

CBPF-NF-020/85

INTERFACE IN POTTS FERROMAGNET: PHASE
DIAGRAM AND CRITICAL EXPONENTS

by

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ABSTRACT

Within a real-space renormalisation-group framework, we treat the q -state Potts ferromagnet in a simple cubic lattice constituted by two different semi-infinite bulks (respectively characterized by the coupling constants J_1 and J_2) separated by a $(1, 0, 0)$ interface (characterized by J_3). The use of a rather sophisticated two-terminal cluster enables a quite reliable discussion of the phase diagram and its universality classes. Four physically different phases are obtained, namely the paramagnetic and the double-bulk, single-bulk and surface ferromagnetic ones. The critical surface contains a multicritical line (associated with $J_1 \neq J_2$) which in turn contains a special point associated with $J_1 = J_2$.

Key-words: Potts ferromagnet; Interface; Phase diagram; Critical exponents.

I INTRODUCTION

Critical phenomena associated with surface or interface magnetism have recently raised increasing interest, due both to its theoretical richness (see Binder 1983 for a recent review) and to its experimental utility (Pierce and Meier 1976, Alvarado et al. 1982 (a,b) Klebanoff et al. 1984). One of the simplest models that can be assumed is the q -state Potts ferromagnet in semi-infinite simple cubic lattice, the free surface and the bulk coupling constants being not necessarily equal. This model has already received some attention within real space renormalisation group (RG) frameworks (Lipowsky 1982 (a,b), Lam and Zhang 1983, Tsallis and Sarmiento 1985). However they addressed mainly the qualitative aspects of the problem. More recently Costa et al 1985 (hereafter referred to as paper I) used, for the same problem, a quite sophisticated cluster (da Silva et al 1984) which enables quantitatively satisfactory results.

In the present paper we assume the system to be constituted by two (not necessarily equal) semi-infinite simple cubic bulks separated by a $(1, 0, 0)$ interface with a coupling constant which might be different from those of the bulks. This model contains the free surface problem (treated in paper I) as well as the planar defect problem (a planar anomaly in a otherwise homogeneous system) as particular cases. All of the present calculations recover those of paper I if one of the semi-infinite bulks is assumed to be the vacuum.

The paper is organized as follows: in section II we introduce the model and the RG formalism, in section III we present the results (q -evolution of the phase diagram and critical exponents), and finally we conclude in section IV.

II MODEL AND FORMALISM

We consider a q-state Potts model whose Hamiltonian is given by

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

where $\langle i,j \rangle$ runs over all pairs of first-neighbouring sites of two semi-infinite simple cubic bulks separated by a $(1, 0, 0)$ interface (square lattice). J_{ij} equals J_1 on one semi-infinite bulk, J_2 on the other one, and J_S on the interface ($J_1, J_2, J_S \geq 0$). Let us introduce the following convenient variables (hereafter referred to as thermal transmissivities: see Tsallis and Levy 1981):

$$t_r \equiv \frac{1 - e^{-qJ_r/k_B T}}{1 + (q-1)e^{-qJ_r/k_B T}} \quad \in [0, 1] \quad (r = 1, 2, S) \quad (2)$$

where T is the temperature and k_B the Boltzmann constant. The following definition will also be useful:

$$\Delta \equiv \frac{J_S}{J_1} - 1 = \frac{\ln \frac{1+(q-1)t_S}{1-t_S}}{\ln \frac{1+(q-1)t_1}{1-t_1}} - 1 \quad (3)$$

where we have used definitions (2).

To establish the RG recursive relations, we renormalize the two-terminal cell (first introduced by da Silva et al 1984 to treat the anisotropic simple cubic lattice) indicated in Fig.1 into a single bond (with renormalized transmissivity) by preserving the partition function. The recurrence for the first bulk is obtained by associating t_1 to each bond of the cell of Fig.1,

and is given by

$$t_1' = f(t_1) \quad (4)$$

where the function $f(t_1)$ (too lengthy to be reproduced herein) has been calculated by using the Break-collapse method (BCM; Tsallis and Levy 1981). Analogously we obtain, for the second bulk,

$$t_2' = f(t_2) \quad (5)$$

For the interface transmissivity recurrence, we associate t_1 , t_2 and t_S on the cluster (which lies now on the interface) precisely as indicated in Fig. 1, and obtain (once more through the BCM)

$$t_S' = g(t_1, t_2, t_S) \quad (6)$$

where the function g is a ratio of two polynomials in (t_1, t_2, t_S) , each of them containing about two thousand terms for arbitrary q . Also we verify that $g(t, t, t) = f(t), \forall t$.

The set of Eqs. (4) - (6) formally closes the RG procedure, and determines both the phase diagram and the various correlation length and crossover critical exponents (respectively denoted by ν and ϕ). The particular case $t_2 = 0$ (or equivalently $t_1 = 0$) precisely recovers the RG constructed in paper I.

III RESULTS

Before we enter into the description of the results obtained within the present RG, let us make a few general considerations. The intuitive expectation for the present system is that various phase transitions could occur. Two of them correspond to the single bulk para-ferromagnetic standard phase transi-

tions, respectively occurring at $T_C^{3D(1)} = n^{3D}(q)J_1/k_B$ and $T_C^{3D(2)} = n^{3D}(q)J_2/k_B$, where $n^{3D}(q)$ is a pure number (e.g., $n^{3D}(2) = 4.511$ (Zinn-Justin 1979)) corresponds to the Ising model). For Δ above a critical value Δ_C (which depends on q and J_2/J_1), the interface is expected to retain a ferromagnetic order even when both bulks have lost theirs, more precisely for temperatures up to a critical value T_C^S which depends on q , J_S/J_1 and J_2/J_1 , and which satisfies $T_C^S \geq T_C^{2D} \equiv n^{2D}(q) J_S/k_B$, where $n^{2D}(q)$ is a pure number (e.g., $n^{2D}(2) = 2.269\dots$). T_C^S approaches T_C^{2D} if and only if J_S is much larger than both J_1 and J_2 . A mean field argument for the Ising model ($4J_S + J_1 + J_2 = 6J_1$, conventionally assuming $J_2 \leq J_1$) yields $\Delta_C = (1 - J_2/J_1)/4$. This implies $\Delta_C = 1/4$ ($\Delta_C = 0$) for the free surface (planar defect) problem which corresponds to $J_2 = 0$ ($J_2 = J_1$). The RG results we are now presenting are different and a priori more reliable.

