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CRITICALITY OF THE SEMI-INFINITE POTTS FERROMAGNET: A RENORMALIZATION GROUP APPROACH

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ABSTRACT

Within a real space renormalisation group framework which uses rather sophisticated clusters, we discuss the phase diagram and the universality classes of a semi-infinite cubic-lattice q-state Potts ferromagnet. In particular, we study the influence, on the surface magnetism, of q and $\Delta \equiv J_S/J_B - 1$ (where J_s and J_B are respectively the surface and bulk coupling constants). The exact d=2 critical temperature T_c^{2D} is recovered for all values of q. The q-dependence of the value Δ_c above which surface magnetic order can exist even if the bulk is disordered, is calculated and, through a convenient extrapolation, reliable results are obtained (for the Ising particular case, i.e. q=2, we obtain the extrapolated value $\Delta_c \simeq 0.569$, which compares satisfactorily with the series result 0.6 ± 0.1 and the Monte Carlo one 0.50 ± 0.03). At the surface-bulk (SB) multicritical point we calculate the q-dependences of the critical amplitude A and the crossover exponent ϕ [defined in the $\Delta \to \Delta_c + 0$ limit through $(T_c^S(\Delta)/T_c^{3D} - 1) \sim A(\Delta/\Delta_c - 1)^{1/\phi}$, where $T_c^S(\Delta)$ and $T_c^{3D} \equiv T_c^S(\Delta_c)$ respectively are the surface and the bulk critical temperatures], as well as the correlation length critical exponent ν_1^{SB}. For the Ising particular case we obtain $\phi \simeq 0.641$ (which compares satisfactorily with the ε-expansion result 0.68 and the Monte Carlo one 0.56 ± 0.04), $A \simeq 0.4$ and $\nu_1^{SB} \simeq 1.623$ (as far as we know, no series or Monte Carlo results are available in the literature for A or ν_1^{SB}).

Key-words: Potts ferromagnet; Criticality; Surface effects; Renormalisation group.

I INTRODUCTION

Surface magnetism presents a quite rich criticality, which has been focused both theoretically (Binder and Hohenberg 1972, 1974, Binder and Landau 1976, Svrakic and Wortis 1977, Burkhardt and Eisenriegler 1977, 1978, Svrakic et al 1980, Reeve and Guttmann 1980, 1981, Reeve 1981, Diehl and Dietrich 1980, 1981 (a,b), 1983, Wortis and Svrakic 1982, Diehl et al 1982, Lam and Zhang 1983, 1984, Aguilera-Granja et al 1983, Sarmento et al 1984, Binder and Landau 1984) and experimentally (Pierce and Meier 1976, Alvarado et al 1982 (a,b)); for a recent review see Binder 1983.

It is by now relatively well established that if we consider a three-dimensional semi-infinite magnetic system with bulk and free surface ferromagnetic (nearest-neighbour) coupling constants J_B and J_S respectively (the interactions might be Ising, anisotropic Heisenberg, Potts or more complex ones), several types of phase transitions are present in the phase diagram (see Fig. 1). At sufficiently low temperatures, more precisely for $T < T_c^{3D} \equiv n^{3D} J_B/k_B$, where n^{3D} is a pure number ($n^{3D} \simeq 4.511$ for the spin 1/2 Ising model in simple cubic lattice), all the spin layers (starting from the free surface, corresponding to height $z=0$, to deep in the bulk, corresponding to a height $z \to \infty$) are magnetically ordered (*bulk ferromagnet*, noted BF); the z-profile of the layer magnetisations increases or decreases with increasing z for $J_S/J_B << 1$ or $J_S/J_B >> 1$ respectively, and is rather flat for the intermediate values of J_S/J_B. When T crosses the value T_c^{3D}, two important cases occur according to whether $\Delta \equiv J_S/J_{B-1} < \Delta_c$ or $\Delta > \Delta_c$, where Δ_c is a pure number satisfying $0 < \Delta_c < n^{3D}/n^{2D} - 1$ (the *strictly* two-dimensional critical temperature is given by $T_c^{2D} \equiv n^{2D} J_S/k_B$, where n^{2D} is a pure num ber; $n^{2D} \simeq 2.269$ for the spin 1/2 Ising model in square lattice, therefore, for semi-infinite simple cubic lattice, it is $0 < \Delta_c < 4.511/2.269 - 1 \simeq 0.988$; in fact, series and Monte Carlo studies for that model provide $\Delta_c \simeq 0.5-0.6$). In the first case ($\Delta < \Delta_c$), all the layer magnetisations $m(z)$ vanish *simultaneously* (see Binder and Landau 1984 and references therein) at T_c^{3D} ($m_B \equiv m(z \to \infty) \propto (T_c^{3D} - T)^{\beta^{3D}}$, β^{3D} being the standard three-dimensional critical expoent; $m_S \equiv m(z=0) \propto (T_c^{3D} - T)^{\beta_1}$ where β_1 is a new critical exponent in general different from both two-and three-dimensional values; the same law $(T_c^{3D} - T)^{\beta_1}$ holds for $0 < z < \infty$), and the *paramagnetic* phase (noted P) emerges. In the second case ($\Delta > \Delta_c$), m_B vanishes ($m_B \propto (T_c^{3D} - T)^{\beta^{3D}}$), whereas $m(0 \leq z < \infty)$ (possibly) present only a soft singularity, retaining a finite value (*surface ferromagnet*, noted SF) up to $T = T_c^S(\Delta)$, where they in turn vanish ($m(0 \leq z < \infty) \propto (T_c^S - T)^{\beta^{2D}}$, β^{2D} being the standard two-dimensional critical exponent), thus restoring the P phase; it is intuitive that T_c^S necessarily satisfies $T_c^S > T_c^{2D}$ (from where it comes that $\Delta_c < n^{3D}/n^{2D} - 1$, as stated before). The marginal case $\Delta = \Delta_c$ corresponds to a multicritical point (referred to as the surface-bulk point, noted SB), which is associated to a new universality class ($m_B \propto (T_c^{3D} - T)^{\beta^{3D}}$, but $m(0 \leq z < \infty) \propto (T_c^{3D} - T)^{\beta_1^{SB}}$, where the critical exponent β_1^{SB} is in general different from all three previously mentioned, namely β^{3D}, β^{2D} and β_1; note $T_c^S(\Delta_c) = T_c^{3D}$). In the neighbourhood of the SB point ($\Delta \to \Delta_c + 0$), one expects $(T_c^S(\Delta)/T_c^{3D} - 1) \sim \sim A(\Delta/\Delta_c - 1)^{1/\phi}$ (see Fig.1), which defines the critical amplitude A and the crossover exponent ϕ.

