ISSN - 0029 - 3865

CBPF-NF-027/85

ANISOTROPIC HEISENBERG SURFACE ON SEMI-INFINITE ISING FERROMAGNET: RENORMALIZATION GROUP TREATMENT

by

Uriel M.S. Costa[1,2], Ananias M. Mariz[1,3]
and Constantino Tsallis[1]

[1]Centro Brasileiro de Pesquisas Físicas - CBPF/CNPq
Rua Dr. Xavier Sigaud, 150 - Urca
22290 - Rio de Janeiro, RJ - Brasil

[2]Departamento de Física
Universidade Federal de Alagoas
Cidade Universitária
57000 - Maceió, AL - Brasil

[3]Departamento de Física Teórica e Experimental
Universidade Federal do Rio Grande do Norte
Campus Universitário
59000 - Natal, RN - Brasil

ABSTRACT

We use a Migdal-Kadanoff-like renormalization group approach to study the critical behaviour of a semi-infinite simple cubic Ising ferromagnet whose (1,0,0) free surface contains anisotropic (in spin space) Heisenberg ferromagnetic interactions. The phase diagram presents three phases (namely the paramagnetic, the bulk ferromagnetic and the surface ferromagnetic ones) which join on a multicritical point. The location of this point is calculated as a function of the anisotropy. The various universality classes of the problem are exhibited.

Key-words: Surface magnetism; Anisotropic Heisenberg model; Phase diagram; Renormalization group.

PACS index: 05.50 +q; 64.60.Cn; 75.40.Dy; 75.40.Fa.

I INTRODUCTION

The appearence of surface effects in magnetic systems has been studied extensively during last years. Both theoretical and experimental efforts have been dedicated to the subject (see Ref. [1] for a recent review) because of its various applications as well as its intrinsic richness. A quite interesting and realistic particular situation is that where the surface magnetic interactions differ, in strength and even in nature, from the bulk ones. A possible experimental implementation of such a situation can be done by adsorbing, on top of the magnetic bulk, a layer of different magnetic atoms. Among the various theoretical approaches that can be used to discuss this type of system, the real-space renormalization-group (RG) is a quite convenient one as it hopefully provides a good description of its criticality [2-6].

In the present paper we discuss a spin 1/2 semi-infinite simple cubic lattice Ising ferromagnet with a (1,0,0) free surface (square lattice) whose interactions are of the anisotropic Heisenberg type. Our approach is a Migdal-Kadanoff-like RG which follows along the lines of Refs. [5] and [7]. In Section II we introduce the model and formalism, in Section III we present the results, and finally we conclude in Section IV; operational details are given in Appendix.

II MODEL AND FORMALISM

We consider the following Hamiltonian:

$$\mathcal{H} = -\sum_{<i,j>} J_{ij}\left[(1-\eta_{ij})(\sigma_i^x\sigma_j^x + \sigma_i^y\sigma_j^y) + \sigma_i^z\sigma_j^z\right] \qquad (1)$$

where $<i,j>$ runs over all pairs of first-neighbouring sites on a semi-inifinite simple cubic lattice with a (1,0,0) free surface (see Fig. 1); the σ's are the standard Pauli matrices; (J_{ij}, η_{ij}) equals $(J_B, 1)$ in the bulk $(J_B \geq 0)$, and equals (J_S, η) on the free surface $(J_S \geq 0,\ 0 \leq \eta \leq 1)$. The $\eta = 1$ and $\eta = 0$ limits respectively correspond to the Ising and isotropic Heisenberg models. We introduce the following convenient variables:

$$K_r \equiv J_r/k_B T \qquad (r = B, S) \qquad (2)$$

$$t_r \equiv \tanh K_r \qquad (r = B, S) \qquad (3)$$

$$\Delta \equiv J_S/J_B - 1 = K_S/K_B - 1 \qquad (4)$$

where T is the temperature and k_B the Boltzmann constant.