The $q = 2$ RG flow diagram is presented in Fig. 2. It qualitatively illustrates the general phase diagram obtained for arbitrary q . We verify the following features:

- (i) Five different phases are present, respectively characterized by the trivial (fully stable) fixed points $(t_1, t_2, t_3) = (0, 0, 0)$ (paramagnetic phase; P), $(1, 0, 1)$ (bulk-1 ferromagnetic phase; BF₁; bulk-1 and interface are ordered, whereas bulk-2 is disordered), $(0, 1, 1)$ (bulk-2 ferromagnetic phase; BF₂; bulk-2 and interface are ordered, whereas bulk-1 is disordered), $(1, 1, 1)$ (bulk-1-2 ferromagnetic phase; BF₁₂; all three regions are ordered), and $(0, 0, 1)$ (surface ferromagnet; SF; the interface is ordered, whereas both bulks are disordered);
- (ii) Eleven semi-stable fixed points are present (see Fig. 2 and Table 1), namely at $(t_1, t_2, t_3) = (t^B(q), 0, 1)$ and $(0, t^B(q), 1)$ (characterising the single-bulk para-ferromagnetic phase tran

sition with three-dimensional correlation length critical exponent ν^{3D} , at $(t^B(q), t^B(q), 1)$ (characterising the double-bulk phase transition whose critical exponent also is ν^{3D}), at $(0, 0, t^S(q))$ (characterising the interface para-ferromagnetic phase transition with critical exponent ν^{2D}), at $(t^B(q), 0, t^{SB}(q))$ and $(0, t_B(q), t^{SB}(q))$ (characterising the surface-single-bulk multicritical lines with critical exponent ν^{3D} for the bulks and $1/\gamma_{t_1}^{SB}$ (Burkhardt and Eisenriegler 1977) for the surface), at $(t^B(q), 0, t^{Sl}(q))$ and $(0, t^B(q), t^{Sl}(q))$ (characterising the *simultaneous* single-bulk and interface para-ferromagnetic phase transition, with critical exponent ν^{3D} for the bulk and $1/\gamma_{t_1}^{SB}$ for the interface), and finally at $(t^B(q), t^B(q), t^{SEB}(q))$ (characterising the simultaneous equal-bulk and interface phase transition, with critical exponent ν^{3D} for the bulks and $1/\gamma_{t_1}^{SEB}$ for the interface).

- (iii) A fully unstable fixed point is present at $(t_1, t_2, t_3) = (t^B(q), t^B(q), t^B(q))$ (characterising a high-order multicritical point with critical exponent ν^{3D} for the bulks and $1/\gamma_{t_1}^{SEB}$ for the interface). Its existence is obvious from the fact that $g(t, t, t) = f(t)$. Its (un)stability deserves however a few comments. Very recently dos Santos et al 1985 treated, within a Migdal-Kadanoff-like RG (whose essential difference with the present treatment comes from the choice of the cluster), the criticality of a quantum anisotropic Heisenberg interface between Ising bulks. That problem shares with the present one a common particular case, namely the $q = 2$ ferromagnet. Consequently, for this particular model, the two approximations can be compared. Both present, on the $t_1 = t_2$ axis, two non trivial fixed points, a fully unstable one and, at a lower t_3 value, a semi-stable one. However, in the dos Santos et al

1985 treatment, the lower fixed point (i.e. the semi-stable one) lies on the axis $t_1=t_2=t_S$, whereas, in the present treatment, it is the higher one (i.e., the fully unstable one) which lies on this axis, as already said. Furthermore, the dos Santos et al 1985 RG yields $t^B(2) = 0.34$ (which is too high with respect to the very accurate series result 0.21811 (Zinn-Justin 1979)), whereas the present RG yields $t^B(2) \approx 0.19$ (which is too low with respect to the series result). All these features put together make the following picture possible. The fact that $g(t, t, t) = f(t)$ (true for both RG's under analysis) implies, as said before, the existence of a non trivial fixed point on the $t_1=t_2=t_S$ axis. The nature of the RG approximations leads to the existence of another non trivial fixed point on the axis $t_1=t_2$, whose t_S coordinate might be higher or lower than that of the fixed point just mentioned. RG clusters which overestimate $t^B(2)$ might belong to one class, and those which underestimate $t^B(2)$ might belong to the other class. If so, an exact RG should correspond to the collision of these two fixed points, and a set of approximations running from one type to the other should correspond to the crossing of these two fixed points and simultaneous stability interchange (as occurs often; see Toulouse and Pfeuty 1975). All this analysis could be clarified by studying the influence of increasingly large clusters; unfortunately this is, computationally speaking, not trivial at all.

In Figs. 3 and 4 we present the q -evolution of the phase diagram. The location of the multicritical point (characterized by the value Δ_c) is presented in Fig. 5 as a function of q and J_2/J_1 .

Let us now focus the values of the various correlation length critical exponents. Eqs.(4)-(6) enable the calculation of the Jacobian matrix $M \equiv \partial(t'_1, t'_2, t'_S)/\partial(t_1, t_2, t_S)$ evaluated at

any relevant fixed point. Its general form is given by

$$M = \begin{pmatrix} a(q) & 0 & 0 \\ 0 & b(q) & 0 \\ d(q) & e(q) & c(q) \end{pmatrix} \quad (7)$$

where $a(q), \dots, e(q)$ depend on the particular fixed point. The eigen values are given by

$$\lambda_1 = a(q) \quad (8.a)$$

$$\lambda_2 = b(q) \quad (8.b)$$

$$\lambda_3 = c(q) \quad (8.c)$$

whose respective eigenvectors are given by

$$\vec{u}_1 \propto \begin{pmatrix} a - c \\ 0 \\ d \end{pmatrix} \quad (9.a)$$

$$\vec{u}_2 \propto \begin{pmatrix} 0 \\ b - c \\ e \end{pmatrix} \quad (9.b)$$

$$\vec{u}_3 \propto \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \quad (9.c)$$

We quickly review now the various types of fixed points appearing in our problem. For the fixed point at $(t_1, t_2, t_3) = (t^B(q), 0, 1)$ we have $b=c=d=e=0$, $a > 1$, and the three-dimensional critical exponent is given by

$$v^{3D}(q) = \ln 3 / \ln a(q) \quad (10)$$

where 3 is the RG linear scale factor. For the fixed point at $(1, t^B(q), 1)$ we have $a = c = d = e = 0$, and $b > 1$; b equals the value of a appearing in Eq.(10). For the fixed point $(t^B(q), t^B(q), 1)$ we have $c = d = e = 0$, and $a = b > 1$; a and b equal the value of a appearing in Eq.(10). For the fixed point $(0, 0, t^S(q))$ we have $a = b = 0$, $d = e$ and $ac > 1$; the two-dimensional critical exponent is given by

$$v^{2D}(q) = \ln 3 / \ln c(q) \quad (11)$$

For the fixed point $(t^B(q), 0, t^{SB}(q))$ we have $b = 0$, d and $e < 1$, and $a, c > 1$; a equals the value appearing in Eq.(10), and the corresponding crossover and critical exponent are respectively given by

$$\phi^{SB}(q) = \ln c(q) / \ln a(q) \quad (12)$$

$$\text{and } 1/y_{t_1}^{SB}(q) = \ln 3 / \ln c(q) \quad (13)$$

For the fixed point $(t^B(q), t^B(q), t^B(q))$ we have $d = e$, $c+d+e = a = b > 1$ and $c > 1$; a and b equal the value appearing in Eq.(10), and the corresponding crossover and critical exponents are respectively given by

$$\phi^{SEB}(q) = \ln c(q) / \ln a(q) \quad (14)$$

$$\text{and } 1/y_{t_1}^{SEB}(q) = \ln 3 / \ln c(q) \quad (15)$$

For the fixed point $(t^B(q), 0, t^{S1}(q))$ we have $b=0$, $c, d, e < 1$ and $a > 1$; a equals the value appearing in Eq.(10). Fi-

nally, for the fixed point $(t^B(q), t^B(q), t^{SEB}(q))$ we have c, d and $e < 1$, $a = b > 1$; a and b equal the value appearing in Eq. (10). The various exponents that have been determined are presented in Table I and Fig. 6.

