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ABSTRACT

Within a real space renormalisation group framework, we study the phase diagram of a semi-infinite cubic-lattice q-state Potts ferromagnet, in which the free surface coupling constant $J_S = (1+\Delta)J_B$ might be different from the bulk one J_B. We calculate the starting value $\Delta_c(q)$ above which surface order is possible even if bulk order is absent. Our results can be alternatively seen as *approximate* for the simple cubic lattice (as a matter of fact, the Ising value $\Delta_c(2)$ we obtain approaches the series result better than any other theory we are aware of; consequently $\Delta_c(q)$ is expected to be quite satisfactory even for $q \neq 2$) or as *exact* for a well defined diamond-like hierarchical lattice. In the $q \to 0$ limit, Δ_c diverges as $1/\sqrt{q}$.

Key-words: Surface; Potts model; Renormalisation group; Phase diagram.

I-INTRODUCTION

Surface magnetism is an interesting problem which, in the last decade, has received both theoretical (Mills 1971, 1973, Weiner 1973, Binder and Hohenberg 1974, Binder and Landau 1976, Burkhardt and Eisenriegler 1977, Lipowsky and Wagner 1981, Sarmento et al 1982, Wortis and Svrakic 1982, Lipowsky 1982, Lam and Zhang 1983, Kaneyoshi et al 1983, Tamura et al 1983, Selzer and Majlis 1983, Aguilera-Granja et al 1983, Sarmento et al 1984) and experimental (Pierce and Meier 1976, Alvarado et al 1982) attention (see Binder 1983 for a review). One of the simplest three-dimensional models that can be assumed is the spin 1/2 Ising one in semi-infinite simple cubic lattice (see Fig. 1), the coupling constant $J_S (J_S \geq 0)$ on the free surface being not necessarily equal to the bulk one $J_B > 0$ (it is convenient to introduce the adimensional parameter $\Delta \equiv J_S/J_B - 1$).

It is intuitive that for $0 \leq J_S \leq J_B$ the free surface acquires, for temperatures low enough, spontaneous magnetisation if and only if the bulk itself acquires such long range order; therefore only two phases are expected, namely the (bulk) ferromagnetic (BF) and the paramagnetic (P) ones. But for Δ high enough a third phase, namely the surface ferromagnetic (SF) one, becomes possible. In this phase, the free surface maintains a *finite* magnetisation which monotonously, goes to zero when one penetrates in the bulk. This phase is expected to occur at an intermediate range of temperatures, separating the low temperature regime (where the BF phase exists) from the high temperature regime (where the P phase is restaured). The SF phase is expected to be possible for $\Delta > \Delta_c$, where Δ_c is a still unknown finite value. A Mean Field Approximation (MFA) argument for the simple cubic lattice ($6J_B = 4J_S + J_B$) yields $\Delta_c = 1/4$ (Mills 1973). More sophisticated theories have provided more reliable values, namely 0.307 and 0.357 (cumulant and cluster renormalisation groups; Burkhardt and Eisenriegler 1977), 0.3068 and 0.3297 (effective field theories; Sarmento et al 1982, Kaneyoshi et al 1983, Tamura et al 1983), 0.4232 (improved effective field theory; Sarmento et al 1984), 0.816 (Bethe approximation; Aguilera-Granja et al 1983). These values are to be compared with the series one 0.6 ± 0.1 (Binder and Hohenberg 1974).

The central purpose of the present paper is to extend this type of calculation (phase diagram in the Δ-T space) to the q-state Potts ferromagnet, which recovers that of Ising for $q = 2$ (and which, for $q \to 1$, is isomorphic to random bond percolation; Kasteleyn and Fortuin 1969). In particular $\Delta_c(q)$ is calculated for arbitrary values of q, and $\Delta_c(2)$ is compared to the above mentioned values. To perform the present study we use a hierarchical-lattice-like real-space renormalisation group (RG) (see, for instance, Tsallis and Levy 1981 and references therein). This type of approach has proved its efficiency in a great variety of situations, commonly found in literature. Nevertheless, to the best of our knowledge this is the first time that this technique is applied to discuss surface magnetism for the d = 3 Potts model for arbitrary values of q.