The phase diagram for the purely Ising case ($\eta = 1$) presents three phases [5,6,8-12], namely the *bulk ferromagnetic* (BF; both the bulk and the surface are magnetized), the *surface ferromagnetic* (SF; finite surface but vanishing bulk magnetizations), and the *paramagnetic* (P; no spontaneous magnetization) ones. We intend to study the evolution of the phase diagram when quantum aspects ($\eta \neq 1$) are introduced in the free surface. To perform this analysis we follow along the lines of Ref. 5 and construct a RG with Migdal-Kadanoff-like clusters [13,14] (see Fig. 2) for both surface and bulk bonds.

The partition function of each cluster is preserved through the renormalization. The clusters of Fig. 2 are reducible in sequencial series and parallel operations. This fact enables the quick (and exact) calculation [15] of the cluster of Fig. 2(a), all the bonds of which are Ising (i.e., classical) interactions. We also take advantage of this fact to make easier the calculation of the cluster of Fig. 2(b). In this case however, quantum effects are present and therefore the result is not exact; nevertheless it constitutes an excellent approximation [7].

For the bulk we obtain the following recursive relation:

$$K_B' = \frac{9}{2}\, \ell n\, \frac{3e^{-K_B} + e^{3K_B}}{3e^{K_B} + e^{-3K_B}} \tag{5}$$

which is equivalent to Eq. (7) of Ref. [5]. This equation admits two trivial (stable) fixed points (at $K_B = 0$ and $K_B = \infty$), as well as a critical (unstable) one (at a finite value of K_B).

The calculation of the recurrence for the surface is more complex. We first solve (see Appendix) a series array of three bonds (each of them associated with (K_S, η)), and obtain the equivalent parameters noted $K_3^S(K_S,\eta)$ and $\eta_3^S(K_S,\eta)$. If the three bonds are of the bulk type (i.e., Ising interactions), the equivalent parameters are $K_3^S(K_B,1)$ and $\eta_3^S(K_B,1) = 1$. We now approach the cluster of Fig. 2(b) by six parallel branches [being three of the type $(K_3^S(K_S,\eta),\ \eta_3^S(K_S,\eta))$ and three of the type $(K_3^S(K_B,1), 1)$] and obtain [7] the following recurrence:

$$K'_S = 3\left[K_3^S(K_S,\eta) + K_3^S(K_B,1)\right] \tag{6}$$

$$\eta' = \frac{3\left[K_3^S(K_S,\eta)\eta_3^S(K_S,\eta) + K_3^S(K_B,1)\right]}{K'_S} \tag{7}$$

Eqs. (5)-(7) formally close the construction of the RG: the flow they determine (in the (K_B,K_S,η) space for instance) yields the phase diagram and exhibits the relevant universality classes.

III RESULTS

The present RG provides the flow diagram indicated in Figs. 3(a) and 3(b) (in the (t_B,t_S,η) space), where we note two interesting invariant subspaces, namely $\eta = 1$ (purely Ising problem) and $\eta = t_B = 0$ (fully bulk-disconnected isotropic Heisenberg free surface). We also note the following facts: (i) three trivial (fully stable) fixed points, namely at $(t_B,t_S,\eta) = (0,0,1)$, $(1,1,1)$ and $(0,1,1)$, characterize the three phases of the system, respectively the P, BF and SF ones; (ii) five main semi-stable fixed points are present, namely at $(t_B,t_S,\eta) = (t_B^{3D},1,1)$ (characterizing the standard $D = 3$ universality class; t_B^{3D} corresponds to the finite critical temperature for the $D = 3$ Ising model), $(t_B^{3D},t_S^1,1)$ (characterizing the non trivial universality class associated with the surface phase transition occurring *simultaneously* with the bulk one; t_S^1 is a finite constant), $(0,t_S^{2D},1)$ (characterizing the standard $D = 2$ universality class; t_S^{2D} corresponds to the finite critical temperature for the D = 2 Ising model), $(t_B^{3D}, t_S^{SB}, 1)$ (characterizing the universality class of the multicritical line where all three P,BF and SF join together) and (0,1,0) (characterizing the universality class of the D=2 isotropic Heisenberg model, whose critical temperature vanishes); (iii) one fully unstable fixed point at $(t_B, t_S, \eta) = (t_B^{3D}, 1, 0)$ which is a special point on the above mentionned multicritical line, and determines by itself a new universality class. In short the universality classes of the problem are Ising-dominated, and the isotropic Heisenberg nature prevails only when no source of Ising symmetry exists at all. In Fig. 4 we present cuts of the critical surface (in the (Δ, T) space) for typical values of the anisotropy η. The location of the multicritical point as a function of η is indicated in Fig. 5; Δ_c is the value of Δ above which surface magnetic order can subsist even if the bulk is disordered). For $\eta = 1$ we recover the result of Ref. 5, i.e., $\Delta_c \simeq 0.74$, which compares reasonably well with the series result [8] 0.6 ± 0.1, the Monte Carlo one [11] 0.50 ± 0.03, and other RG result [6] 0.569.