If we focuse the correlation length rather than the magnetisation, we expect, consistently with what said before, the following critical exponents: whereas the bulk correlation length diverges at T_c^{3D} as $|T-T_c^{3D}|^{-\nu^{3D}}$ for all values of Δ, the surface correlation length diverges, on the P - BF line ($\Delta<\Delta_c$), as $|T-T_c^{3D}|^{-\nu_1}$, on the multicritical point ($\Delta=\Delta_c$), as $|T-T_c^{3D}|^{-\nu_1^{SB}}$, and, on the P - SF line ($\Delta > \Delta_c$), as $|T-T_c^{S}(\Delta)|^{-\nu^{2D}}$. In addition to that, a soft singularity might be present in the surface correlation length on the BF-SF line ($\Delta > \Delta_c$).

The picture described above has already been satisfactorily (although partially) exhibited for the spin 1/2 Ising model in semi-infinite simple cubic lattice; in particular the following (reliable) numerical values have been obtained: $\Delta_c=0.6 \pm 0.1$ (series, Binder and Hohenberg 1974) and 0.50 ± 0.03 (Monte Carlo, Binder and Landau 1984), and $\phi=0.68$ (ε-expansion, Diehl and Dietrich 1980) and 0.56 ± 0.04 (Monte Carlo, Binder and Landau 1984). No such (relatively "hard") information is available for the q--state Potts ferromagnet, which recovers the spin 1/2 Ising model for q=2, and bond percolation for q=1 (Kasteleyn and Fortuin 1969). Some real space renormalisation group (RG) approaches have already been performed (Lipowsky 1982 (a,b), Lam and Zhang 1983, Tsallis and Sarmento 1984) but they stress the qualitative aspects of the problem more than the quantitative ones.

In the present paper we develope a RG calculation which precisely follows along the lines of Tsallis and Sarmento 1984; however we use (instead of the Migdal-Kadanoff-like cluster therein introduced) a recent cluster (da Silva et al 1984) which has already exhibited high performance for the simple cubic lattice. As a consequence of the quality of this cluster (whose size is such that quite heavy computation is involved), it has been possible to obtain *quantitatively* satisfactory q-dependence of Δ_c, ϕ, A,

ν_1^{SB} and $T_c^S(\Delta)$ (the results for $T_c^S(\Delta)$, and consequently for Δ_c and A, have been improved by performing a convenient extrapolation on top of the RG treatment).

In Section II we introduce the model and the formalism; in Section III we present the results, compare them with other available works, and discuss the bond percolation problem; finally we conclude in Section IV.

II MODEL AND FORMALISM

We consider the system whose Hamiltonian is given by

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

where <i,j> runs over all pairs of nearest-neighbouring sites of a semi-infinite simple cubic lattice; J_{ij} equals $J_S (J_S \geq 0)$ if *both* sites belong to the free surface, and equals $J_B (J_B > 0)$ otherwise. Let us introduce the following convenient variable (*thermal transmissivity*; Tsallis and Levy 1981 and references therein)

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

therefore

$$\Delta \equiv \frac{J_S}{J_B} - 1 = \frac{\ln \dfrac{1+(q-1)t_S}{1-t_S}}{\ln \dfrac{1+(q-1)t_B}{1-t_B}} - 1 \qquad (3)$$

We construct now a RG following along the lines of Tsallis and Sarmento 1984 (where two-terminal graphs are used). The recursive relation for the bulk transmissivity is given by

$$t_B' = f(t_B) \tag{4}$$

where $f(t_B)$ is the equivalent transmissivity associated with the cluster of Fig. 2 (see da Silva et al 1984); $f(t_B)$ is a very long ratio of polynomials in t_B with q-dependent coefficients which has been calculated through analytic implementation (in computer) of the Break-Collapse Method (Tsallis and Levy 1981). Analogously the recursive relation for the surface transmissivity is given by

$$t_S' = g(t_S, t_B) \tag{5}$$

where $g(t_S, t_B)$ is the equivalent transmissivity associated with the cluster of Fig. 3; to calculate $g(t_S, t_B)$ we have used once more the program just mentioned.

The flow, in the $t_B - t_S$ space, associated with Eqs.(4) and (5) yields, for arbitrary q, the phase diagram (and therefore Δ_c, ϕ and A) as well as the thermal critical exponents ν^{2D}, ν^{3D} and ν_1^{SB}.

III RESULTS

III.1 Flow diagram

The flow diagram is, for any value of q, of the type indicated in Fig.4. (qualitatively similar to that appearing in Tsallis and Sarmento 1984). In what follows we present the main features:

i) the trivial (stable) fixed points $(t_B,t_s)=(0,0)$, $(0,1)$ and $(1,1)$ respectively correspond to the P, SF and BF phases;

ii) the critical (semi-stable) fixed points $[(t_B,t_S)=(0,1/\sqrt{q}+1)]$ recovers the *exact* two-dimensional critical point;

iii) the critical (semi-stable) fixed points $B_1[(t_B,t_S) = (t_B^{3D}, t_S^{(1)})]$ and $B_2[(t_B,t_S) = (t_B^{3D},1)]$ respectively correspond to the cases where m_B and m_S vanish and do not vanish simultaneously; t_B^{3D} is, for let us say $q \leq 4$, about 10% lower than the best available values (see Table I);

iv) the multicritical (fully unstable) fixed point $SB[(t_B,t_S) = (t_B^{3D},t_S^{SB})]$ constitutes a universality class by itself;

v) the critical lines P-SF, P-BF and SF-BF belong to the universality classes respectively associated with the S, B_1 and B_2 fixed points.

III.2 Extrapolation

The P-SF critical line in the (t_B,t_S) space can be quantitatively improved through a very simple extrapolation procedure which consists in a streching of the t_B-axis (without any distortion of the t_S-axis) such that t_B^{3D} coincides, by construction, with the best available value (referred to as t_B^{3D}(exact)). In other words (t_B,t_S) becomes $(t_B\,t_B^{3D}(\text{exact})/t_B^{3D},\ t_S)$. This extrapolation consistently improves $T_c^S(\Delta)$, Δ_c and A (see Figs. 5 and 6). For example, Δ_c is given by Eq. (3) where t_B is replaced by t_B^{3D} (exact), and t_S is replaced by t_S^{SB}.