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

II-MODEL AND FORMALISM

Let us consider the following Potts Hamiltonian:

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

where <i,j> run over all pairs of first-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. We introduce the following convenient variables (*thermal transmissivity*; Tsallis and Levy 1981 and references therein):

$$t \equiv \frac{1 - e^{-qJ_B/k_BT}}{1 + (q-1)e^{-qJ_B/k_BT}} \in [0,1] \tag{2}$$

$$s \equiv \frac{1 - e^{-qJ_S/k_BT}}{1 + (q-1)e^{-qJ_S/k_BT}} \in [0,1] \tag{3}$$

where T is the temperature and k_B the Boltzmann constant. From Eqs. (2) and (3) we obtain

$$\Delta \equiv \frac{J_S}{J_B} - 1 = \frac{\ln\frac{1+(q-1)s}{1-s}}{\ln\frac{1+(q-1)t}{1-t}} - 1 \tag{4}$$

To discuss the phase diagram corresponding to the present system we shall construct an appropriate RG. The cells we use are Mygdal-Kadanoff like, and are indicated in Fig. 2; the corresponding linear expansion factor b equals 3. These cells generate, through the standard procedure (illustrated in Fig. 3

for cells which are simpler), two different diamond-like hierarchical lattices. The transformation indicated in Fig. 2(a) approaches, through the standard bond-moving procedure, the bulk of our system. The transformation indicated in Fig. 2(b) is of the same type: the larger cell is assumed to lay on the free surface of our system in such a way that 1/3 of its "initial" 27 bonds are *outside* of the semi-infinite lattice, and therefore 9 bonds are absent (i.e. their transmissivities vanish).

The series and parallel composition laws of two arbitrary transmissivities t_1 and t_2 are respectively given (Tsallis and Levy 1981) by

$$t_s = t_1 t_2 \qquad \text{(series)} \tag{5}$$

and

$$\frac{1 - t_p}{1 + (q-1)t_p} = \frac{1 - t_1}{1 + (q-1)t_1}\,\frac{1 - t_2}{1 + (q-1)t_2} \qquad \text{(parallel)} \tag{6}$$

Consequently the RG recursive relations associated with Figs. 2(a) and 2(b) are given by

$$t' = \frac{1 - \left[\frac{1 - t^3}{1 + (q-1)t^3}\right]^9}{1 + (q-1)\left[\frac{1 - t^3}{1 + (q-1)t^3}\right]^9} \tag{7}$$

and

$$s' = \frac{1 - \left[\frac{1 - s^3}{1 + (q-1)s^3}\right]^3\left[\frac{1 - t^3}{1 + (q-1)t^3}\right]^3}{1 + (q-1)\left[\frac{1 - s^3}{1 + (q-1)s^3}\right]^3\left[\frac{1 - t^3}{1 + (q-1)t^3}\right]^3} \tag{8}$$

The flow, in the t-s space, determined by Eqs. (7) and (8) provides, for arbitrary q, the desired phase diagram (in particular Δ_c), the universality classes and the thermal and crossover critical exponents.

III- RESULTS

The RG flux diagrams we obtain are, for all values of q, as illustrated in Fig. 4 for $q = 2$. The evolution with q is indicated in Fig. 5 (in the t - s space) and in Fig. 6 (in the Δ-T space). A diagram such as that of Fig. 4 is rich in information:

i) the three trivial (stable) fixed points at the corners of the unitary square characterize the possible phases, namely the BF phase [$(t,s) = (1,1)$], the SF phase [$(t,s) = (0,1)$] and the P phase [$(t,s) = (0,0,)$];

ii) the two bulk semi-stable fixed points, namely B_1 [$(t,s) = (t_B, s_B)$] and B_2 [$(t,s) = (t_B, 1)$] are two equivalent mathematical representations for the $d = 3$ phase transition;

iii) the single surface semi-stable fixed point, namely S [$(t,s) = (0, s_S)$] corresponds to the $d = 2$ phase transition;

iv) the surface-bulk unstable fixed point SB [$(t,s) = (t_B, s_{SB})$] presents a multicritical nature, constituting a universality class by itself;

v) the critical line $t = t_B$ (excepting, as said before, for the SB point) belongs to the $d = 3$ universality class;

vi) the critical line joining the SB point and the S point belongs to the $d = 2$ universality class.

From the quantitative point of view, our main result, namely $\Delta_c(q)$ (value of Δ above which the SF phase becomes possible) is obtained by using Eq. (4) (with $s = s_{SB}$ and $t = t_B$), and is indicated in Fig. 7.

All the considerations made in this Section strictly apply only for standard second order phase transitions, i.e., for $q < 4$ for $d = 2$ (Baxter 1973, Straley and Fisher 1973), and $q < q_c$ (with $q_c \simeq 3$; Jensen and Mouritsen 1979, Pytte 1980) for d=3. However the $d = 3$ phase transition being only slightly first order for $q_c < q \leq 4$, the overall picture can be retained for $0 \leq q \leq 4$.