IV CONCLUSION

We have used a simple renormalization group approach, with Migdal-Kadanoff-like clusters, to study surface critical effects in semi-infinite lattices of spins 1/2 which interact through standard Ising ferromagnetic couplings in the bulk, and through anisotropic Heisenberg ferromagnetic couplings on the free surface. The anisotropy η is assumed to vary between 0 (isotropic Heisenberg free surface) and 1 (purely Ising problem, relatively well discussed in the literature). The present results can alternatively be applied to the hierarchical lattice determined by the topological recurrence in Fig. 2, and for such system they are strictly *exact* for $\eta = 1$ [17] and *approximate* otherwise [7]; or be applied to the semi-infinite simple cubic Bravais lattice with a (1,0,0) free surface, and for such system they are, for all values of η, *approximate* (although qualitatively correct). The phase diagram presents three phases, namely the paramagnetic, the bulk ferromagnetic and the surface ferromagnetic ones. All three phases join, for a given value of η, on a multicritical point, whose location can be characterized by Δ_c (defined as the particular value of $\Delta \equiv J_S/J_B - 1$ above which surface ordering can exist even in the absence of bulk ordering). Δ_c monotonously and continuously decreases while η increases from 0 to 1; it attains its maximum at $\eta = 0$, where it presents a *finite* value ($\Delta_c \simeq 2.5$). This behaviour is in disagreement with recent results [16] obtained for the FCC lattice which suggest the existence of a *finite positive* critical value η_c below which the surface ferromagnetic phase cannot exist: the present treatment yields $\eta_c \leq 0$. Δ_c attains its minimum for $\eta = 1$, where we obtain $\Delta_c \simeq 0.74$ which compares satisfactorily with other values available in the literature.

As intuitively expected, most regions of the critical surface belong to the universality classes associated with the lowest symmetry of the problem, the Ising model in our case. In particular all points but one (corresponding to $\eta = 0$) of the multicritical line (on which all three phases join) belong to the bulk-surface Ising universality class; the $\eta = 0$ point constitutes a non trivial universality class by itself.

APPENDIX

We consider a series array of three (K,η) bonds and four sites (see Fig. 6, where (K',η') is to be identified with (K_3^S, η_3^S) of the main body of the paper). The array is characterized by the dimensionless Hamiltonian

$$\mathcal{H}_{1234} = K\Big[(1-\eta)(\sigma_1^x\sigma_3^x + \sigma_1^y\sigma_3^y + \sigma_3^x\sigma_4^x + \sigma_3^y\sigma_4^y + \sigma_4^x\sigma_2^x + \sigma_4^y\sigma_2^y) + (\sigma_1^z\sigma_3^z + \sigma_3^z\sigma_4^z + \sigma_4^z\sigma_2^z)\Big] \quad \text{(A.1)}$$

This array is renormalized into a single bond whose dimensionless Hamiltonian is given by

$$\mathcal{H}'_{12} = K'_0 + K'\Big[(1-\eta')(\sigma_1^x\sigma_2^x + \sigma_1^y\sigma_2^y) + \sigma_1^z\sigma_2^z\Big] \quad \text{(A.2)}$$

where K'_0, K' and η' are to be found as functions of (K,η) by imposing

$$e^{\mathcal{H}'_{12}} = \operatorname*{Tr}_{3,4} e^{\mathcal{H}_{1234}} \quad \text{(A.3)}$$

where $\operatorname*{Tr}_{3,4}$ denotes the trace over the internal sites of the series array.