All the results we are discussing strictly hold for standard second order (or at least continuous) phase transitions, i.e. for $0 \leq q \leq 4$ for two dimensions, and $0 \leq q \leq q_c$ (with $q_c \approx 3$) for three dimensions. Nevertheless, whenever the transition is a first order one, the latent heat is quite small in the interval $q \in [0, 4]$; it is due to this fact that we present our results (see Table I and Fig.6) up to $q = 4$.

IV CONCLUSIONS

Within a real space renormalisation group approach, we have treated the criticality of the q -state Potts ferromagnetic model in a inhomogeneous lattice constituted by two semi-infinite simple cubic bulks (characterized by the coupling constants J_1 and J_2 respectively) separated by a $(1, 0, 0)$ square lattice interface (characterized by the coupling constant J_S). The approach extends that devised by Costa et al 1985 and uses a rather sophisticated cluster introduced by da Silva et al 1984 for the homogeneous system ($J_1=J_2=J_S$). The phase diagram presents, for all values of q , four physically different phases, namely the paramagnetic, the ferromagnetic single-bulk, the ferromagnetic double-bulk, and the ordered surface ones. The paramagnetic, single-bulk and surface phases join on a multicritical line whose universality class for $J_1 \neq J_2$ is that corresponding to the free surface case ($J_2/J_1=0$). All four phases join on a special point (corresponding to $J_1 = J_2$) whose nature is not sufficiently clarified within the present (re

latively small) cluster approach. The exact critical temperature is recovered for the two-dimensional limit ($J_1, J_2 \ll J_S$).

The location of the multicritical line can be characterized by the value $\Delta \equiv J_S/J_1 - 1$ above which surface magnetic order can exist even if it has disappeared from both bulks (see Fig. 4). We present, for the first time as far as we know, the evolution of Δ with q and J_2/J_1 . For the Ising model ($q=2$) we obtain, for the free surface case ($J_2/J_1 = 0$), $\Delta \approx 0.76$ (to be compared with the series result 0.6 ± 0.1 by Binder and Hohenberg 1974, the Monte Carlo result 0.5 ± 0.03 by Binder and Landau 1984, and with the mean field value 0.25); for the equal bulk case ($J_1 = J_2$) we obtain $\Delta \approx 0.10$, to be compared with the mean field value 0.

With respect to the critical exponents, we obtained that all ν 's monotonously decrease with increasing q , whereas the crossover exponents ϕ 's present the opposite tendency.

We acknowledge valuable discussions with E.M.F. Curado and A.M. Mariz.

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CAPTION FOR FIGURES AND TABLE

- Fig. 1 - RG cell for the (1,0,0) interface in double semi-infinite simple cubic lattice. The full (dotted) bonds represent the bulk-1 (bulk-2) coupling t_1 (t_2). The dashed line represents the interface coupling t_s . The arrows indicate the terminal nodes of the cell.
- Fig. 2 - $q=2$ RG flux diagram in the (t_1, t_2, t_s) space. ■ denotes trivial (fully stable) fixed points; ● denotes the multicritical and the critical (semi-stable) fixed points ($SB_1, SB_2, S, \text{etc.}$); ○ denotes the high-order multicritical (SB_{12}) (fully unstable) fixed point. The five possible phases are indicated: the two single-bulk ferromagnetic (BF_1, BF_2), the double-bulk ferromagnetic (BF_{12}), the surface ferromagnetic (SF) and the paramagnetic (P) ones.
- Fig. 3 - q -evolution of the phase diagram indicated in Fig.2 (a) for $t_2=0$; (b) for $t_2=t_1$.
- Fig. 4 - Same q -evolution appearing in Fig. 3, but in the Δ - T space ($\Delta \equiv \frac{J_s}{J_1} - 1$). (a) for $J_2/J_1=0$; (b) for $J_2/J_1=.5$; (c) for $J_2/J_1=1$.
- Fig. 5 - q -evolution of Δ_c for several ratios J_2/J_1 ; the $J_2/J_1=0$ case reproduces the results obtained in paper I.
- Fig. 6 - q -dependence of the thermal-type critical exponents (ν 's and γ 's) and the crossover exponents (ϕ 's).
- Table 1 - Present RG (upper value) and exact or series or Monte Carlo or similar (lower value) results for the main critical points and exponents. (a) de Magalhães et al. 1981; (b) Gaunt and Ruskin 1978; (c) Zinn-Justin 1979; (d) Jensen and Mouritsen 1979; (e) calculated from value appearing in Zinn-Justin 1979 and Binder and Hohenberg 1974; (f) calculated from value appearing in Zinn-Justin 1979 and Binder and Landau 1984; (g) Wu 1982 and references therein; (h) den Nijs 1979; (i) Heerman and Stauffer 1981; (j) Le Guillou and Zinn-Justin 1980; (k) Diehl and Dietrich 1980; (l) Binder and Landau 1984; (m) Costa et al. 1985; (n) Binder and Hohenberg 1974.

