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# CRITICALITY OF THE BOND-DILUTED ISING FERROMAGNET IN A SEMI-INFINITE SIMPLE CUBIC LATTICE

by

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ABSTRACT

We study the phase diagram and universality classes of the quenched bond-diluted spin 1/2 Ising ferromagnet in a semi-infinite simple cubic lattice with a (0,0,1) free surface. The approach (herein formulated for arbitrary values of the number of states q of the Potts model) is a real space renormalization group which preserves two-spin correlation functions and uses clusters which have already proved to be very appropriate for the present structure. We observe that surface ferromagnetism persists below the d=2 percolation threshold $p_c^{2D}=1/2$, in fact down to $p_c \simeq 0.42$. In addition to that we check that a conjectural extension of the Kasteleyn and Fortuin theorem is satisfied in the present particular case.

Key-words: Surface magnetism; Bond-dilution; Phase diagram; Semi-infinite cubic lattice.

# 1 - INTRODUCTION

Surface magnetism is nowadays an expanding subject of research which presents both theoretical and experimental richness, besides various applications such as catalysis and corrosion. For details, the reader is referred to various recent reviews: that of Binder[1] for a general introduction, that of Diehl [2] for reciprocal space renormalization group treatments and that of Tsallis[3] for real space ones. Several studies are available for non-random systems (pure Ising, q-state Potts, anisotropic Heisenberg models) but very few have been devoted to random ones,[4-6] none of them with purposes of numerical accuracy.

Here we focus the criticality associated with the quenched bond-diluted spin 1/2 Ising ferromagnet in a semi-infinite simple cubic lattice with a (0,0,1) free surface. The coupling constant and bond concentration are assumed to be respectively $J_S$ and $p_S$ on the surface, and $J_B$ and $p_B$ everywhere else. The phase diagram (in the space $(k_BT/J_B,\ J_S/J_B, p_B,\ p_S)$ for instance) of this system is still unknown within a reasonable degree of accuracy. The main purpose of the present work is to perform such a study, as well as to establish the corresponding universality classes. Special emphasis will be given to the role played by dilution ($0\leq p_S,\ p_B\leq 1$). To do this study we construct a real space renormalization group (RG) which preserves two-spin correlation functions and uses sophisticated clusters which have already proved to be quite efficient for both infinite [7] and semi-infinite [8] simple cubic lattices.

The RG formalism will be established for the q-state Potts model for arbitrary q. For simplicity we shall proceed as follows. Dilution will be assumed *only* on the free surface (i.e., $p_B=1$ and $0\leq p_S\leq 1$). The value q=2 will give to us the $p_B=1$ section of the phase diagram we are looking for. The value q=1 will give to us (through the Kasteleyn and Fortuin theorem[9]) the T=0 section (bond percolation diagram in the *full* $(p_B,p_S)$ space) of the phase diagram of the q=2 system under analysis.

In addition to what has been said up to now, the present work illustrates a conjectural extension by Tsallis[10] of the Kasteleyn and Fortuin theorem. Indeed bond percolation in an arbitrary finite or infinite system is expected to be isomorphic not only with the *pure* version of the $q\to 1$ Potts ferromagnet, but also with *any* quenched bond-random version of it, the probability law $P(J_{ij})$ being an *arbitrary* one with ferromagnetic coupling constants (i.e., $P(J_{ij})=0$ if $J_{ij}<0$).

In Section 2 we present the model and formalism; in Section 3 we present the results and discuss the $q\to 1$ limit; we finally conclude in Section 4.

## 2 - MODEL AND FORMALISM

We consider the following Potts Hamiltonian

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

where the sum runs over all pairs of nearest-neighbouring sites on a semi-infinite simple cubic lattice with a (0,0,1) free surface. When both i and j sites belong to the free surface, $J_{ij}$ is given by the following probability law:

$$P_S(J_{ij}) = (1-p_S)\delta(J_{ij}) + p_S\delta(J_{ij}-J_S) \tag{2}$$

with $0 \leq p_S \leq 1$ and $J_S \geq 0$. Otherwise, the following law holds:

$$P_B(J_{ij}) = (1-p_B)\delta(J_{ij}) + p_B\delta(J_{ij}-J_B) \tag{3}$$

with $0 \leq p_B \leq 1$ and $J_B \geq 0$.

Let us introduce the following convenient variable (*thermal transmissivity* ; Ref.[11] and references therein):

$$t \equiv \frac{1-\exp(-qJ/k_BT)}{1+(q-1)\exp(-qJ/k_BT)} \in [0,1] \tag{4}$$

which defines $t_S$ and $t_B$ from $J_S$ and $J_B$ respectively. Eqs.(2) and (3) can be rewritten as follows:

$$P_S(t) = (1-p_S)\delta(t) + p_S\delta(t-t_S) \tag{5}$$

and

$$P_B(t) = (1-p_B)\delta(t) + p_B\delta(t-t_B) \tag{6}$$

To construct the RG we shall use the clusters of Figs.1(a) and 1 (b) (noted $G_B$ and $G_S$) for the bulk and surface respectively: with each continuous (dashed) bond we associate $P_B(t)$ ($P_S(t)$). We shall note $P_{G_B}(t)$ ($P_{G_S}(t)$) the distribution associated with $G_B$ ($G_S$). $P_{G_B}(t)$ and $P_{G_S}(t)$ do not preserve, through successive renormalizations, the simple binary form of Eqs.(5) and (6). One possible way out is to numerically follow the RG evolution of $P_{G_B}(t)$ and $P_{G_S}(t)$ until they achieve invariant forms: this type of approach has been followed, for different systems, by Stinchcombe and Watson[12] and others. Another way out, much simpler and nevertheless very precise if convenient averages are chosen, consists in respectively approximating $P_{G_B}(t)$ and $P_{G_S}(t)$ by the following binary distributions