IV-CONCLUSION

We have studied some surface effects in a semi-infinite cubic-lattice q-state Potts ferromagnet, in which the surface coupling constant $J_S = (1+\Delta)J_B$ might be different from that (J_B) in the bulk. The phase diagram (in the Δ-T space, for instance; see Fig. 6) presents three phases, namely the bulk ferromagnetic (BF), the surface ferromagnetic (SF) and the paramagnetic (P) ones. The BF-P, BF-SF and P-SF critical lines join in a multicritical point which presents its own set of critical exponents (with a typical crossover to either $d = 2$ or $d = 3$ universality classes). The BF-P and BF-SF critical lines have the $d = 3$ set of critical exponents, and the P-SF critical line has the $d = 2$ one. From the quantitative standpoint we have calculated the q-evolution of Δ_c (value of

Δ above which the SF phase becomes possible). The result Δ_c = 0.7360 we obtain for the Ising model ($q = 2$) is quite satisfactory: it approaches the series result 0.6 ± 0.1 more than any other theory we are aware of. Consequently the results we obtain for other values of q (see Fig. 7) become satisfactorily reliable; in particular, in the $q \to 0$ limit, Δ_c diverges as $1/\sqrt{q}$. We are presently trying, by using better renormalisation group cells, to numerically improve $\Delta_c(q)$ with consistent improvements in the $d = 2$ and $d = 3$ results, in order to achieve numerical reliability for the critical exponents associated with the above mentioned multicritical point.

All the results we are discussing strictly hold for standard second order phase transitions, i.e. for $0 \leq q < 4$ for $d = 2$, and $0 \leq q < q_c$ (with $q_c \simeq 3$) for $d = 3$. However, the transitions being only slightly first order (small latent heat) in the range $q_c < q \leq 4$, we can retain, as a resonable approximation, the phase diagrams (Figs. 6 and 7) for the entire range $0 \leq q \leq 4$.

An alternative point of view is to consider the hierarchical lattice generated (through the standard procedure illustrated in Fig. 3) by the transformation of Fig. 2(b) (where the transformation of Fig. 2(a) has to be used also). In this case all our results are *exact* and hold for $q \geq 0$. In the $q \to \infty$ limit, Δ_c vanishes as $1/\ln q$.

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CAPTION FOR FIGURES

Fig. 1 - Cell of a semi-infinite simple cubic lattice. The full (dashed) bonds represent the bulk (free surface) couplings $J_B(J_S)$. On each site a q-state Potts random variable is localized.

Fig. 2 - Renormalisation group cell transformation: (a) for the bulk (transmissivity t); (b) for the free surface (transmissivity s). o represent the terminals, and ● represent the internal nodes (which are being decimated).

Fig. 3 - Illustration of the procedure for generating hierarchical lattices: (a) for the "bulk" medium; (b) for the "semi-infinite" medium. o (●) represents the terminal (internal) nodes.

Fig. 4 - q = 2 renormalisation group flux diagram in the t (bulk transmissivity)-s(free surface transmissivity) space. ■ denotes trivial (stable) fixed points; ● denotes critical (semi-stable) fixed points; o denotes the multicritical (unstable) fixed point. The dashed lines are indicative, Three phases are possible: bulk ferromagnetic (BF), surface ferromagnetic (SF), and paramagnetic (P).

Fig. 5 - q-evolution of the t-s phase diagram indicated in Fig. 4

Fig. 6 - Same q-evolution appearing in Fig. 5, but in the Δ-T space.

Fig. 7 - q-evolution of Δ_c as obtained in the present renormalisation group theory. The available q = 2 (Ising model) results are indicated as well: MFA (mean field approximation, Mills 1973), RG_1 and RG_2 (renormalisation groups

Burkhardt and Eisenriegler 1977), EFA (effective field approximations; EFA_1: Sarmento et al 1982 and Kaneyoshi et al 1983; EFA_2: Tamura et al 1983; EFA_3: Sarmento et al 1984), series (Binder and Hohenberg 1974), BA (Bethe approximation, Aguilera-Granja et al 1983).

