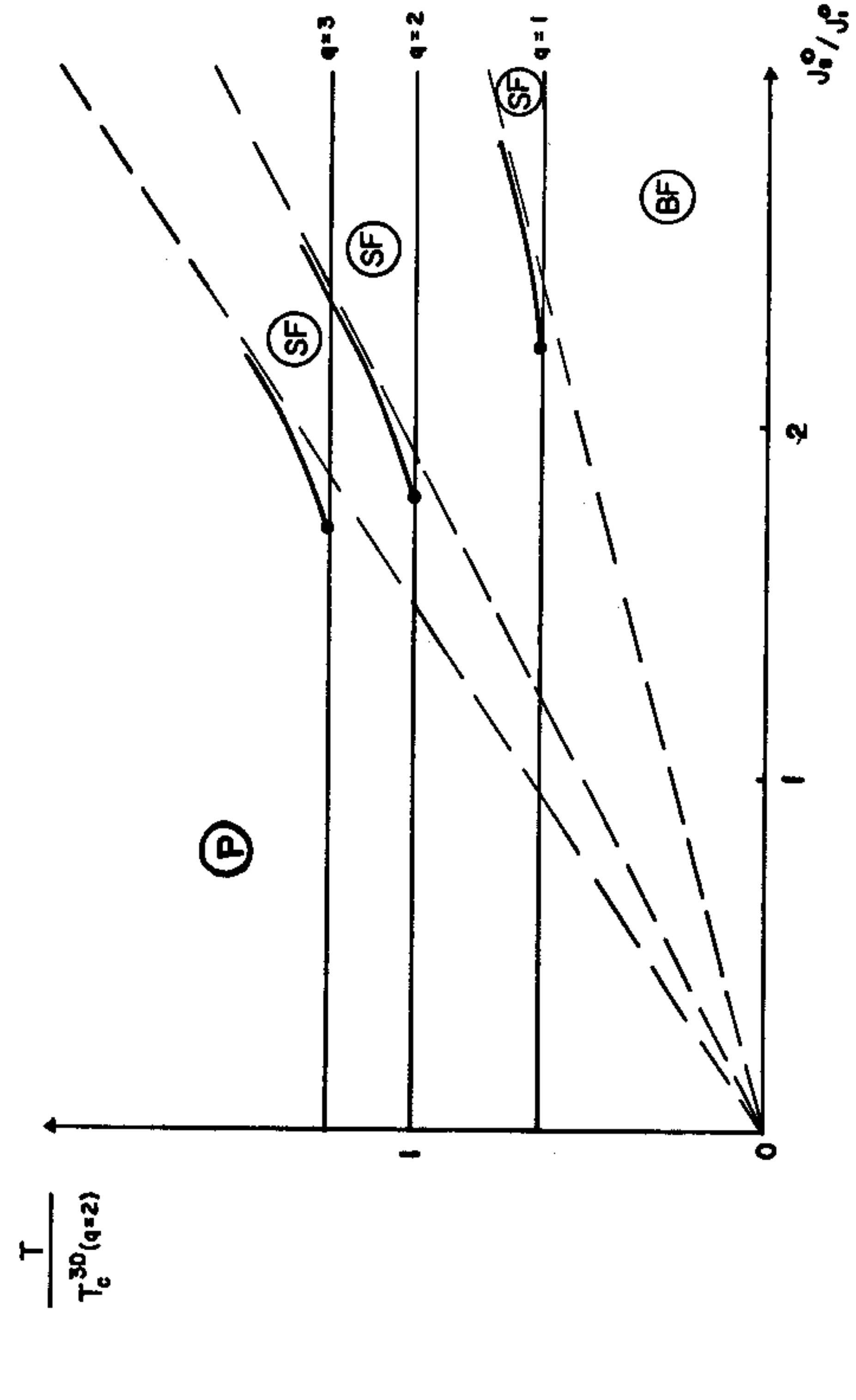

FIG. 7

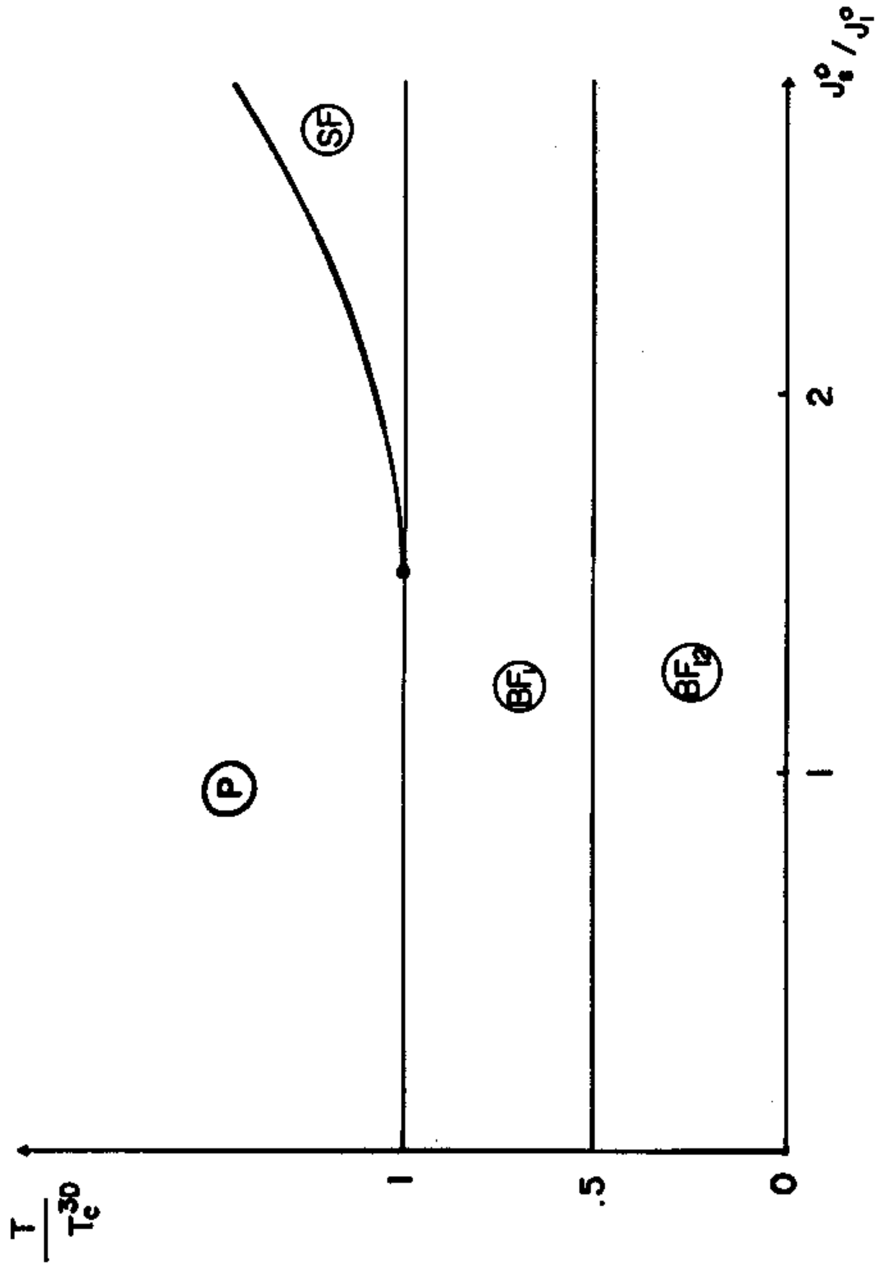

FIG. 8

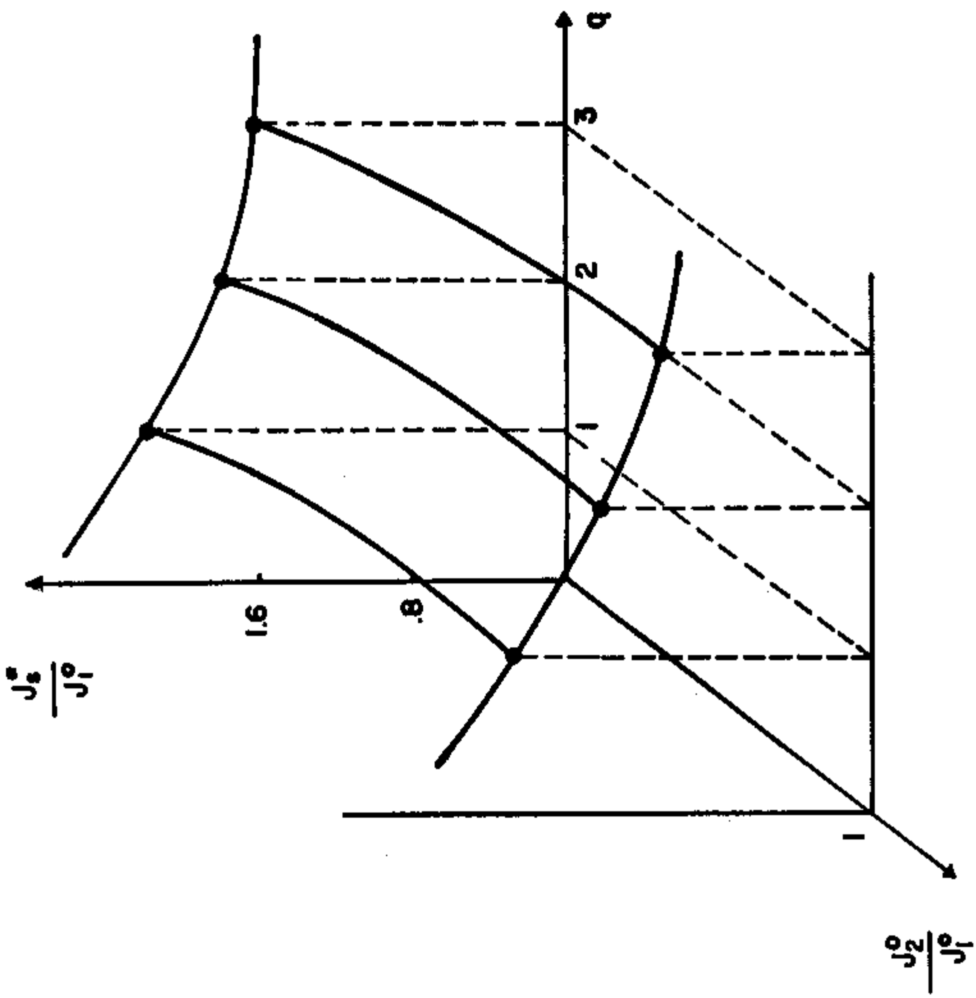

FIG. 9

REFERENCES

[1] K.Binder, "Critical behaviour surfaces" in "Phase transitions and Critical Phenomena", ed. C.Domb and J.L.Lebowitz, vol.8 (Academic Press, 1983)

[2] C.Tsallis, "Influence of dilution and nature of the interaction on surface and interface magnetism", in volume edited by L.M.Falicov (to be published by Springer-Verlag)

[3] A.R.Ferchmin and W.Maciejewski, J.Phys.C 12, 4311 (1979)

[4] C.Tsallis, E.F.Sarmento and E.L.Albuquerque, J.Magn.Magn. Mat. 54-57, 667 (1986)

[5] S.B.Cavalcanti and C.Tsallis, to be published (J.Phys.C)

[6] C.Tsallis and E.F.Sarmento, J.Phys.C 18, 2777 (1985)

[7] L.R.da Silva, C.Tsallis and E.F.Sarmento, to be published

[8] C.Tsallis and S.V.F.Levy, Phys.Rev.Lett. 47, 950 (1981)

[9] A.B.Harris, J.Phys.C 7, 1671 (1974)

[10] M.F.Sykes and J.W.Essam, Phys.Rev.Lett. 10, 3 (1963)

[11] M.F.Sykes, D.S.Gaunt and M.Glen, J.Phys.A 9, 1705 (1976)

[12] D.S.Gaunt and H.Ruskin, J.Phys.A 11, 1369 (1978)