$$P'_B(t) = (1-p'_B)\delta(t) + p'_B\delta(t-t'_B) \tag{7}$$

and

$$P'_S(t) = (1-p'_S)\delta(t) + p'_S\delta(t-t'_S) \tag{8}$$

where $t'_B$, $t'_S$, $p'_B$ and $p'_S$ are to be found as functions of $t_B$, $t_S$, $p_B$ and $p_S$. To perform this we impose

$$\langle t\rangle_{P'_B} = \langle t\rangle_{P_{G_B}} \tag{9}$$

$$\langle t^2\rangle_{P'_B} = \langle t^2\rangle_{P_{G_B}} \tag{10}$$

$$\langle t\rangle_{P'_S} = \langle t\rangle_{P_{G_S}} \tag{11}$$

$$\langle t^2\rangle_{P'_S} = \langle t^2\rangle_{P_{G_S}} \tag{12}$$

which formally closes the RG procedure. In practice however $P_{G_B}$ contains almost $2^{35} \simeq 3\times 10^{10}$ delta's ! (and $P_{G_S}$ contains almost $2^{22}$ delta's). To make the problem more tractable we shall proceed as follows. We consider the particular case $p_B=1$, hence Eqs. (9) and (10) become one and the same equation, namely

$$t'_B = f_q(t_B) \tag{13}$$

where $f_q(t_B)$ is a ratio of polynomials and can be calculated by using the Break-collapse method[11]. For example, the particular case q=2 (Ising model) yields[7]

$$f_2(t_B) = (27t_B^3 + 218t_B^5 + 1410t_B^7 + 7153t_B^9 + 28640t_B^{11} + 84805t_B^{13}$$

$$+ 183265t_B^{15} + 273834t_B^{17} + 263475t_B^{19} + 151028t_B^{21}$$

$$+ 46924t_B^{23} + 7221t_B^{25} + 546t_B^{27} + 29t_B^{29} + t_B^{31})/$$

$$(1 + 8t_B^2 + 64t_B^4 + 599t_B^6 + 3342t_B^8 + 14907t_B^{10} + 50759t_B^{12}$$

$$+ 130256t_B^{14} + 236165t_B^{16} + 284318t_B^{18} + 214054t_B^{20}$$

$$+ 91983t_B^{22} + 19772t_B^{24} + 2255t_B^{26} + 131t_B^{28} + 2t_B^{30}) \quad (14)$$

Also equations (11) and (12) become much simpler for $p_B=1$ because $P_{G_S}(t)$ contains, in this case, slightly less than $2^9=512$ delta's, and is therefore easily tractable in computer. Eqs.(11) and (12) can be rewritten as follows:

$$p_S' t_S' = \langle t \rangle_{P_{G_S}} \equiv F(t_B, t_S, p_S) \quad 15)$$

$$p_S'(t_S')^2 = \langle t^2 \rangle_{P_{G_S}} \equiv G(t_B, t_S, p_S) \quad (16)$$

hence

$$p_s' = \frac{[F(t_B, t_S, p_S)]^2}{G(t_B, t_S, p_S)} \quad (17)$$

and

$$t'_S = \frac{G(t_B,t_S,p_S)}{F(t_B,t_S,p_S)} \tag{18}$$

Summarizing, Eqs.(13), (17) and (18) give the RG recurrence in the $(t_B,t_S,p_S)$-space. Therefore the criticality corresponding to the $p_B=1$ particular case of the Ising ferromagnet (q=2) can be considered as a tractable problem. The other particular case (namely the T=0 limit of the Ising ferromagnet) we are interested in can be solved (through the Kasteleyn and Fortuin theorem) by considering the $p_B=1$ particular case of the $q\to1$ model.

## 3 RESULTS AND THE $q\to1$ LIMIT

The RG flow diagram associated with the $p_B=1$ $q=2$ model is indicated in Fig.2. Three phases are observed characterized by trivial (fully stable) fixed points, namely the *paramagnetic* (PM; $(p_S,t_B,t_S) = (0,0,0)$), *bulk ferromagnetic* (BF; $(p_S,t_B,t_S) = (1,1,1)$) and *surface ferromagnetic* (SF; $(p_S,t_B,t_S) = (1,0,1)$) phases. The PM-BF, SF-BF and SF-PM critical surfaces correspond to the so called [13] *ordinary*, *extraordinary* and *surface* phase transitions; the PM-BF-SF critical line corresponds to the *special* transition.

With respect to the universality classes, Fig.2 shows that:

(i) The pure model ($p_S=1$) presents the well known four universality classes (characterized by four semi-stable fixed points), namely the d=3 and d=2 standard Ising phase transitions, and the behaviour of the surface quantities on the ordinary and on the special phase transitions;

(ii) Surface dilution is irrelevant at any finite temperature, the universality classes of the surface, ordinary, extraordinary and special transitions being those of the pure Ising system;

(iii) At T=0 the universality class of the surface quantities is that of the d=2 percolation, excepting for a very special point (T=0 special phase transition, characterized by a fully unstable fixed point) which by itself constitutes a new universality class.

We present, in Fig.3, sections of the critical surface of Fig.2 for typical values of $p_S$. We observe that surface ferromagnetism persists *below* the d=2 percolation threshold $p_c^{2D}=1/2$, in fact down to $p_c \simeq 0.42$. This constitutes a nice illustration of bulk-assisted surface percolation. Finally, in Fig.4, the same type of sections of the critical surface are indicated in the $(T, J_S/J_B)$ space. The effect of the dilution on the location (value of $J_S/J_B$) of the special phase transition is indicated in Fig.5.