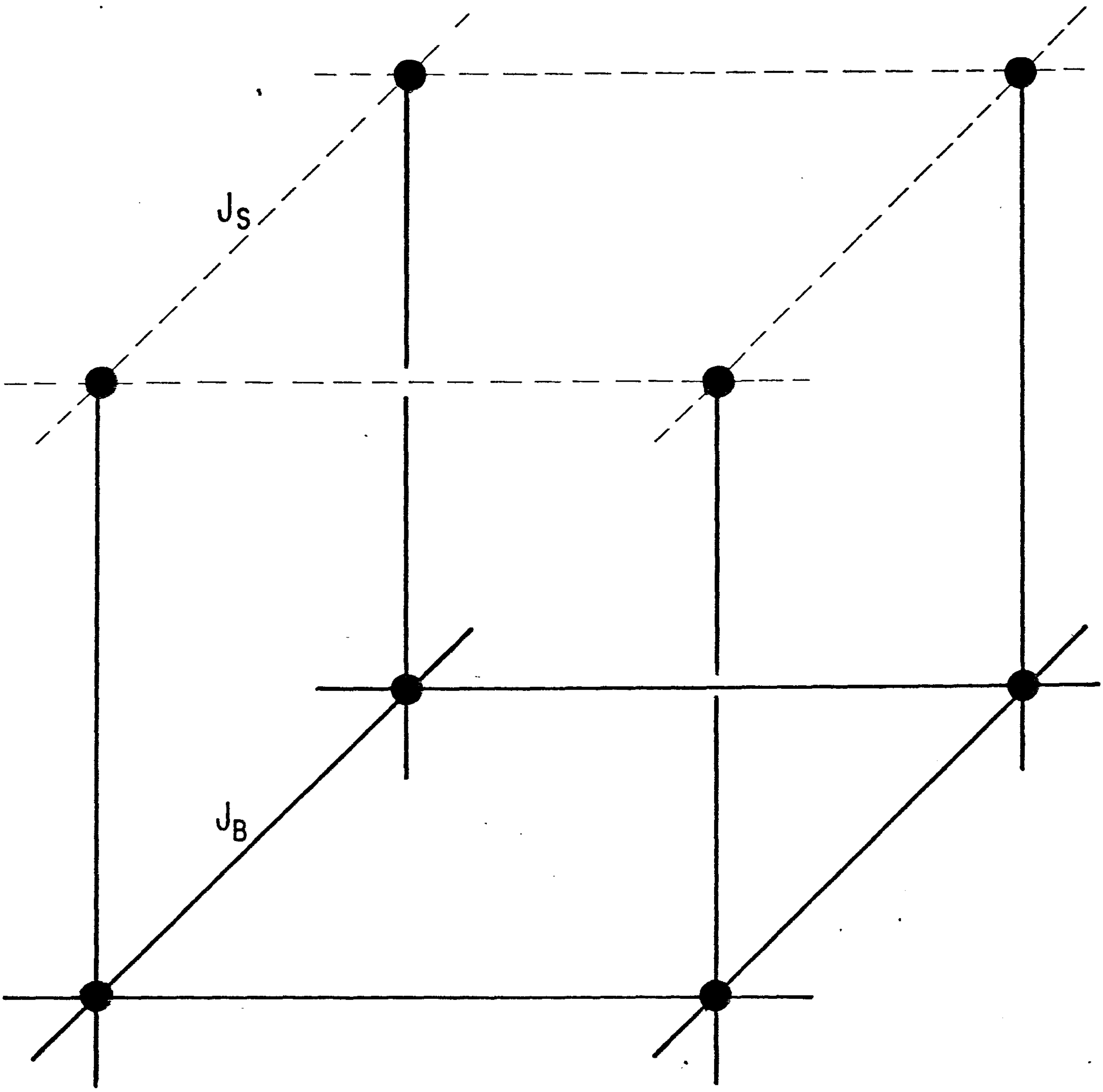

FIG.1