III.3 Critical exponents

The Jacobian matrix $M \equiv \partial(t_B', t_S')/\partial(t_B, t_S)$ evaluated at a particular fixed point of the present RG recursion is given by

$$M = \begin{pmatrix} \lambda_B & 0 \\ \mu & \lambda_S \end{pmatrix} \tag{6}$$

where λ_B, λ_S and μ are positive numbers, the first two being the eigenvalues. By evaluating M at the S, B_1, B_2 and SB fixed points, by taking into account that the RG linear expansion factor b equals 3 (Melrose 1983 (a,b) arguments indicate this value rather than b=2 previously adopted by da Silva et al 1984), and by using the following formulae (see, for example, Svrakic and Wortis 1977, Burkhardt and Eisenriegler, 1977, 1978)

$$\nu^{2D} = \ell n\ b/\ell n\ \lambda_S^S \tag{7}$$

$$\nu^{3D} = \ell n\ b/\ell n\ \lambda_B^{B_1} = \ell n\ b/\ell n\ \lambda_B^{B_2} = \ell n\ b/\ell n\ \lambda_B^{SB} \tag{8}$$

$$\nu_1^{SB} = \ell n\ b/\ell n\ \lambda_S^{SB} \tag{9}$$

$$\phi = \nu^{3D} / \nu_1^{SB} \tag{10}$$

we obtain the set of critical exponents we were looking for (see Table I and Fig. 7).

III.4 Bond percolation

It is worthly to note that through the isomorphism (Kasteleyn and Fortuin 1969) between the q → 1 Potts ferromagnet and bond percolation, and by identifying $p_B \equiv t_B(q=1)$ and $P_S \equiv t_S(q=1)$ (see, for example, Tsallis and Levy 1981), we can exhibit the phase diagram (see Fig. 8) of a geometrical problem, namely bonds present ("active") with probability p_s in the surface, and p_B in the bulk. Three phases are possible: the non percolating one (NP), the bulk percolating one (BP), and finally the surface percolating one (SP), where percolation has disappeared in the bulk but not in the surface. For $p_s > 0.417$, surface percolation becomes possible, even in the absence of bulk percolation (i.e., $p_B < 0.247$): in this case, the bulk helps the surface to percolate, *although not percolating itself*.

IV CONCLUSION

Within a real space renormalisation group which uses quite sophisticated clusters, we have substantially improved and completed the results recently obtained (Tsallis and Sarmento 1984) for the criticality of the semi-infinite q-state Potts ferromagnet in simple cubic lattice. The *exact* critical point is recovered in the two-dimensional asymptotic limit ($\Delta \equiv J_S/J_B - 1 \rightarrow \infty$) for all values of q.

The present RG three-dimensional critical points exhibit a discrepancy of about 10% with the best available results (series among others). This discrepancy is eliminated through a simple extrapolation. The phase diagrams ($k_B T/J_B$ vs.Δ) are consequently believed to be *quantitatively* quite reliable. From these phase diagrams we have extracted $\Delta_c(q)$ (value of Δ above which surface magnetism becomes possible even in the absence of bulk magnetism) and $A(q)$ (critical amplitude in the surface-bulk multicritical point). For the Ising particular case we have obtained $\Delta_c(2) \simeq 0.569$, to be compared with the series result (Binder and Hohenberg 1974) 0.6 ± 0.1, and the Monte Carlo one (Binder and Landau 1984) 0.50 ± 0.03; we have obtained also $A(2) \simeq 0.4$ (as far as we know, no other values are available for comparison at the moment in the literature; the same holds for $\Delta_c(q)$ and $A(q)$ for $q \neq 2$). The present treatment yields, in the $q \to 0$ limit, $\Delta_c(q) \simeq 2/\sqrt{q}$.

At the surface-bulk multicritical point, the present theory provides also the crossover exponent $\phi(q)$, and the thermal critical exponent $\nu_1^{SB}(q)$ (these quantities have been left free of any extrapolation). For the Ising case, we have obtained $\nu_1^{SB}(2) \simeq 1.623$, and $\phi(2) \simeq 0.641$; the latter is to be compared with the ε-expansion result 0.68 (Diehl and Dietrich 1980), and the Monte Carlo one 0.56 ± 0.04 (Binder and Landau 1984).

In contrast with the theory by Lipowsky 1982 (a,b), our treatment presents no indication of new phases for q high enough. This might be a real evidence, or a mathematical artefact of the approximation: we have no clear-cut arguments discriminating among these two possibilities.

All of the above results concern the simple cubic lattice and only hold for second order phase transitions. Consequently q has to be smaller than a critical value q_c (q_c=4 for strict ly two-dimensional systems (Baxter 1973, Straley and Fisher 1973); $q_c \simeq 3$ for three-dimensional systems (Jensen and Mouritsen 1979, Pytte 1980)). However the latent heat is small for $q \geq q_c$, and consequently the whole picture can be retained up to $q=4$.

An alternative point of view (see Berker and Ostlund 1979) the hierarchical lattice associated with the clusters (two-terminal graphs; see da Silva et al 1984) of Figs. 2 and 3 (see also Tsallis and Sarmento 1984). For this lattice, all the (non extrapolated) results presented in this work are exact, and hold for all $q \geq 0$.

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CAPTION FOR FIGURES AND TABLE

Fig. 1 - The simple cubic lattice Ising (q=2) phase diagram in the $k_BT/J_B - J_S/J_B$ space. BF, SF and P respectively denote the bulk ferromagnetic, surface ferromagnetic and paramagnetic phases. All three phases join at the SB (surface-bulk) multicritical point. The dot-dashed line corresponds to the limiting case where the d=2 surface is completely desconnected from the d=3 bulk.

Fig. 2 - Bulk RG cell; each bond is associated with the bulk coupling constant J_B; the arrows indicate the terminal nodes.

Fig. 3 - Free surface RG cell; the dashed (full) bonds are associated with the surface (bulk) coupling constant $J_S(J_B)$; the arrows are located at the terminal nodes.

Fig. 4 - q=2 RG flux diagram in the t (bulk transmissivity) - s (free surface transmissivity) space. ■, o and ● respectively denote trivial (stable), multicritical (unstable) and critical (semi-stable) fixed points. The dashed lines are indicative. The three phases are bulk ferromagnet (BF), surface ferromagnet (SF) and paramagnet (P).

Fig. 5 - q - evolution of the Δ - T phase diagram indicated in Fig. 1.

Fig. 6 - q - evolution of Δ_c and A (as well as of their extrapolated values, Δ_c^* and A^* respectively) as obtained in the present renormalization group. o, ♦, □ and ■ respectively locate Binder and Hohenberg 1974, Binder and Landau 1984, Sarmento et al 1982 and Mean Field Approximations results for Δ_c corresponding to the Ising model.

Fig. 7 - RG q - dependence of the correlation length critical exponents, ν^{2D}(d=2), ν_1^{SB} (at the surface-bulk multicritical point), ν^{3D}(d=3), as well as the crossover exponent ϕ. The dot-dashed line indicates den Nijs 1979 exact result for ν^{2D}. ♦ and ϕ respectively are Diehl and Dietrich

1980, and Binder and Landau 1984 results for ϕ, while o and ● respectively are Le Guillou and Zinn-Justin 1982 (q=2) and Heerman and Stauffer 1981 (q=1) results for ν^{3D}.