Let us now turn our attention onto the $q \to 1$ limit. Sections, for typical values of $p_S$, of the q=1 $p_B=1$ critical surface are presented in Fig.6. Let us consider its $p_S=1$ curve. According to the Kasteleyn and Fortuin theorem, it might be interpreted as follows: the abcissa $t_B$ and ordinate $t_S$ are respectively changed into $p_B$ and $p_S$, and the curve thus represents the T=0 phase diagram (bond percolation diagram) of the q=2 system (in fact, of the system for arbitrary value of q) where *both* surface and bulk are assumed diluted. As before, the various universality classes are indicated by the RG flow on the critical lines.

Let us now focus the $p_S<1$ curves of Fig.6: they provide an illustration of the conjectural extension of the Kasteleyn and Fortuin theorem proposed by Tsallis[10]. Assume an arbitrary finite or infinite graph, the bond between the i-th and j-th sites of it representing a random ferromagnetic ($J_{ij}>0$) q-state Potts interaction with probability law $P_{ij}(J_{ij})$ or more conveniently $P_{ij}(t_{ij})$, $t_{ij}$ being the corresponding thermal transmissivity. We then calculate, for each bond of the graph, $\langle t_{ij}\rangle_{P_{ij}} \equiv \int_0^1 dt_{ij}\, t_{ij} P_{ij}(t_{ij})$ and then take the q→1 limit of all these quantities. The above mentionned conjecture states that the system thus obtained is fully isomorphic with the bond percolation system through the variable transformation $\lim_{q\to 1} \langle t_{ij}\rangle_{P_{ij}} \leftrightarrow p_{ij}$, $p_{ij}$ being the occupancy probability of the (ij) bond. The standard Kasteleyn and Fortuin theorem is recovered as the particular case $P_{ij}(t_{ij})=\delta(t_{ij}-t^0_{ij})$, $\forall(i,j)$. If we are dealing with an infinite system (Bravais lattice, hierarchical lattice or any other) which, in the q→1 limit, presents a phase diagram represented by the equation $\varphi(\{\lim_{q\to 1}\langle t_{ij}\rangle_{P_{ij}}\})=0$, Tsallis conjecture implies that then and only then the same system presents a bond percolation phase diagram represented by the equation $\varphi(\{p_{ij}\})=0$. In other words, if we represent a q=1 critical frontier in the $\{t_{ij}\}$ variables, *it does not depend on* $\{P_{ij}\}$. For example, Eqs. (5) and (6) imply that, if represented in the $(p_S t_S, p_B t_B)$ variables, the q=1 critical lines would be the same for all $(p_S,p_B)$, hence the same as that associated with $p_B=p_S=1$. This last statement can be checked on Fig. 6. Indeed, the $p_S<1$ curves of that figure satisfy the following (numerical) facts:

(i) all curves with $1>p_S>0.5$ can be transformed into the $p_S=1$ curve through the ordinate transformation $p_S t_S(t_B;p_S) \leftrightarrow t_S(t_B;1)$ (e.g., if we multiply by 0.6 the ordinates of the critical line associated with $p_S=0.6$ we precisely obtain the ordinates of the critical line associated with $p_S=1$, the abcissas being the same);

(ii) all curves with $0.5 \gtrsim p_S \gtrsim p_c = 0.42$ can be transformed into the $p_S=1$ curve through the transformation $(t_B^*,p_S) \leftrightarrow (t_B^*, t_S(t_B^*;p_S=1))$ where $t_B^*$ is, for a given $p_S$, the value of $t_B$ associated with the point at $t_S=1$ (e.g., for $p_S=0.47$, $t_B^*=0.17$, and we verify that the point $(t_B,t_S) = (0.17,0.47)$ belongs to the $p_S=1$ critical line).

## 4 CONCLUSION

We have focused the criticality of the quenched bond-diluted spin 1/2 Ising ferromagnet in a semi-infinite simple cubic lattice with a (0,0,1) free surface. To do this we have developed a RG formalism for the q-state Potts model for arbitrary q, and have obtained the phase diagrams (and discussed the corresponding universality classes) for q=2 and q=1. Within this framework, the semi-infinite Bravais lattice has been approached by a suitable hierarchical lattice (see Fig.1). The d=2 results we obtain for this hierarchical lattice are exact in the pure (non diluted) case, and almost exact for the diluted case. All the phase transitions in the hierarchical lattice are of the second-order type *for all* $q$; this is in contrast with the results known for Bravais lattices, where first-order phase transitions are expected for $q>q_c$ ($q_c=4$ for strictly d=2 systems, and $q_c\simeq 3$ for d=3 ones).

In Fig.4 we present the evolution of the phase diagram as a function of (surface) dilution: it exhibits an interesting and general scheme for bond percolation (and phase transitions of random ferromagnets) in semi-infinite systems. As presented in Fig.4, the results are believed to be exact within an error not larger than 1% everywhere. In particular, we estimate in $p_c=0.42 \pm 0.01$ the bond percolation threshold in bulk-assisted surface percolation in the present case (i.e., $p_c$ jumps from 1/2 to 0.42 if any non vanishing Potts coupling constant is assumed between the free surface and the bulk).

In addition to the above results, the present formalism has enabled, in the $q\rightarrow 1$ limit, an illustration of the Tsallis conjectural extension[10] of the Kasteleyn and Fortuin theorem.

We are deeply indebted to Prof. G.Schwachheim for fruitful computational assistance; interesting remarks from A.C.N. de Magalhães are acknowledged as well.

## CAPTION FOR FIGURES

Fig.1 - Bulk (a) and surface (b) two-rooted graphs. The arrows indicated the "entrances" (one of the roots) and the "exits" (the other root) of the graph. Continuous (dashed) lines indicate bulk (surface) interactions. Within the present RG the bulk (surface) graph is renormalized into a bulk (surface) single bond. Infinite iteration of this procedure generates an hierarchical lattice.