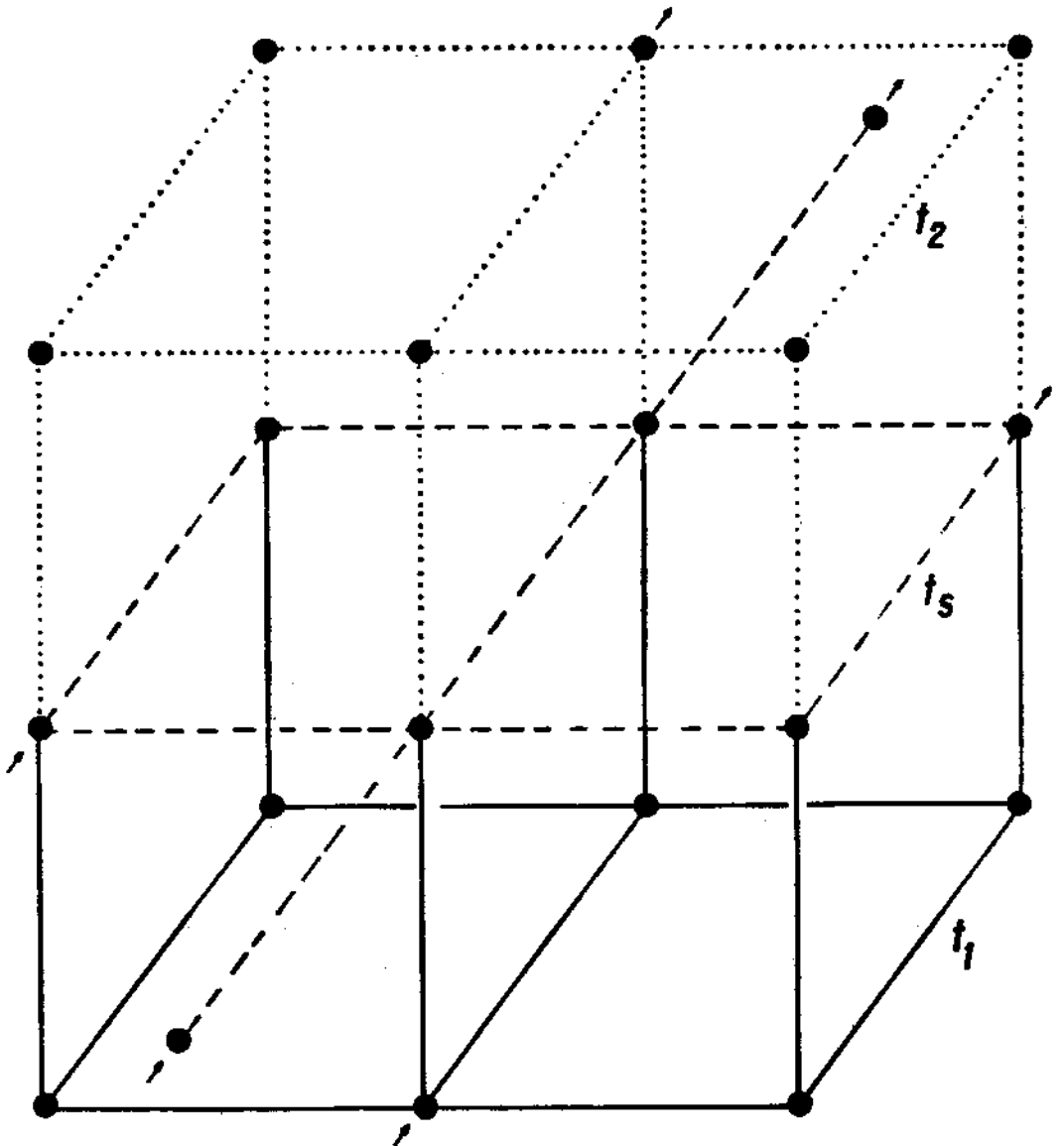


FIG.1

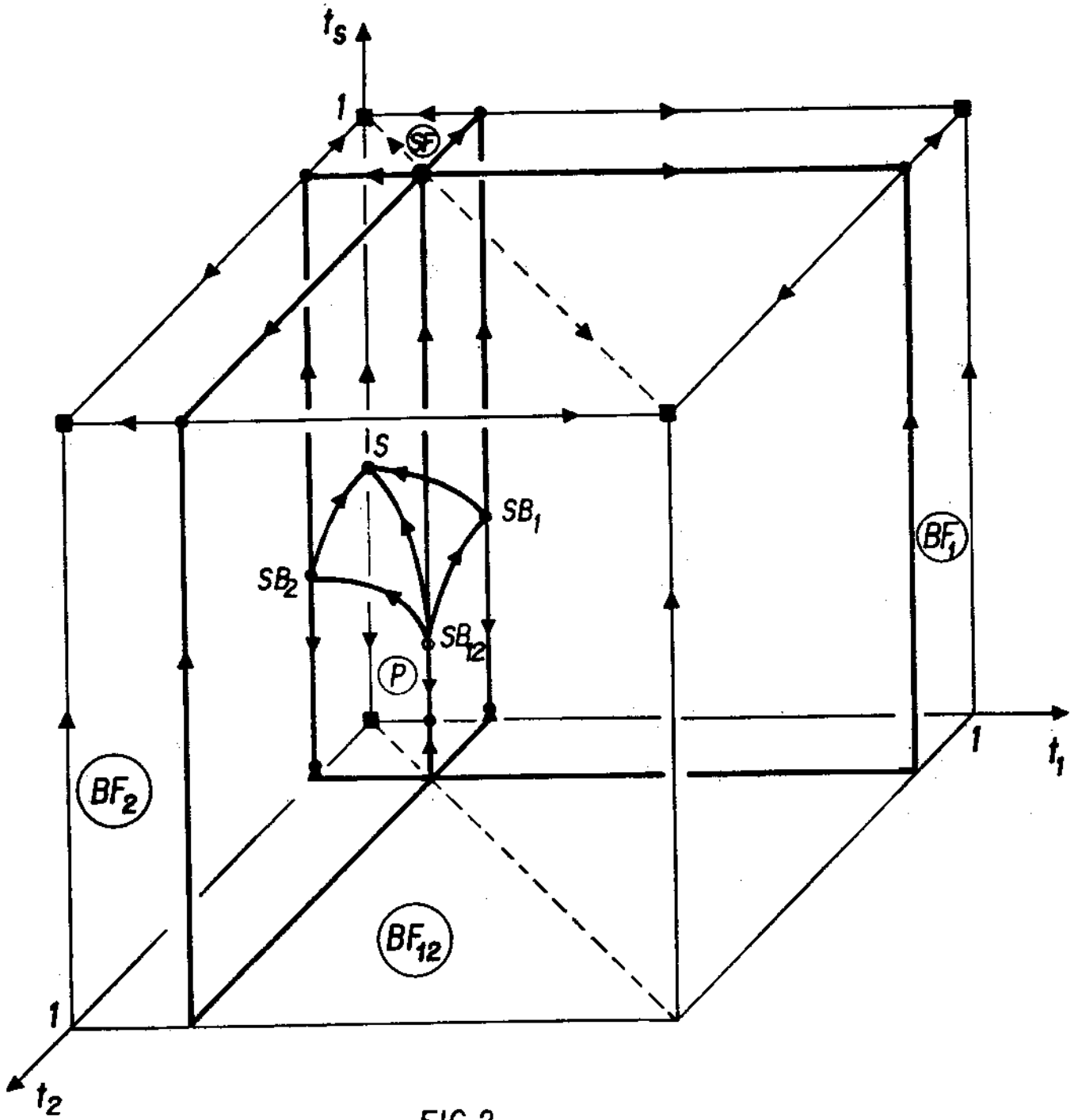


FIG. 2

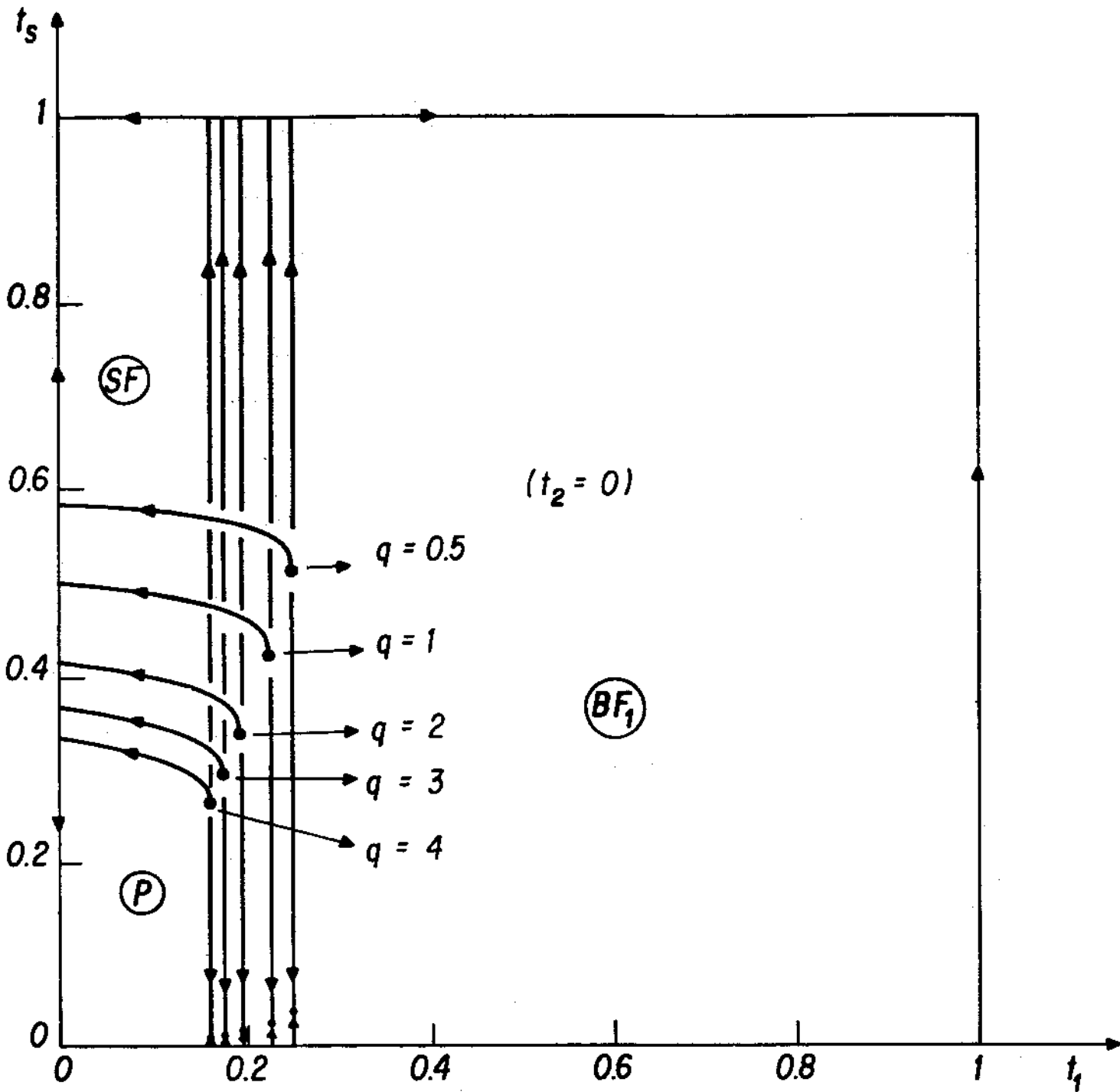


FIG.3-a

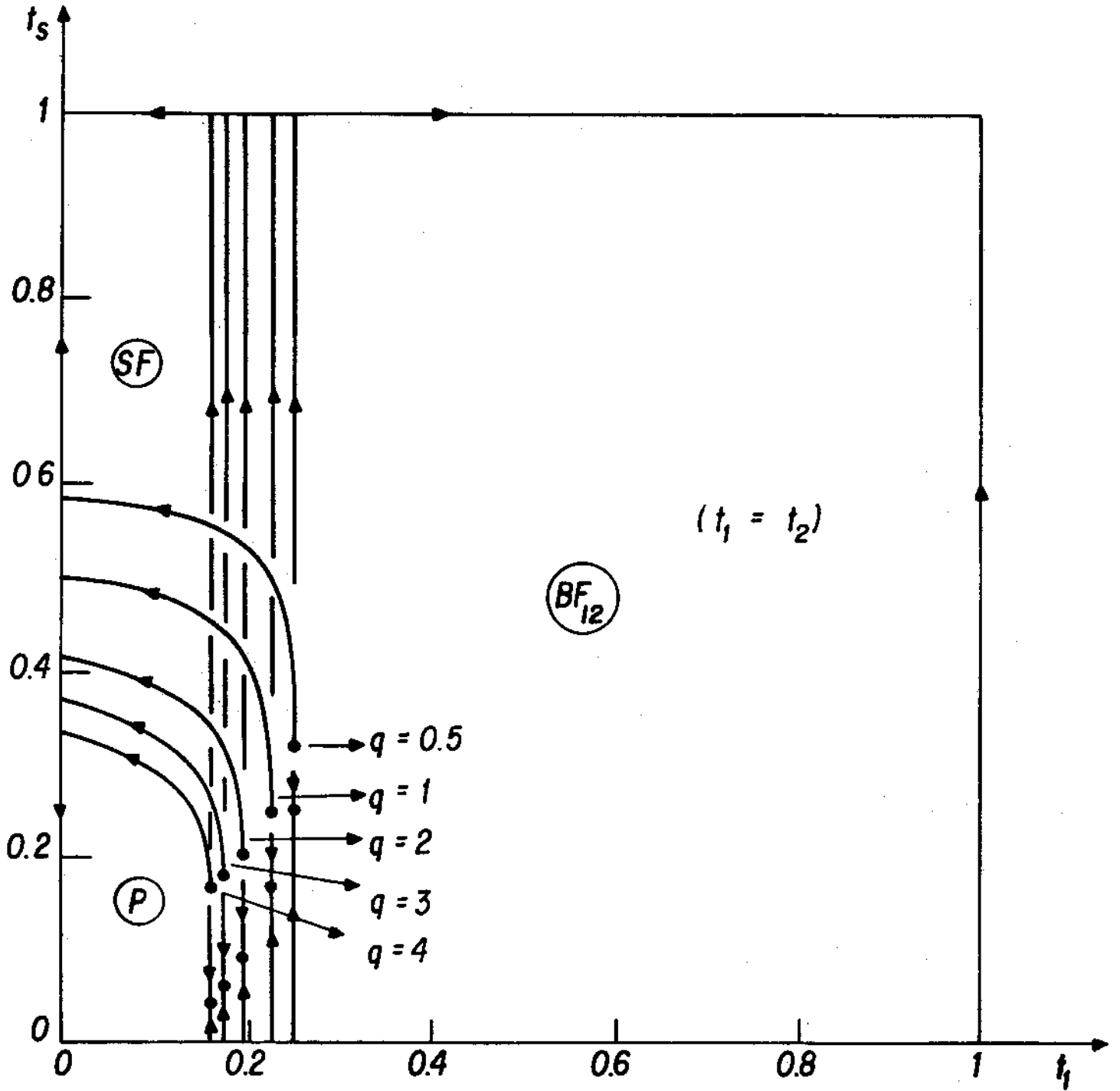


FIG.3-b

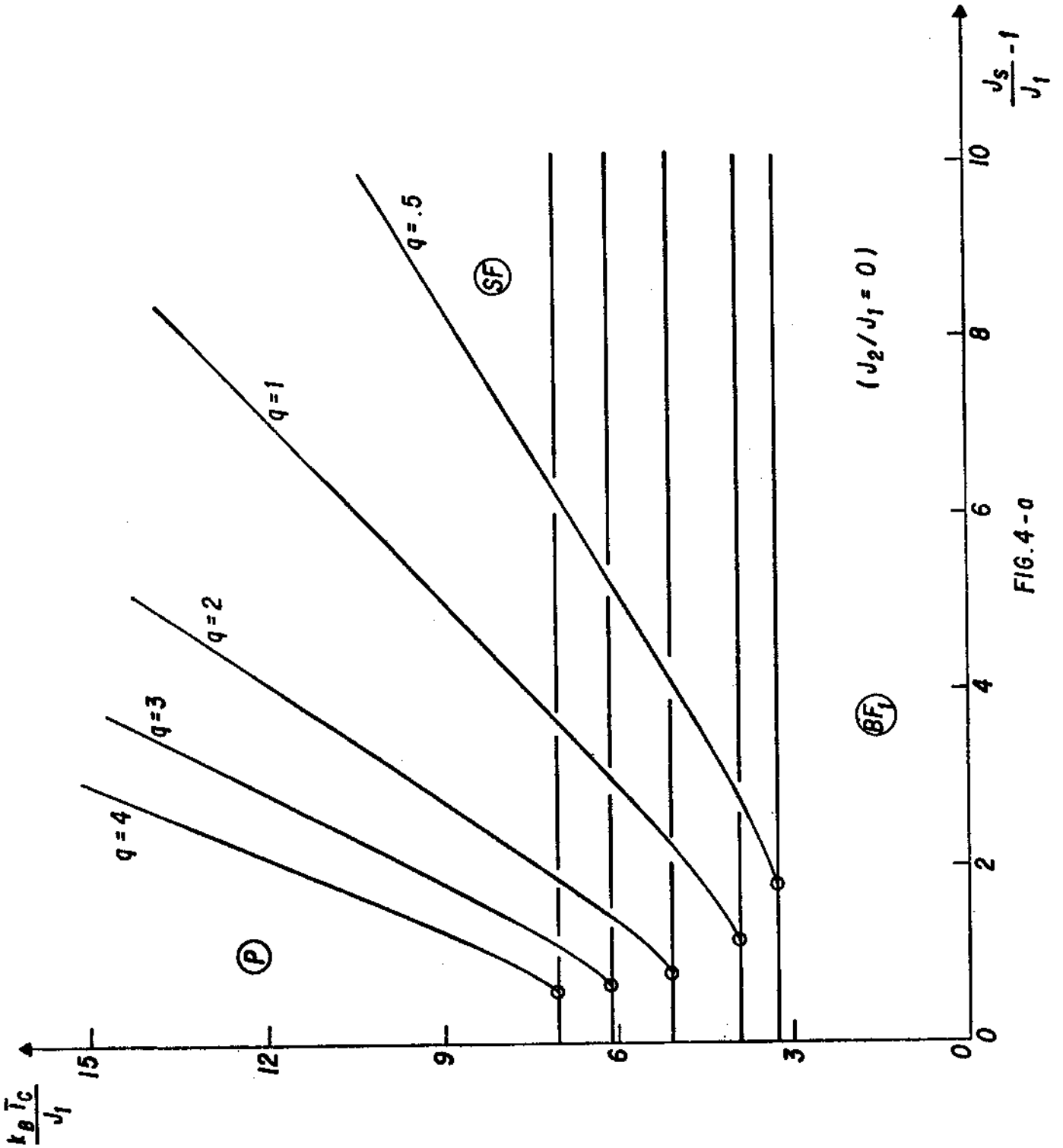


FIG. 4-0