Fig. 8 - Bond percolation phase diagram in the p_S (surface probability) - p_B (bulk probability) space. Three phases are possible, namely the non percolating (NP), the bulk percolating (BP) and the surface percolating (SP) ones.

Table 1- Present RG and exact (or series) results for the critical points t_B and t_S (the RG recover the exact result for all q), exponents ν^{2D}(d=2), ν^{3D}(d=3), ν_1^{SB} (at the surface--bulk (SB) multicritical point) and ϕ (crossover exponent), the critical amplitude A and the adimensional parameter $\Delta_c \equiv J_S/J_B - 1$ which locates the SB multicritical point. * denotes our proposal (extrapolated); (a) Magalhães and Tsallis 1981; (b) Gaunt and Ruskin 1978; (c) Zinn-Justin 1979; (d) Jensen and Mouritsen 1979; (e) den Nijs MPM 1979; (f) Heerman and Stauffer 1981; (g) Le Guillon and Zinn--Justin 1980; (h) Diehl and Dietrich 1980; (i) Binder and Landau 1984; (j) Binder and Hohenberg 1974.

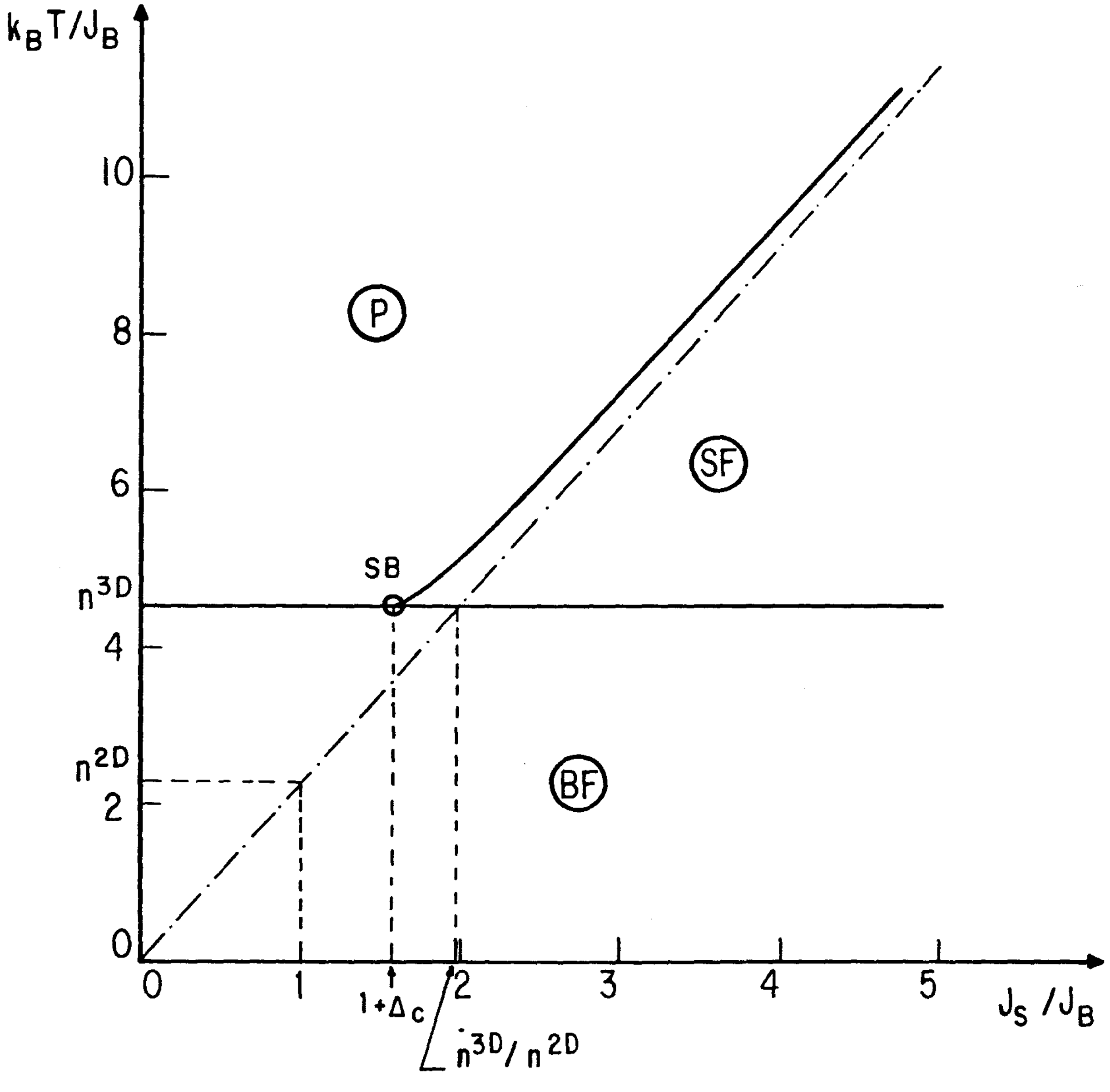

FIG. 1

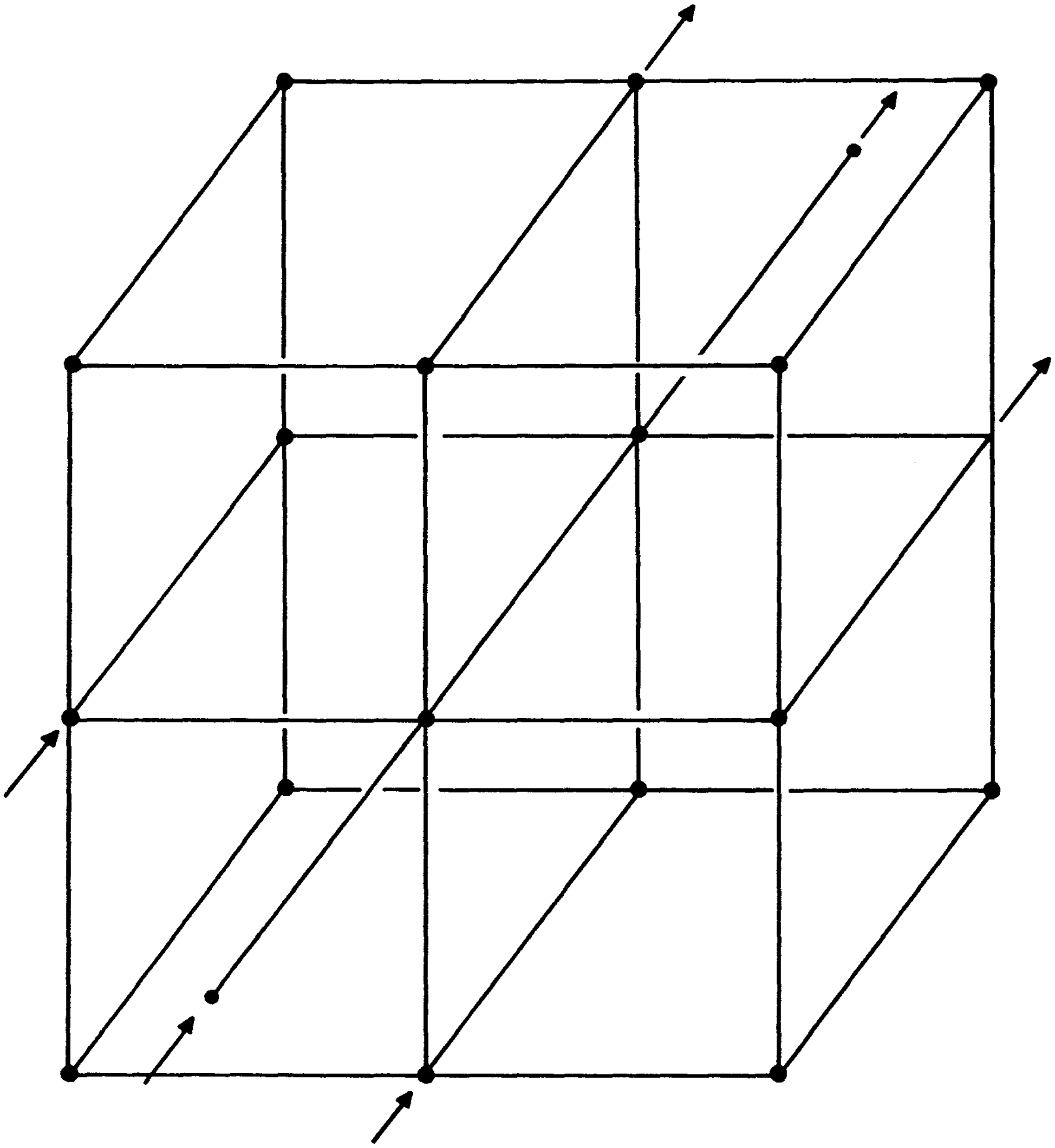

FIG.2

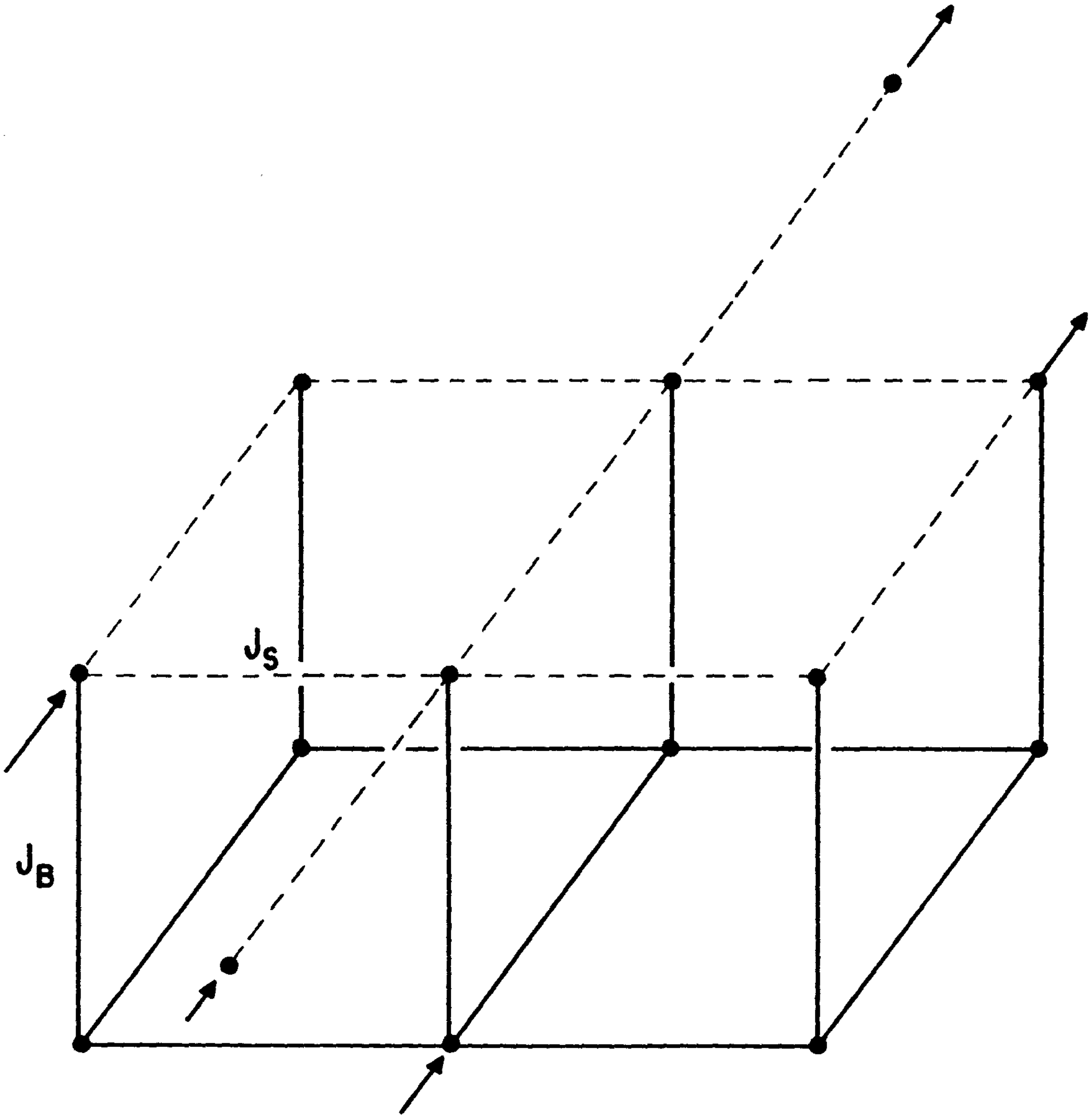