Fig.2 - RG flow of the surface diluted ($p_B=1$) Ising model. ■ , ● and O respectively denote trivial (fully stable), critical (semi-stable) and multicritical (fully unstable) fixed points. PM, BF and SF respectively denote the paramagnetic, bulk ferromagnetic and surface ferromagnetic phases.

Fig.3 - Sections of the critical surface of Fig.2 for typical values of $p_S$.

Fig.4 - The same results of Fig.3 represented in the $(T/T_c^{3D}, J_S/J_S^{SB}, (p_S=1))$ space, where $T_c^{3D}$ and $J_S^{SB}$ respectively are the critical temperature of the d=3 pure model($p_B=1$)and the location of the special transition of the semi-infinite pure model($p_B=p_S=1$). The exact results $p_c^{2D}=1/2$ [14] and $k_BT^{2D}/J_S=2.269...$ [15] are reproduced herein. For $(J_B/k_BT_c^{3D})$ and $(J_S^{SB}/J_B)_{p_B=p_S=1}$ we obtain 0.1949 (to be compared with the series result

0.2181[16] and 1.762 (to be compared with the series 1.6±0.1[17], Monte Carlo 1.5±0.03[18] and extrapolated RG 1.569[19] results).

Fig.5 - Evolution of $(J_S^{SB}/J_B)_{p_B=1}$ with $p_S$ ; $p_c$=0.42.

Fig.6 - Same as Fig.3 (q=1 model instead of q=2). See the text for transforming the $p_S<1$ information into the $p_S=1$ one.