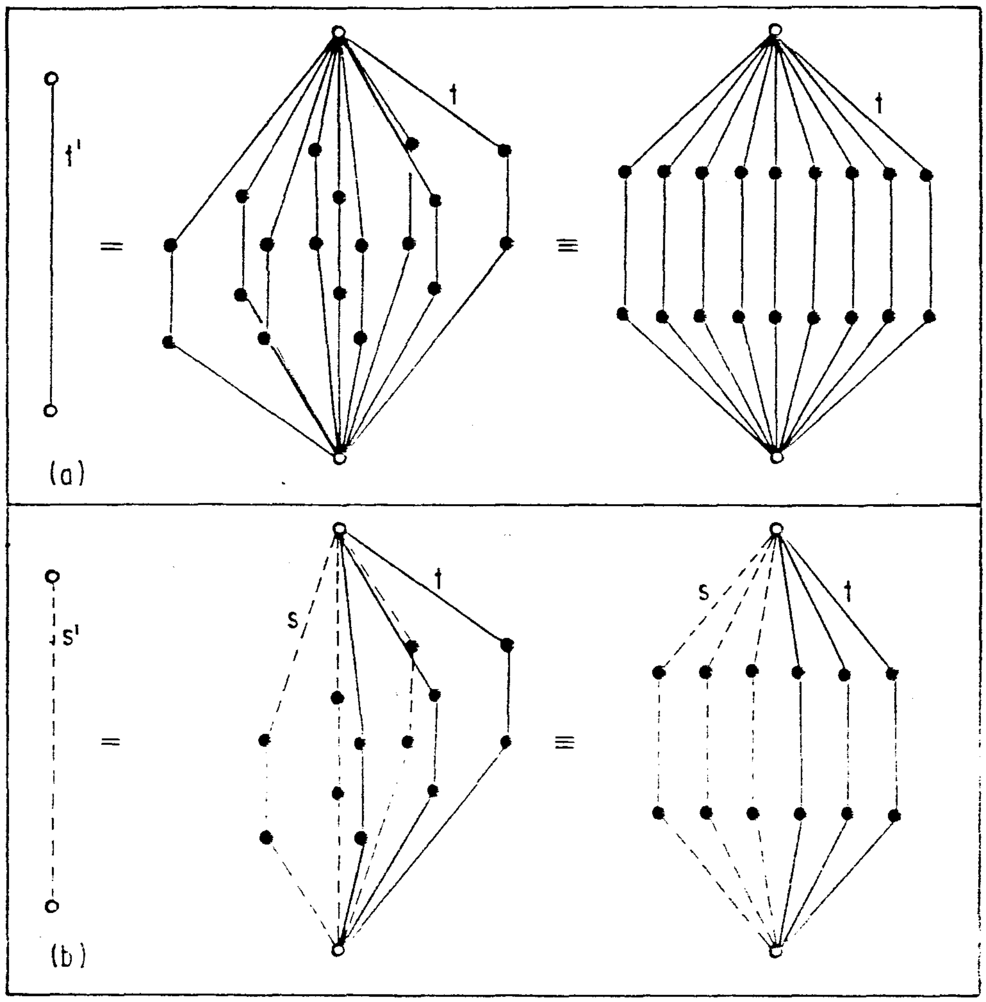

FIG.2

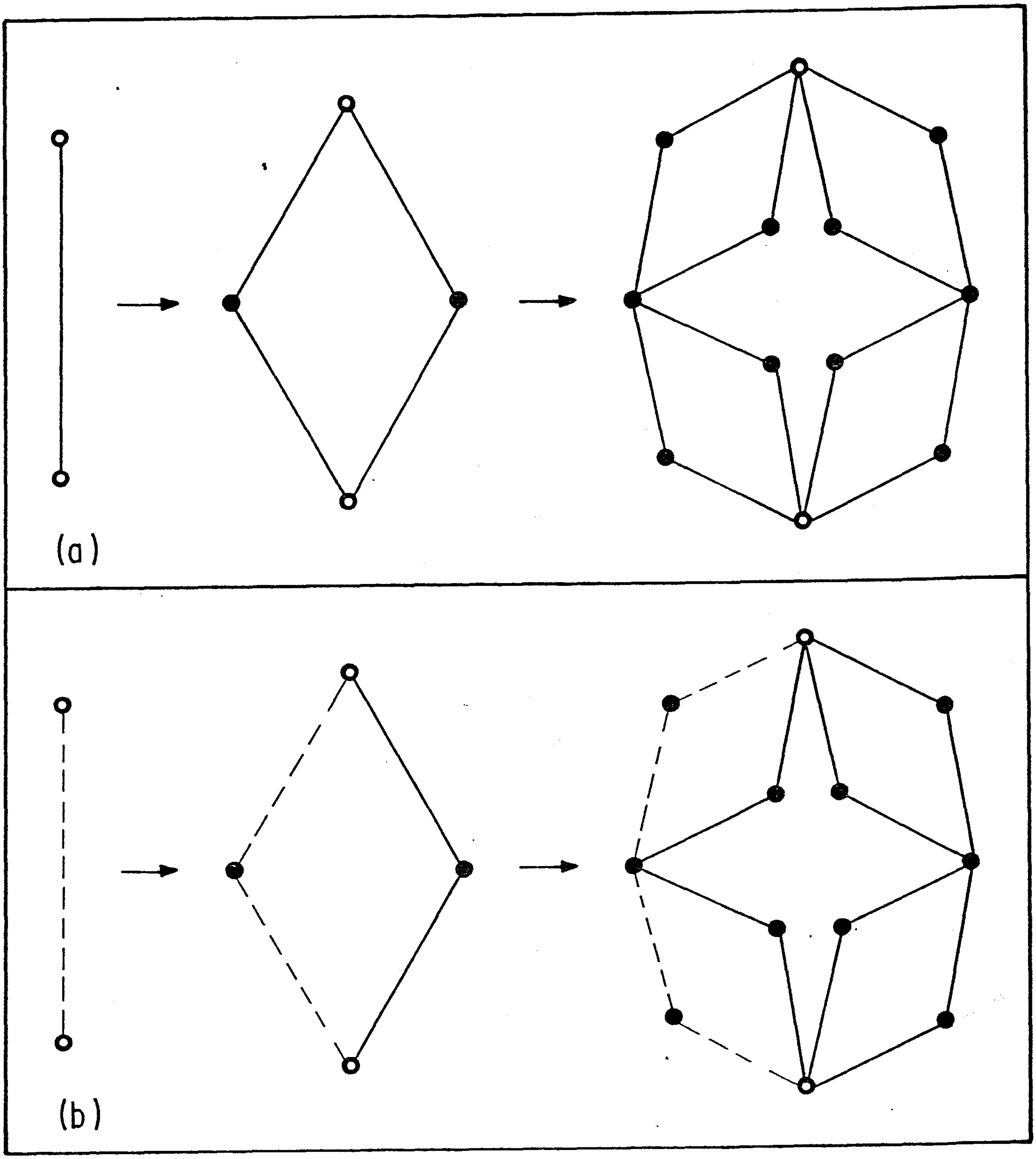