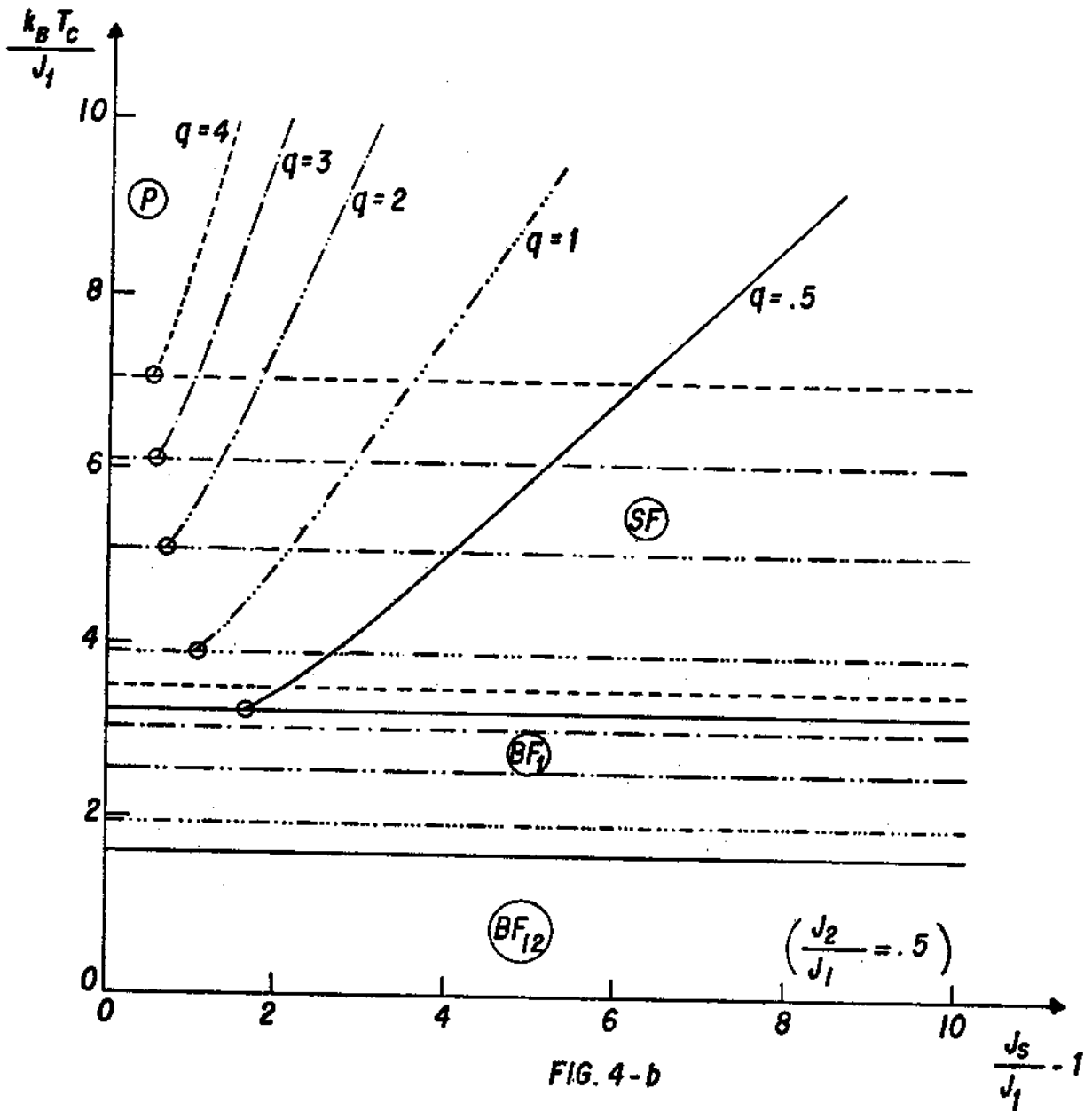


FIG. 4-b

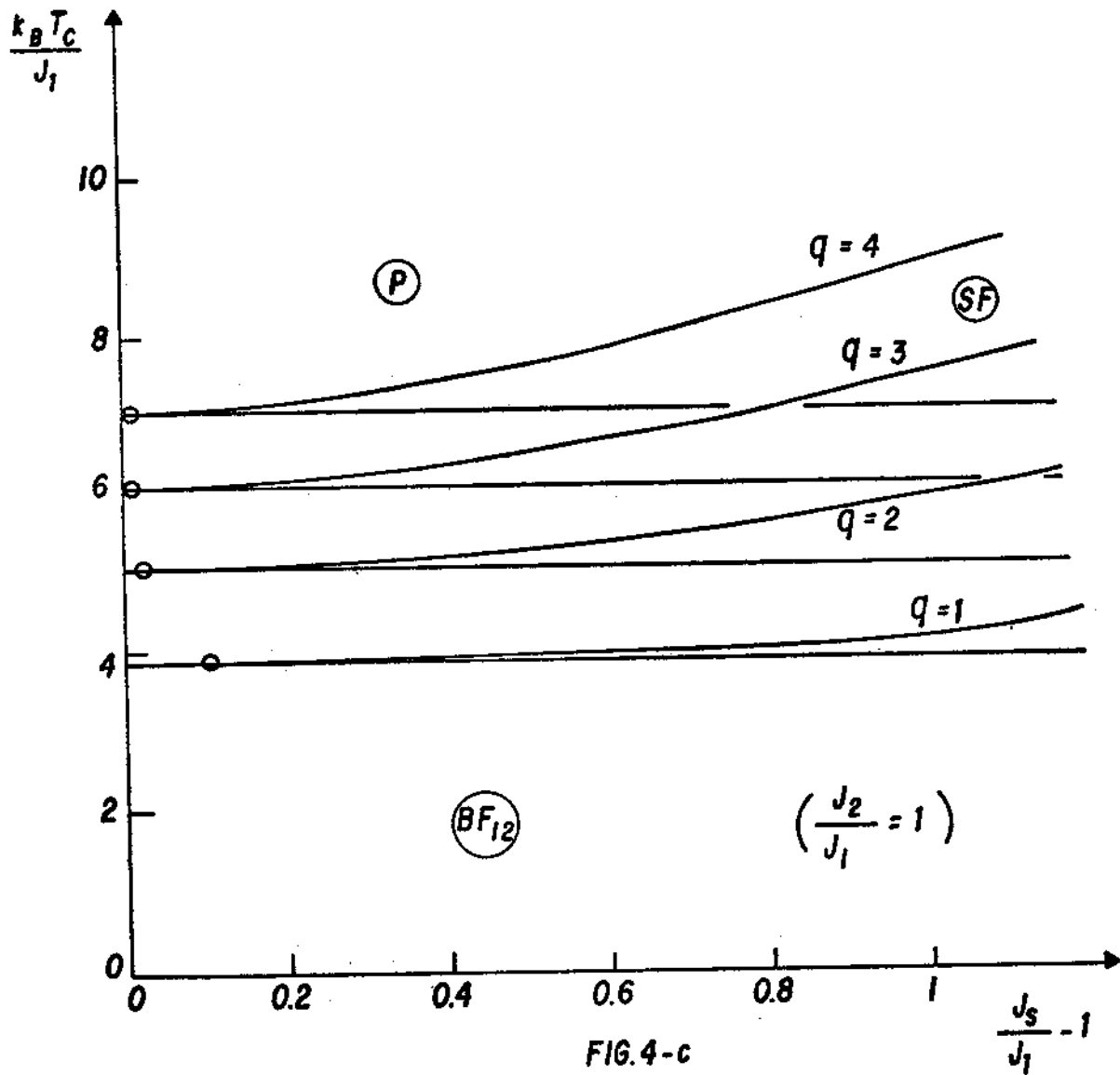


FIG.4-c

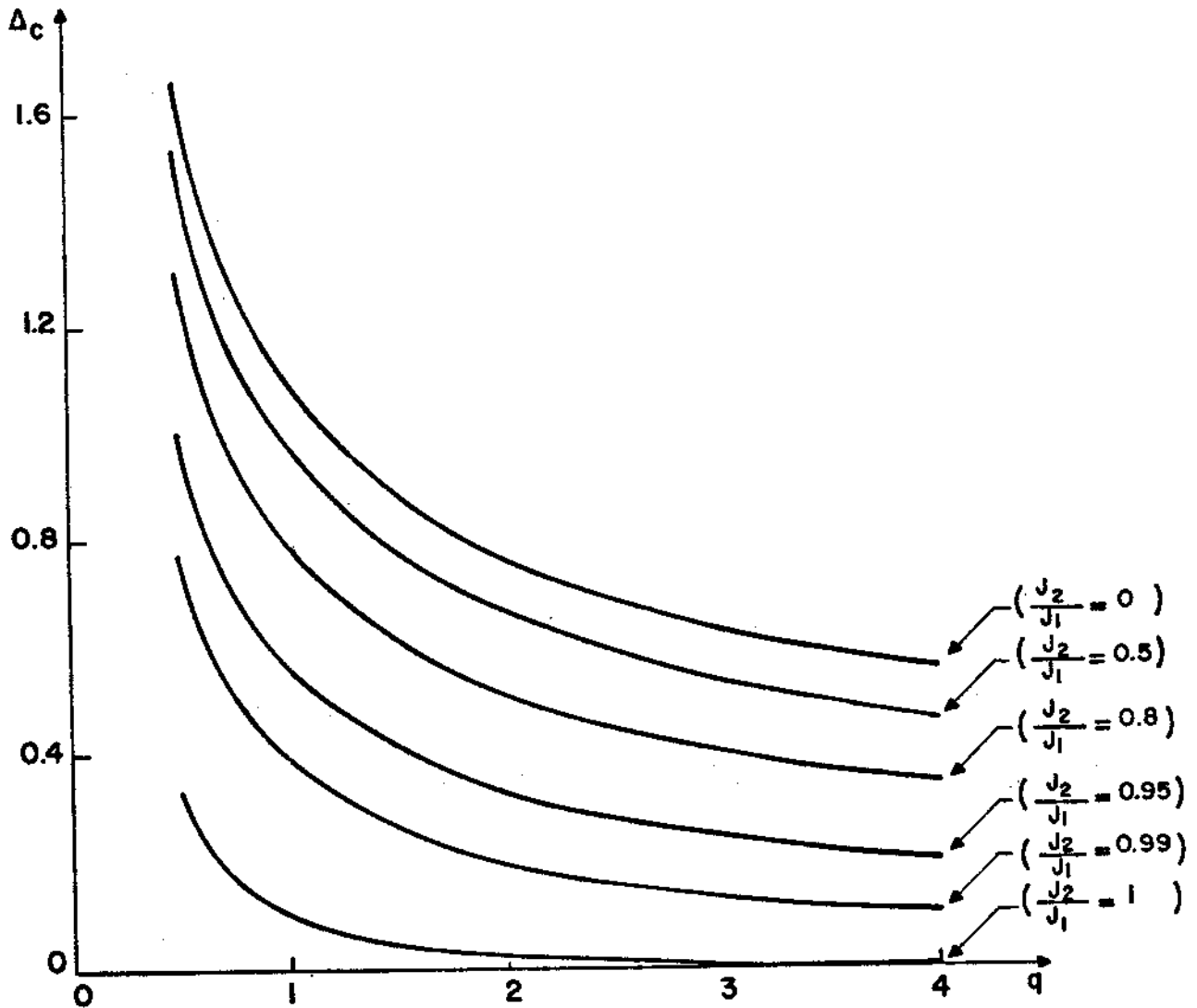


FIG.5

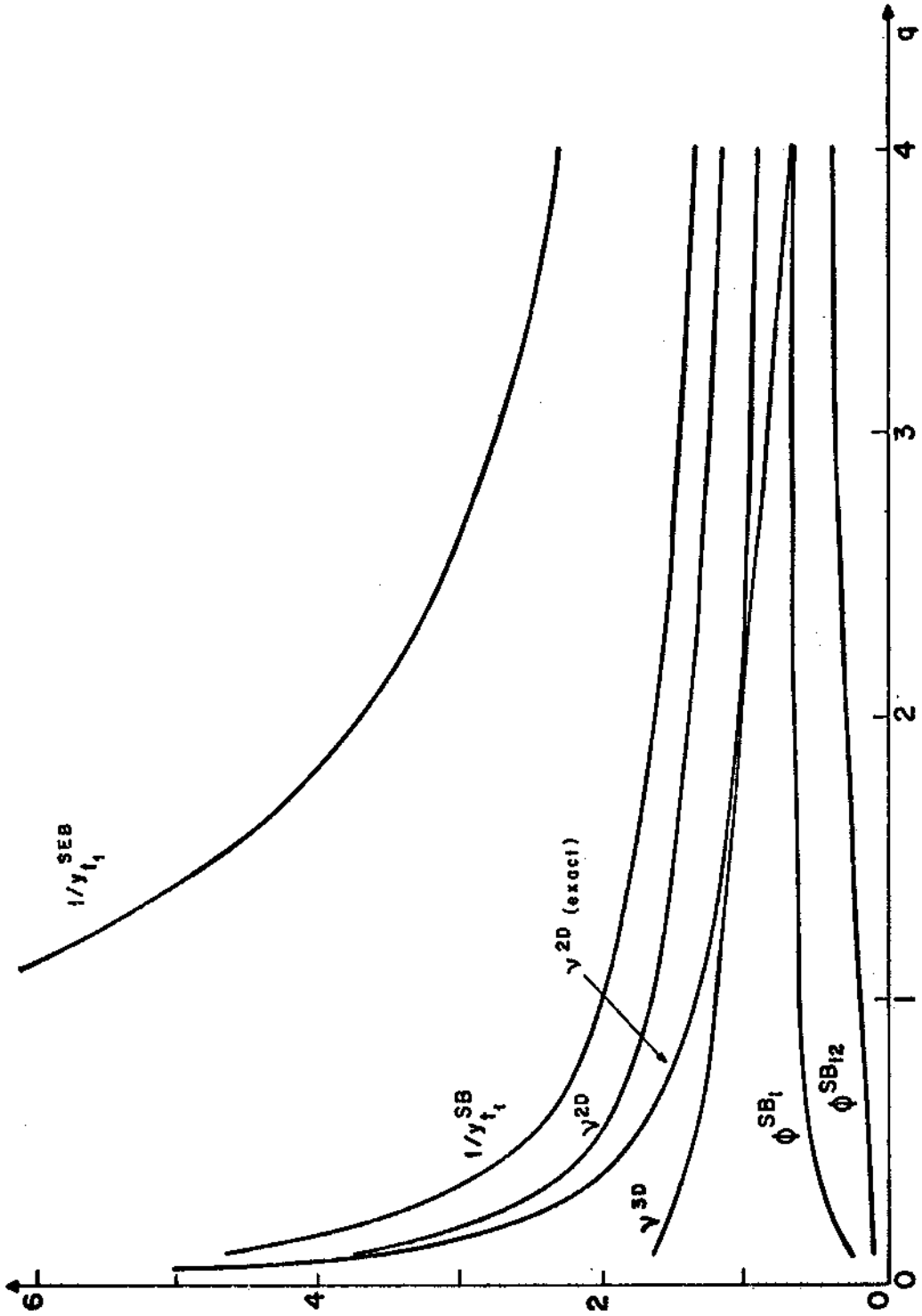


FIG. 6

TABLE 1

q	1/2	1.	2	3	4