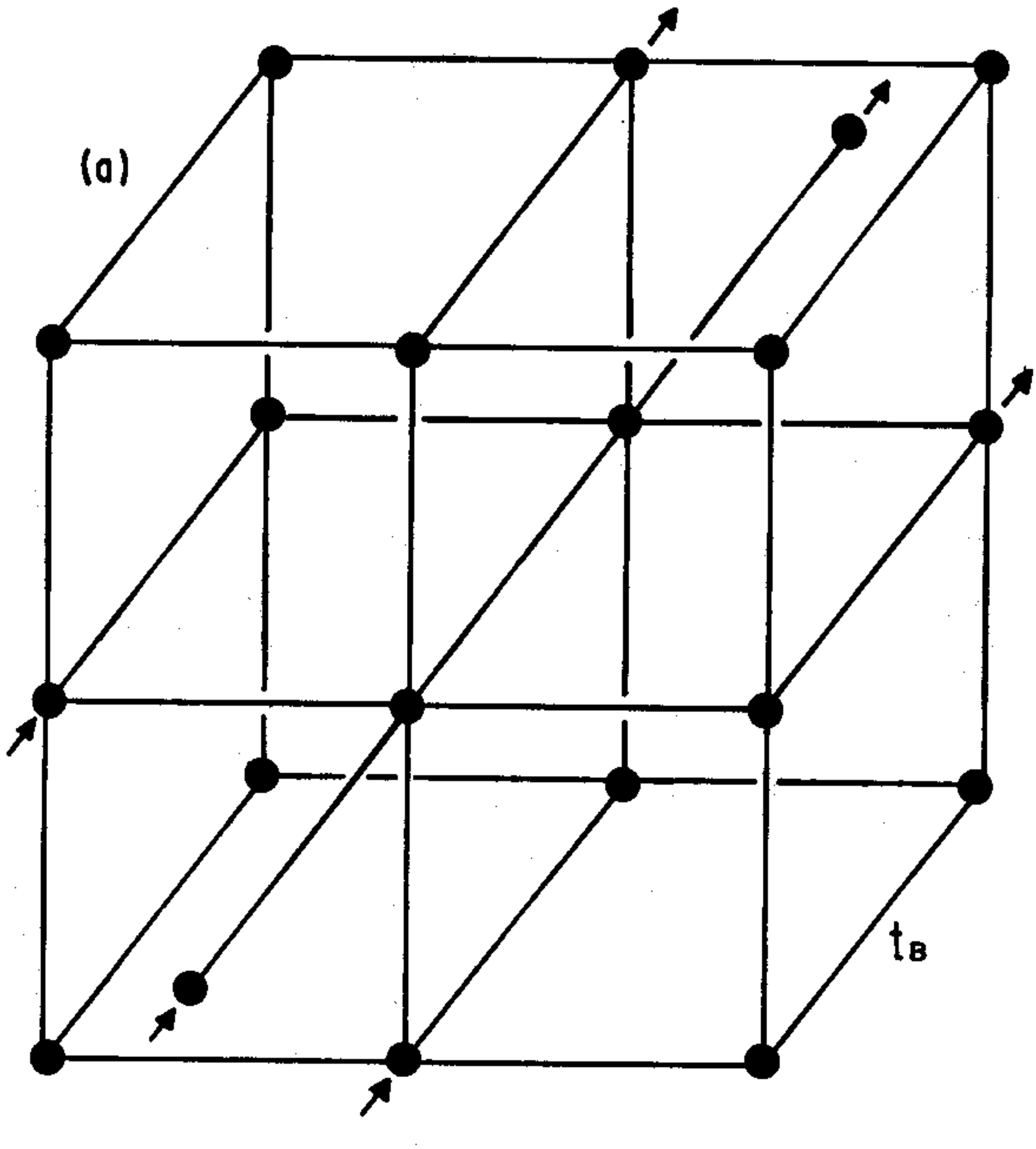



FIG. 1

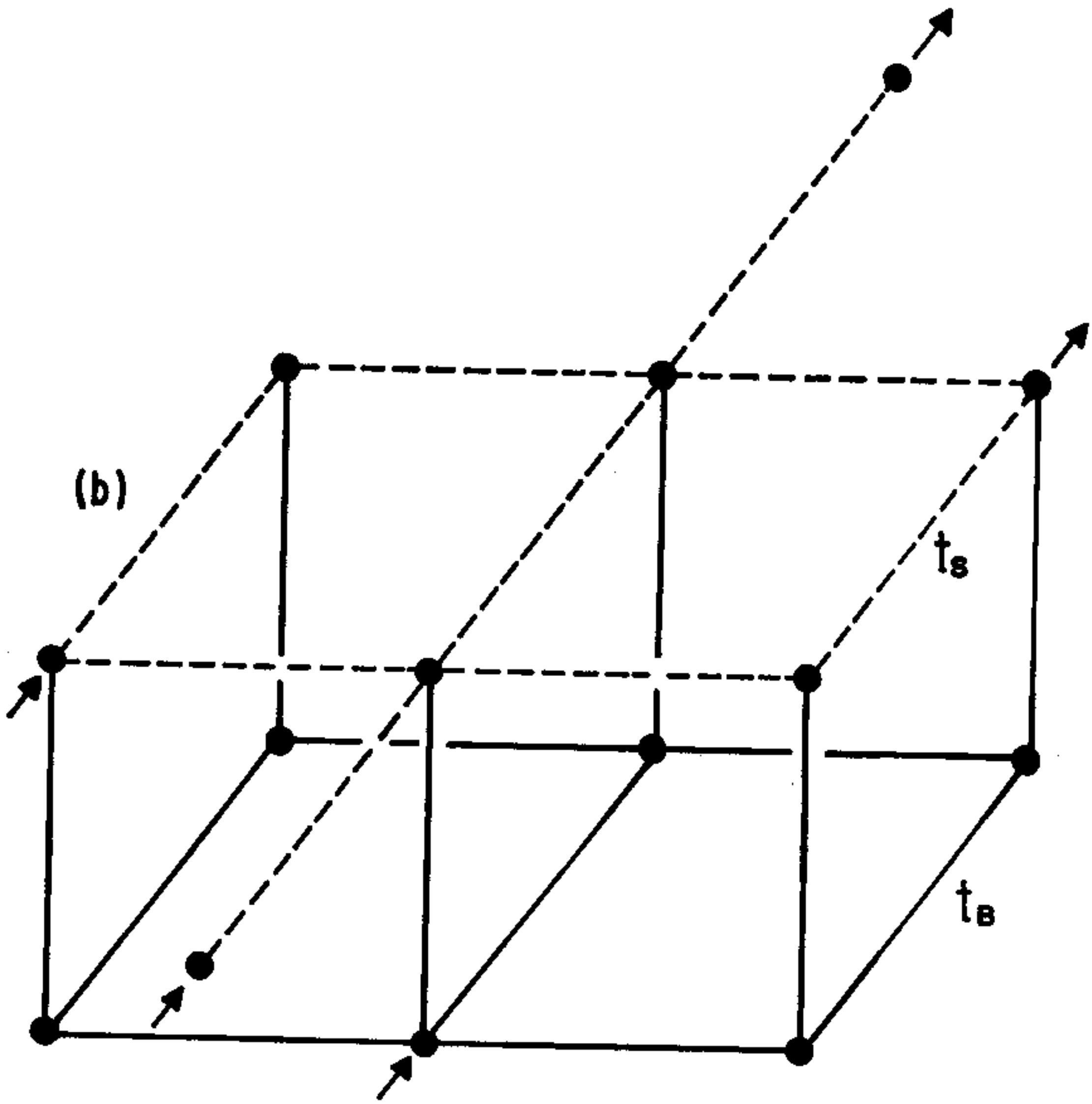



FIG. 1

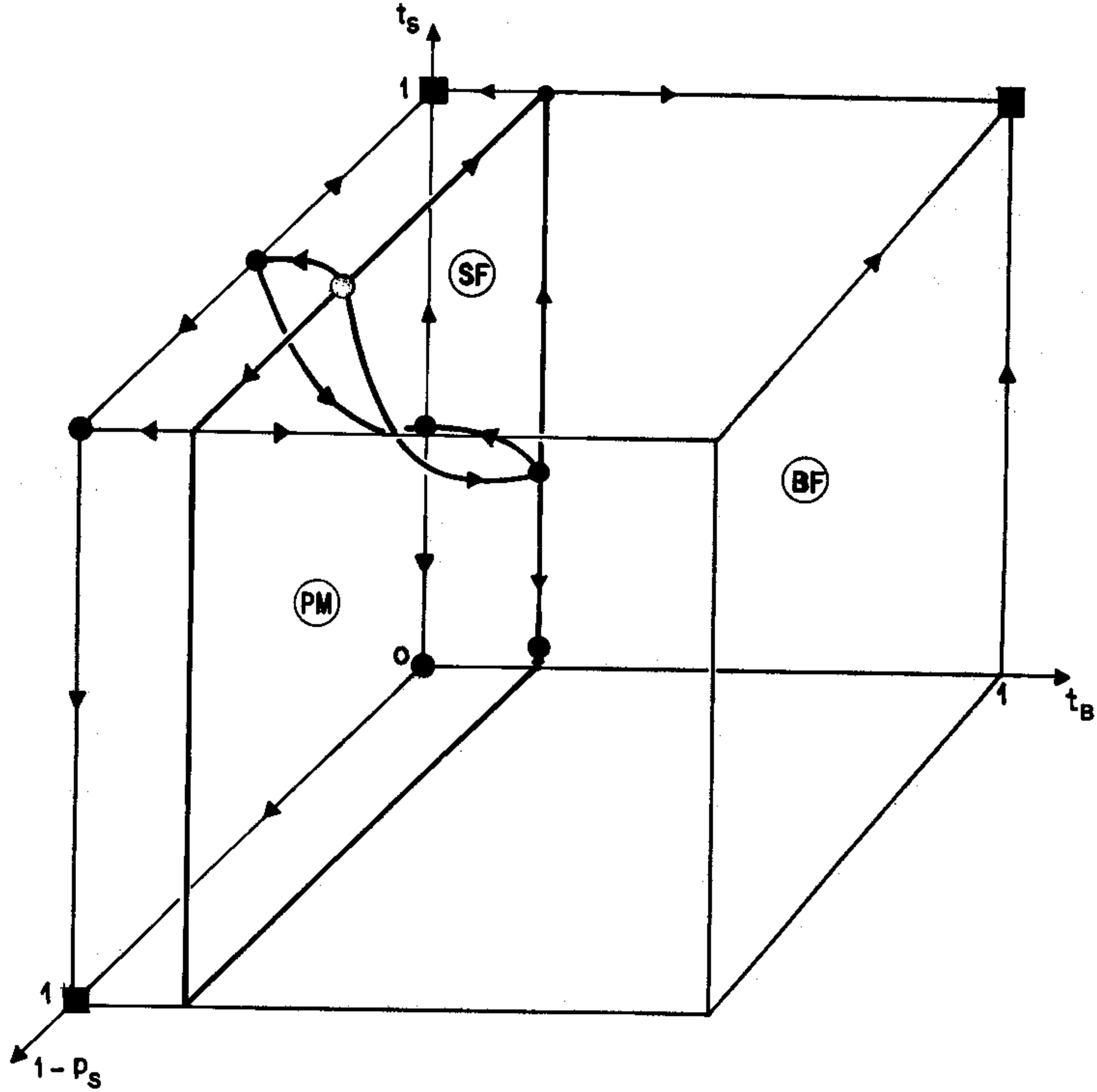



FIG. 2

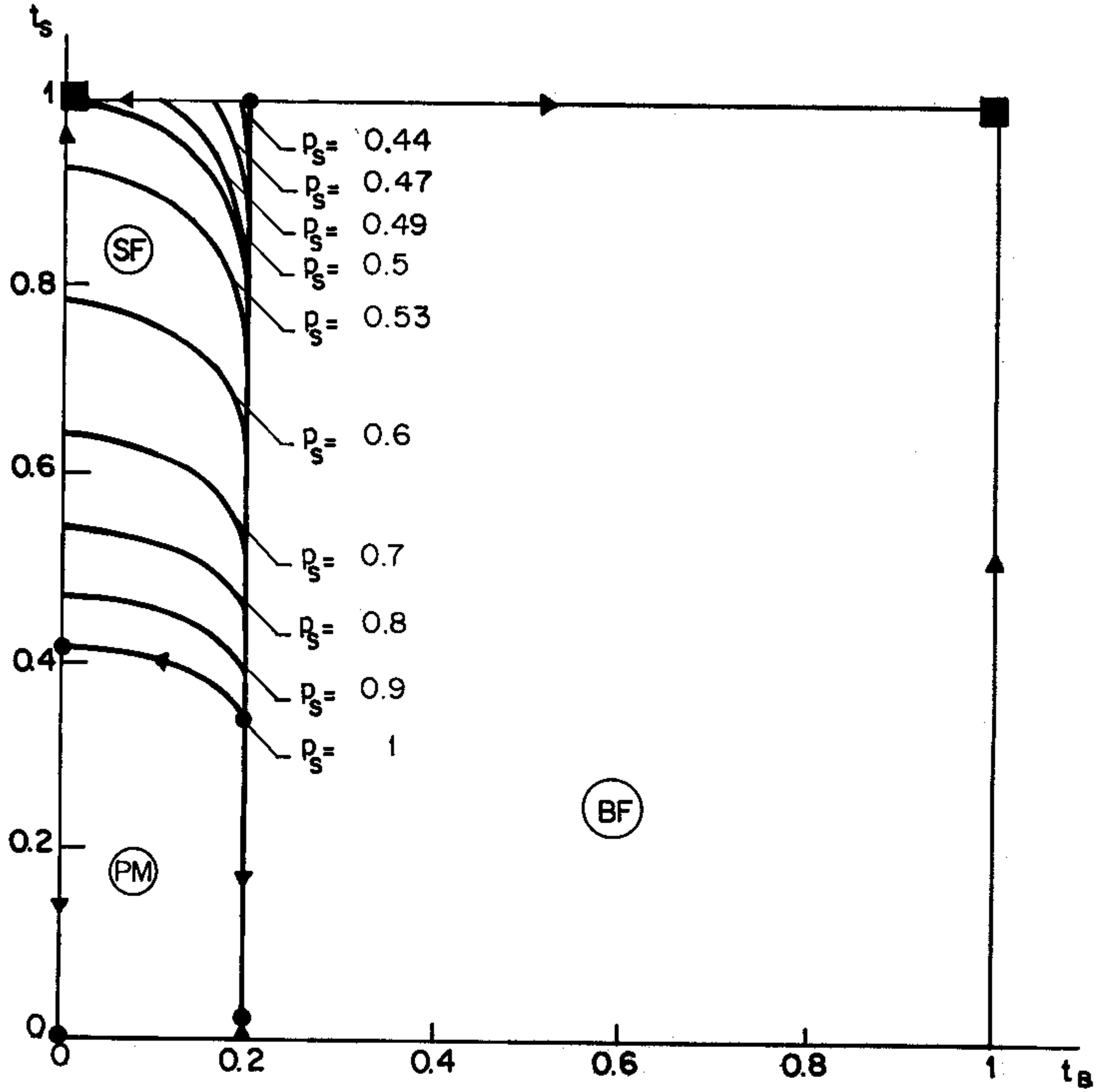

$t_S$
1
0.8
0.6
0.4
0.2
0
SF
PM
BF
$p_S$= 0.44
$p_S$= 0.47
$p_S$= 0.49
$p_S$= 0.5
$p_S$= 0.53
$p_S$= 0.6
$p_S$= 0.7
$p_S$= 0.8
$p_S$= 0.9
$p_S$= 1
0
0.2
0.4
0.6
0.8
1
$t_B$