FIG. 3

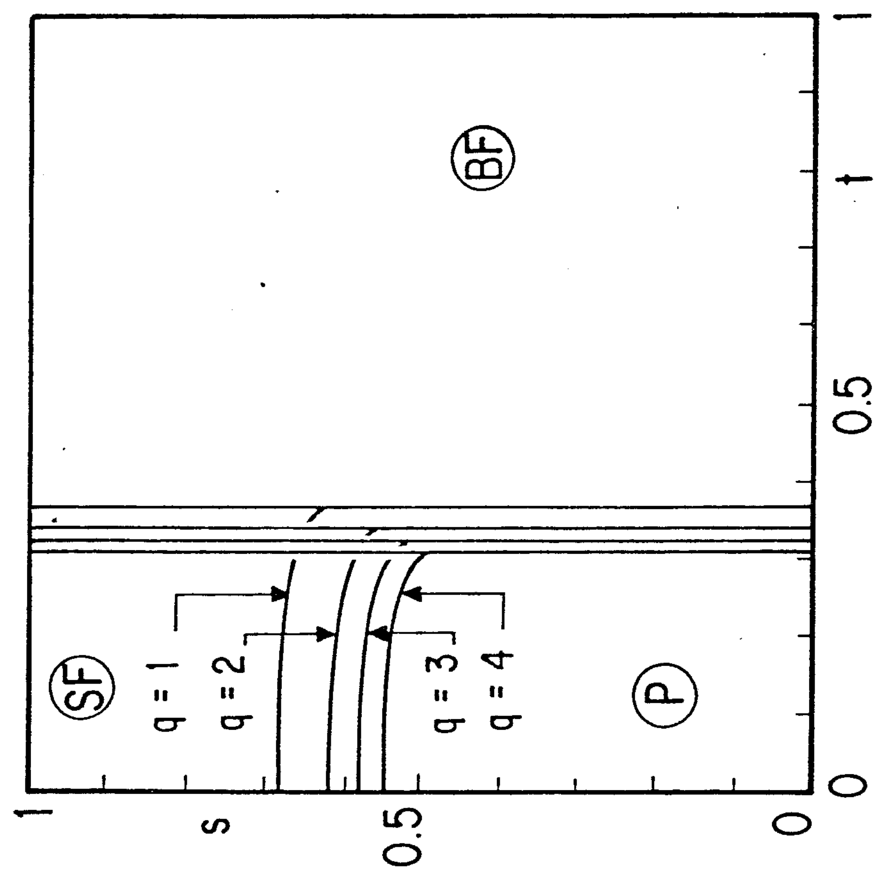

FIG.5