FIG.3

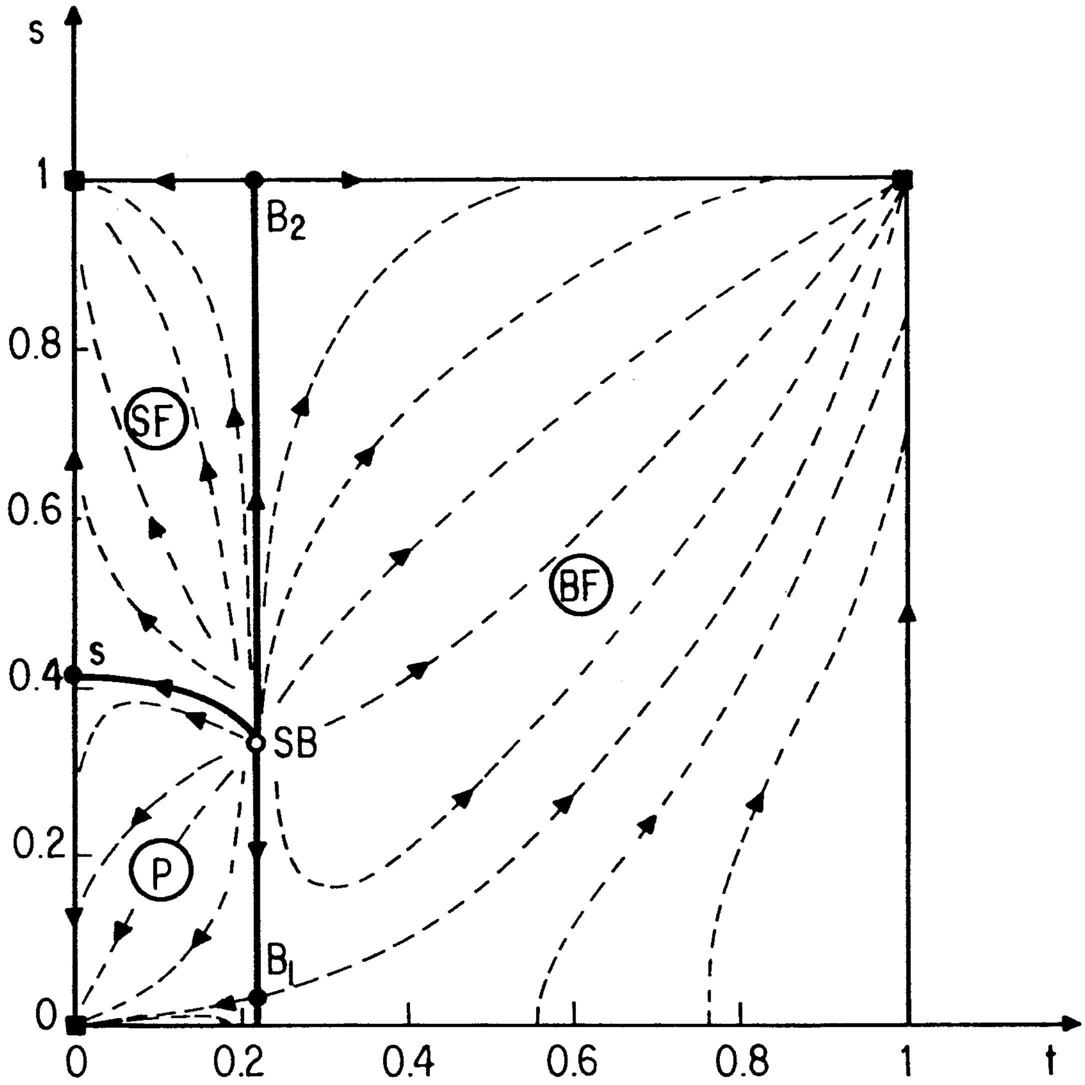

FIG.4

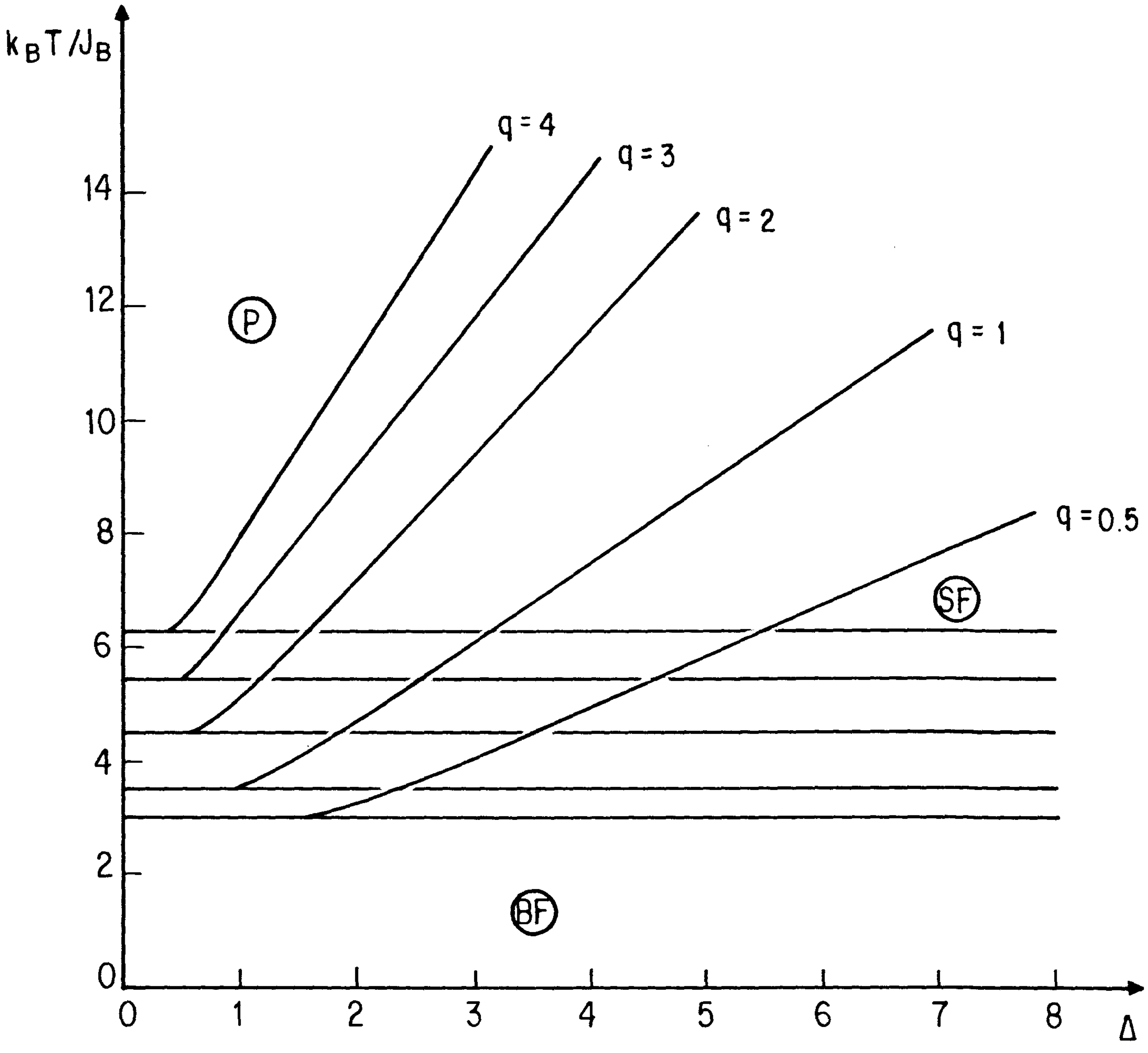

FIG. 5

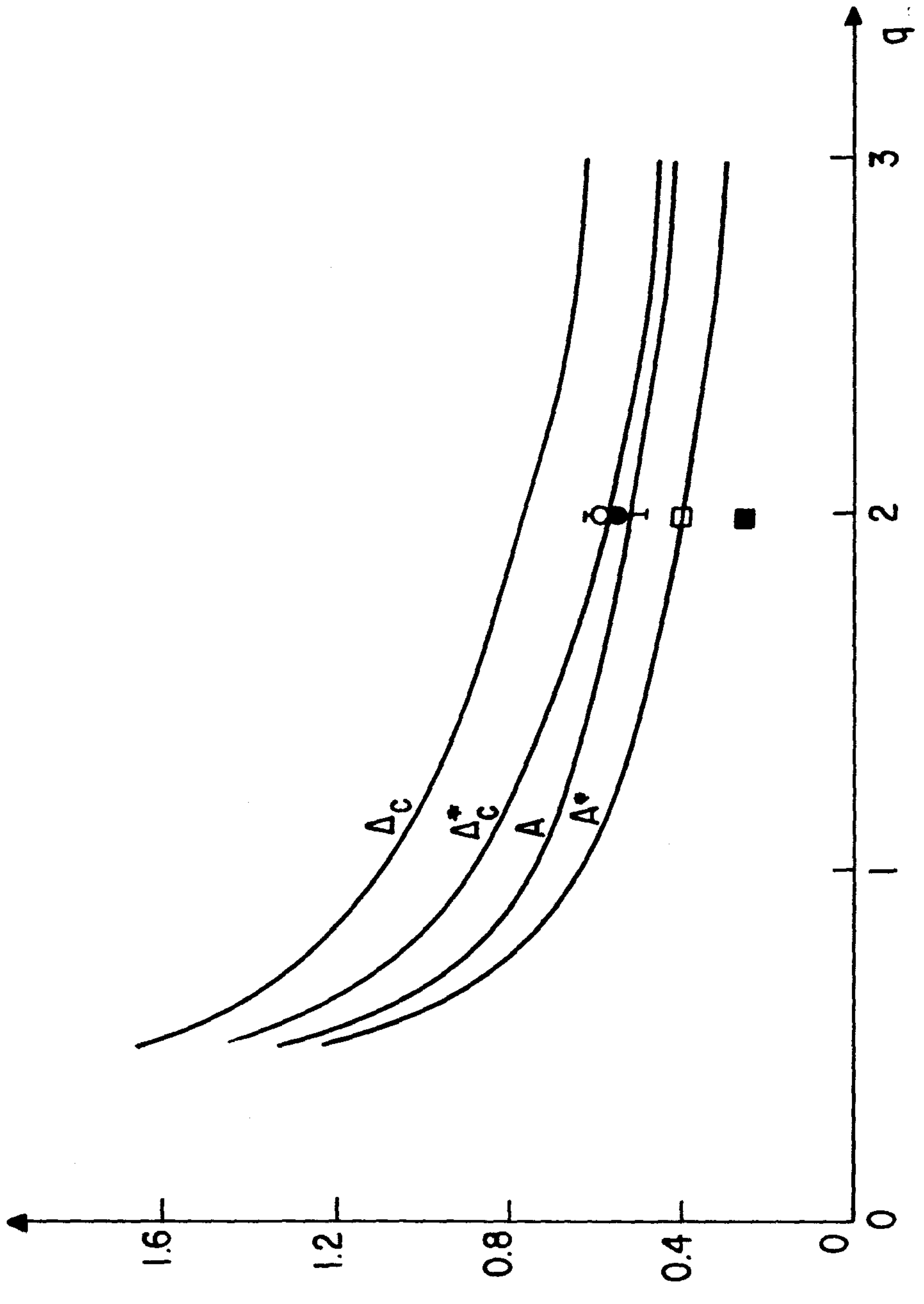

FIG.6

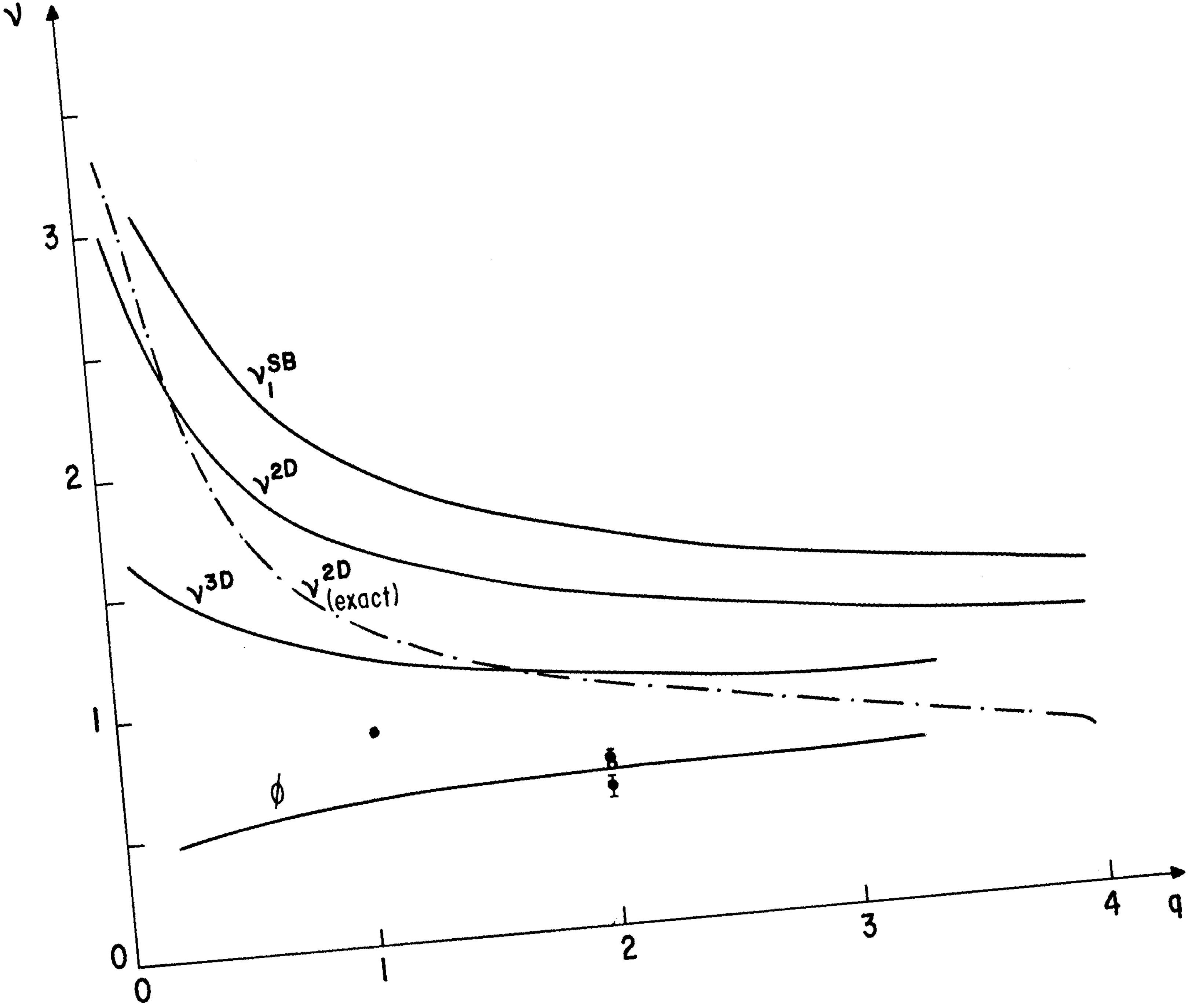

FIG. 7

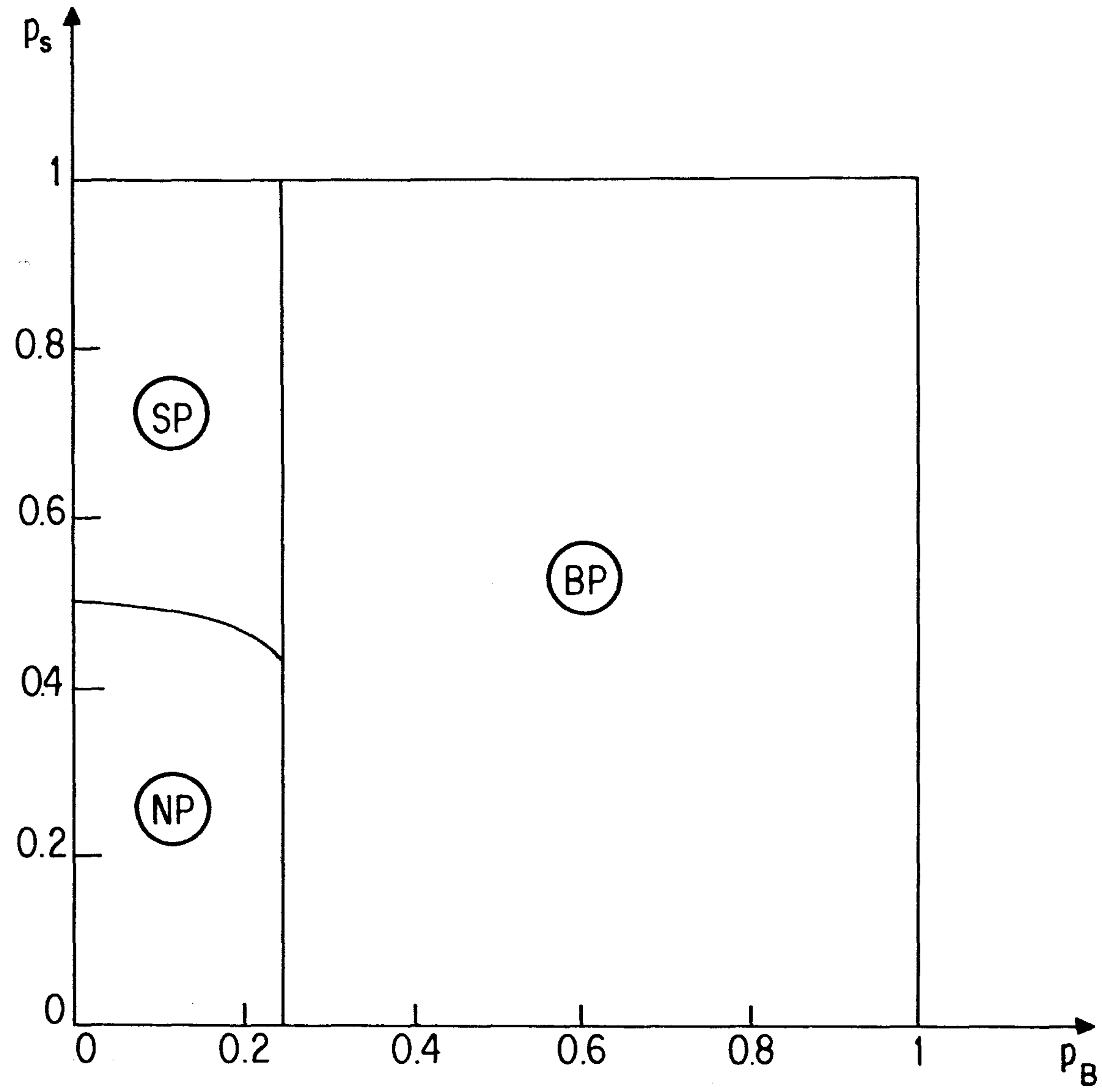

FIG.8

q	1/2	1	2	3
t_B	0.25102 0.2668[a]	0.22604 0.247[b]	0.19492 0.21811[c]	0.17505 0.1966[d]
t_S	0.50580	0.41658	0.33448	0.29195
ν^{2D}	2.035 1.772[e]	1.651 4/3[e]	1.369 1[e]	1.244 5/6[e]
ν^{3D}	1.361 —	1.198 0.88[f]	1.041 0.630[g]	0.960 —
ν_1^{SB}	2.531	2.008	1.623	1.452
ϕ	0.538 —	0.597 —	0.641 0.68[h] 0.56 ± 0.04[i]	0.661 —
A	1.3 1.1 *	0.7 0.6 *	0.5 0.4*	0.4 0.3 *
Δ_c	1.668 1.473* —	1.103 0.899* —	0.762 0.569* 0.6 ± 0.1[j] 0.5 ± 0.3[i]	0.630 0.458* —

TABLE 1