FIG. 3

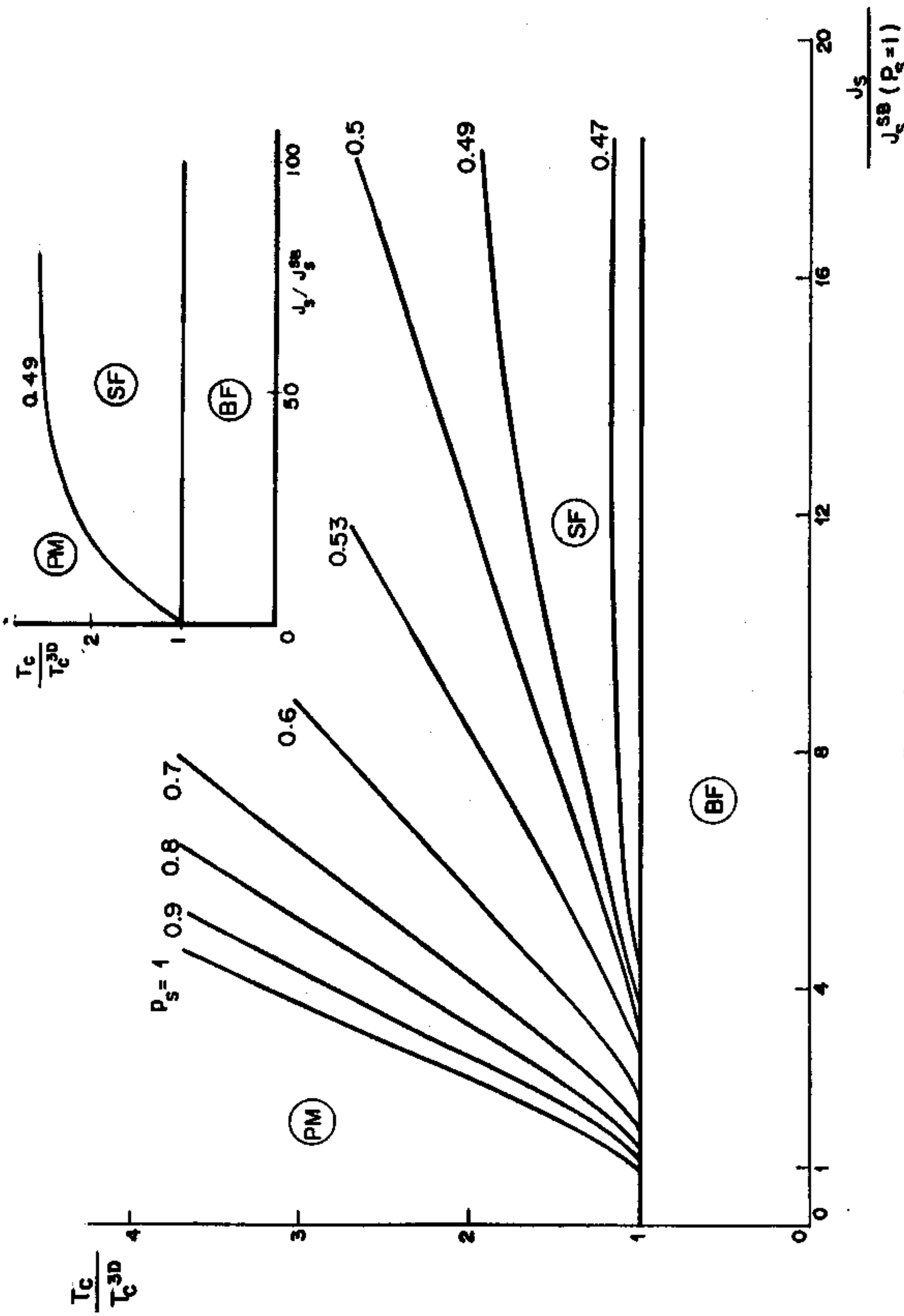

$T_c/T_c^{3D}$
0
1
2
3
4
0
1
4
8
12
16
20
$J_s/J_s^{SB}(P_s=1)$
$P_s = 1$
0.9
0.8
0.7
0.6
0.53
0.5
0.49
0.47
PM
SF
BF
$T_c/T_c^{3D}$
$J_s/J_s^{SB}$
50
100
0.49