t^B	.2510 .2668 ^a	.2260 .247 ^b	.1949 .2181 ^c	.1750 .1966 ^d	.1607 -
t^{SB}	.5058 -	.4166 -	.3345 .3405 ^e .3208 ^f	.2911 -	.2626 -
t^S	.5858 .5858 ^g	.5 .5 ^g	.4142 .4142 ^g	.3660 .3660 ^g	.3333 .3333 ^g
v_{2D}	2.0481 1.7823 ^h	1.6510 4/3 ^h	1.3692 1 ^h	1.2440 5/6 ^h	1.1692 2/3 ^h
v_{3D}	1.3622	1.1988 .88 ⁱ	1.0410 .630 ^j	1.9599 -	.9092 -
$1/y_{t_1}^{SB}$	2.5320 -	2.0071 -	1.6236 -	1.4518 -	1.3497 -
$1/y_{t_1}^{SEB}$	9.8787 -	6.5141 -	3.6628 -	2.7227 -	2.2880 -
ϕ^{SB}	.5380 -	.5973 -	.6412 .68 ^l .56±04 ^m	.6612 -	.6736 -
ϕ^{SEB}	.1379 -	.1840 -	.2842 -	.3526 -	.3974 -
$\Delta_C (J_2/J_1=0)$	1.6678 1.473 ⁿ	1.1032 .899 ⁿ	.7620 .569 ⁿ .6±.1 ^o .5±.03 ^m	.6298 .458 ⁿ	.5574 -
$\Delta_C (J_2/J_1=.5)$	1.5323 -	.9832 -	.6568 -	.5323 -	.4649 -
$\Delta_C (J_2/J_1=1)$.3321 -	.1011 -	.0204 -	.0077 -	.0030 -