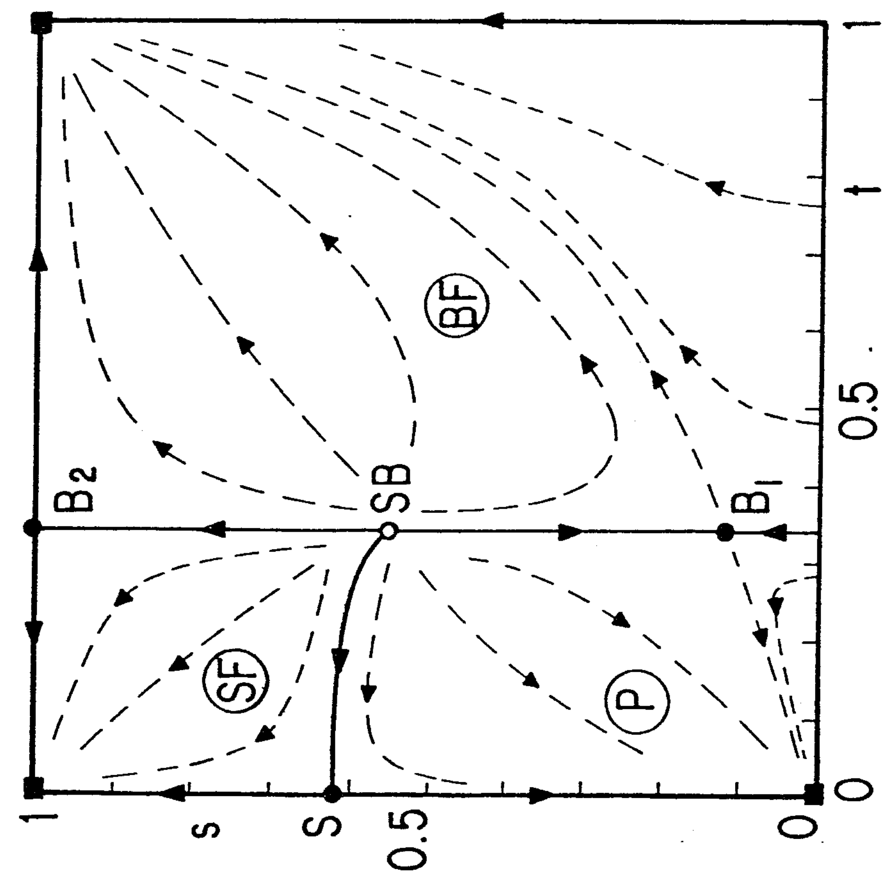

FIG.4

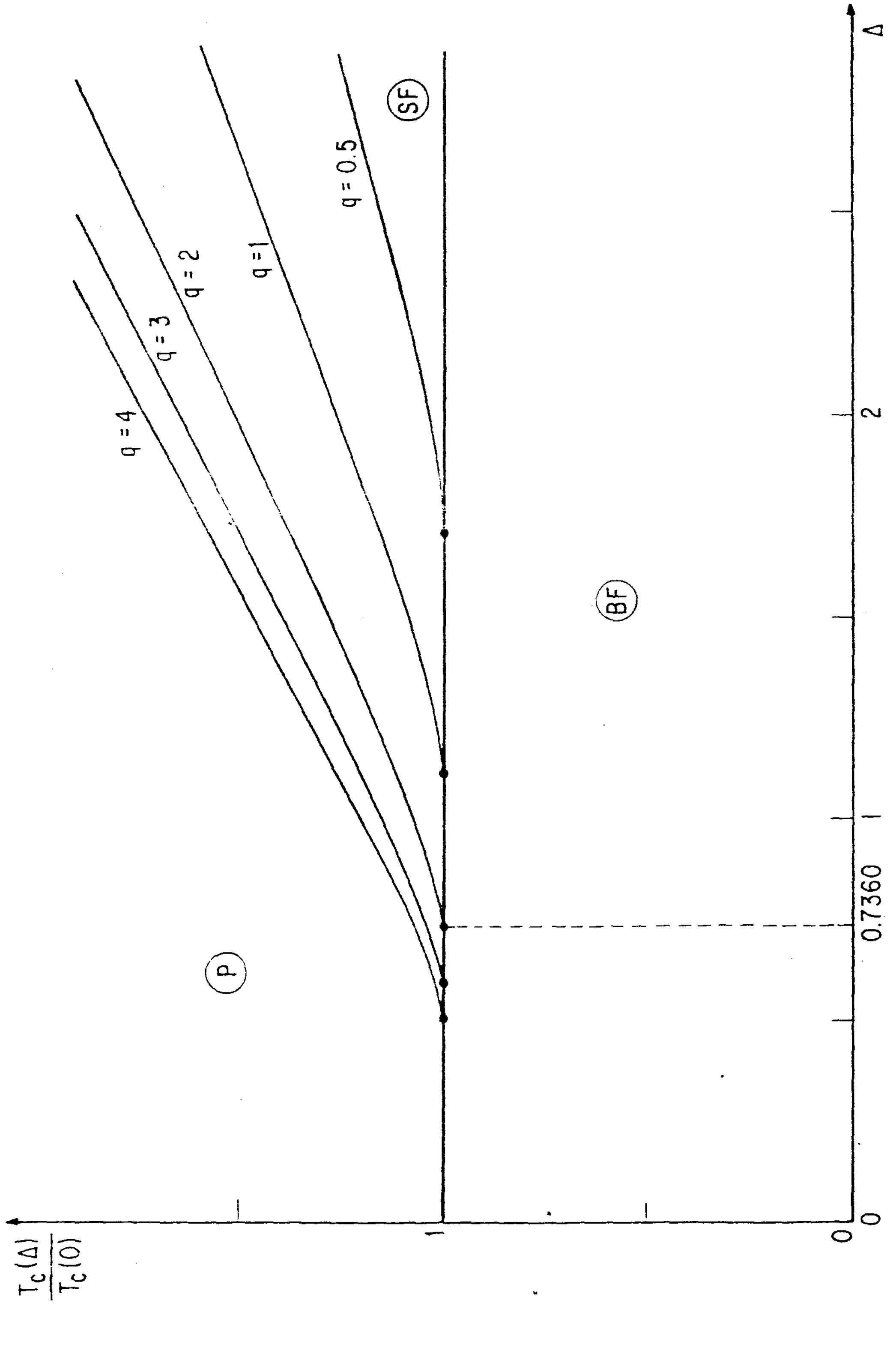