FIG. 4

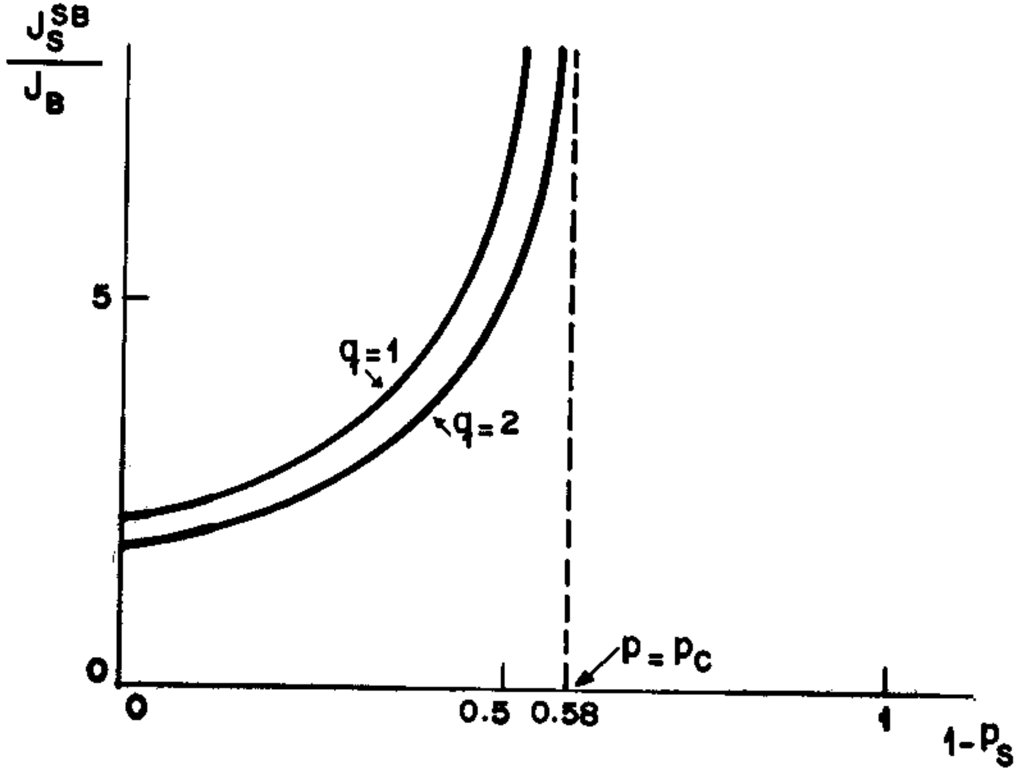
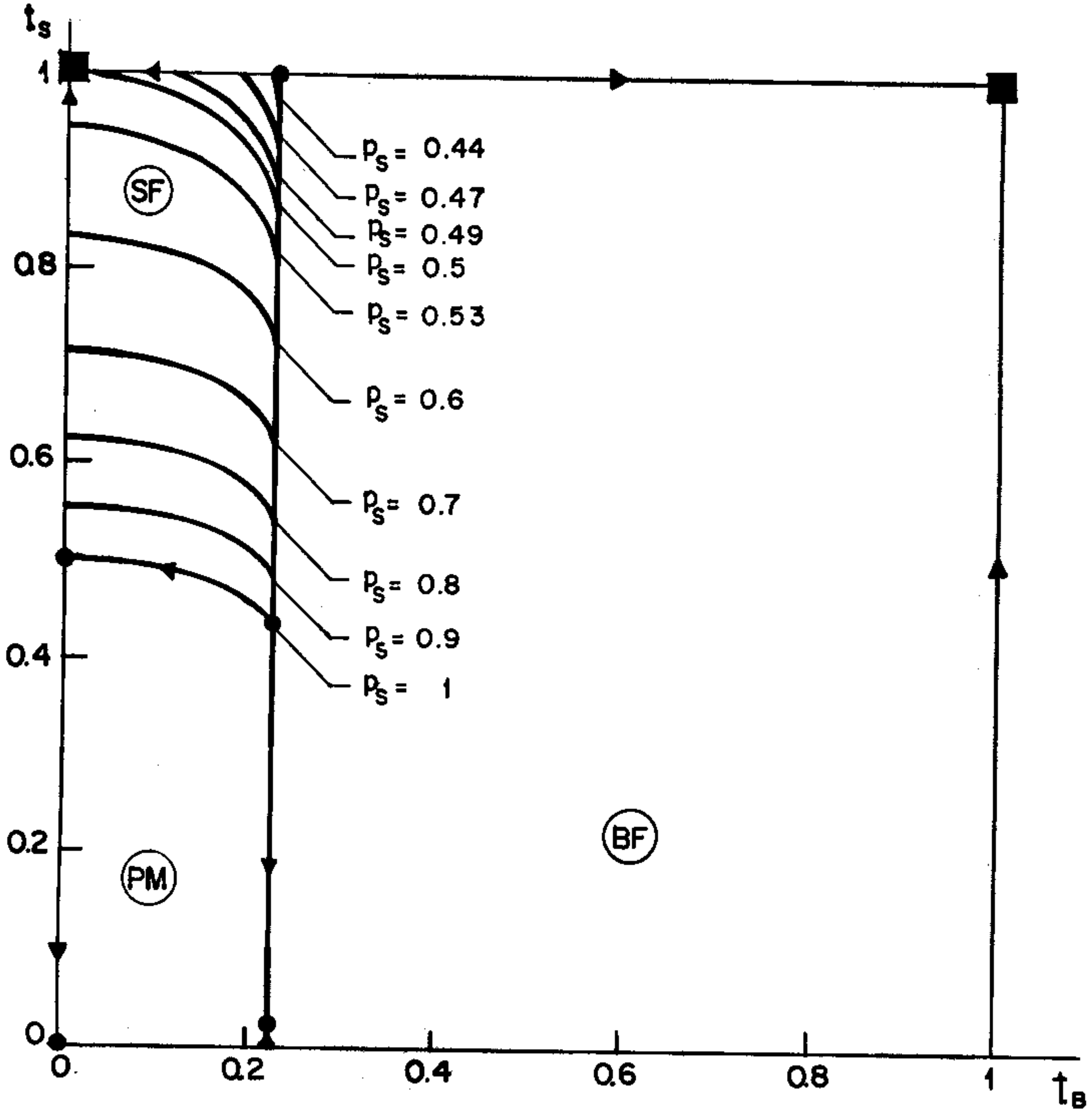



FIG. 5



$t_S$
1
0.8
0.6
0.4
0.2
0
SF
PM
BF
$p_S$ = 0.44
$p_S$ = 0.47
$p_S$ = 0.49
$p_S$ = 0.5
$p_S$ = 0.53
$p_S$ = 0.6
$p_S$ = 0.7
$p_S$ = 0.8
$p_S$ = 0.9
$p_S$ = 1
0.
0.2
0.4
0.6
0.8
1
$t_B$


FIG.6

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