FIG. 6

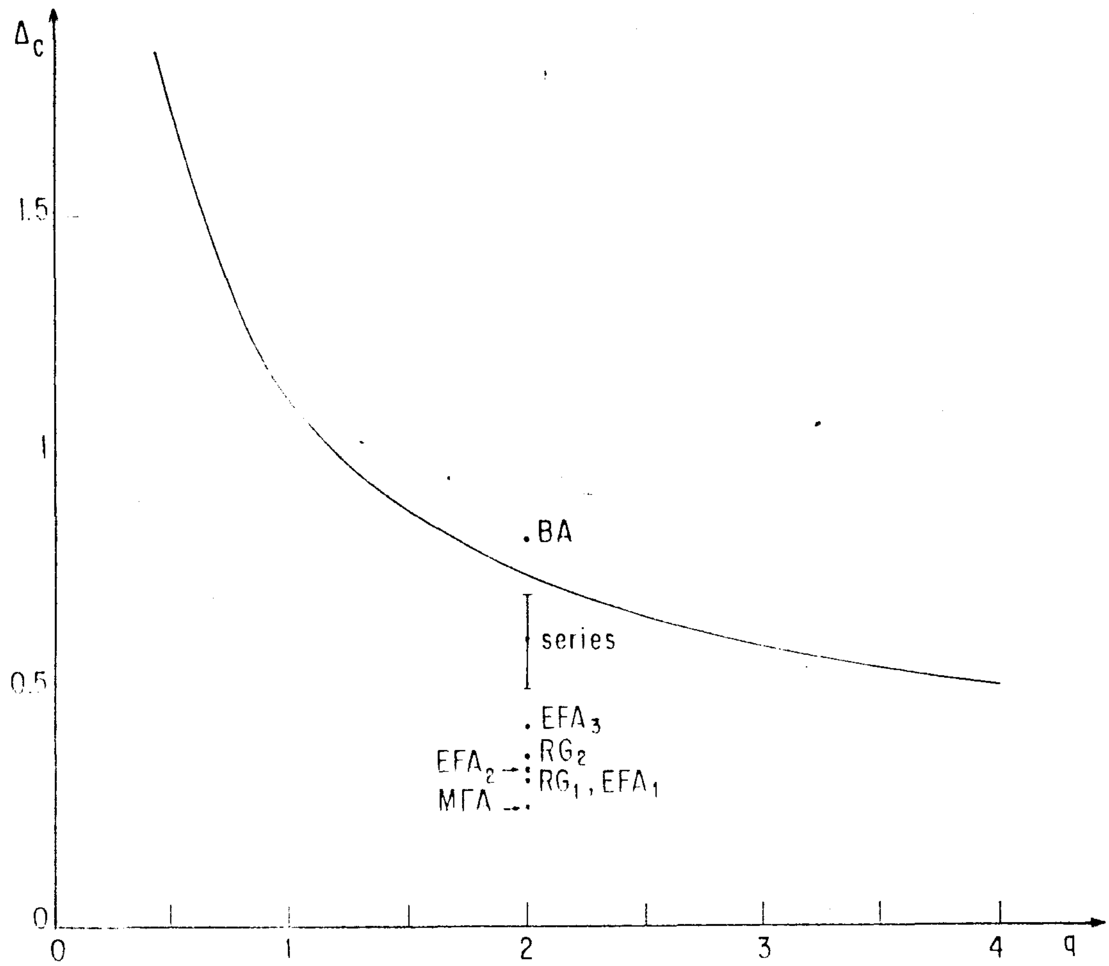

FIG.7