Let us now outline the intermediate steps of the calculation which follows along the lines of Ref. [7]. We first expand both sides of Eq. [A.3], and obtain

$$e^{\mathcal{H}'_{12}} = a' + b'_{12}(\sigma_1^x\sigma_2^x + \sigma_1^y\sigma_2^y) + c'_{12}\sigma_1^z\sigma_2^z \qquad (A.4)$$

and

$$e^{\mathcal{H}_{1234}} = a + \sum_{i<j}\left[b_{ij}(\sigma_i^x\sigma_j^x + \sigma_i^y\sigma_j^y) + c_{ij}\sigma_i^z\sigma_j^z\right] + \sum_{\substack{i<j\\ k<\ell\\ (i,j)\neq(k,l)}}\left[d_{ij}(\sigma_i^x\sigma_j^x + \sigma_i^y\sigma_j^y)\sigma_k^z\sigma_\ell^z\right] + e(\sigma_1^x\sigma_2^x + \sigma_1^y\sigma_3^y)(\sigma_3^x\sigma_4^x + \sigma_3^y\sigma_4^y) + f\sigma_1^z\sigma_2^z\sigma_3^z\sigma_4^z \qquad (A.5)$$

These two expressions replaced into Eq. (A.3) immediately yield

$$a' = 4a \qquad (A.6)$$

$$b'_{12} = 4b_{12} \qquad (A.7)$$

$$c'_{12} = 4c_{12} \qquad (A.8)$$

By expressing $\mathcal{H}'_{12}$ in the basis which diagonalizes it we can easily find $K'_0 = K'_0(a',b'_{12},c'_{12})$, $K' = K'(a',b'_{12},c'_{12})$ and $\eta' = \eta'(a',b'_{12},c'_{12})$. By diagonalizing $\mathcal{H}_{1234}$ we can similarly find $a = a(K,\eta)$, $b_{12} = b_{12}(K,\eta)$ and $c_{12} = c_{12}(K,\eta)$. All these relations together with Eqs. (A.6) - (A.8) provide the relations $K'_0 = K'_0(K,\eta)$, $K' = K'(K,\eta)$ and $\eta' = \eta'(K,\eta)$ we were looking for. We obtain the following expressions:

$$K' = \frac{1}{4}\,\ell n\,\frac{F_3^2}{F_1F_2} \tag{A.9}$$

$$\eta' = 1 - \frac{\ell n(F_1/F_2)}{\ell n(F_3^2/F_1F_2)} \tag{A.10}$$

where

$$F_1 = \frac{1}{\lambda_1}\Big[(\lambda_1 - \omega + K)e^{\omega+\lambda_1} + (\lambda_1 + \omega - K)e^{\omega-\lambda_1}\Big] + \frac{(\lambda_2 - K - \omega)^2}{4\lambda_2(\lambda_2 - K)}\,e^{-K+2\lambda_2} +$$

$$\frac{(\lambda_2 + K + \omega)^2}{4\lambda_2(\lambda_2 + K)}\,e^{-K-2\lambda_2} + \sum_{i=1}^{3}\left(\frac{b_i+1}{x_i}\right)^2 e^{E_i} \tag{A.11}$$

$$F_2 = \frac{1}{\lambda_1}\Big[(\lambda_1 + \omega + K)e^{\omega+\lambda_1} + (\lambda_1 - \omega - K)e^{\omega-\lambda_1} + \frac{(\lambda_2 - K + \omega)^2}{4\lambda_2(\lambda_2 - K)}\,e^{-K+2\lambda_2} +$$

$$\frac{(\lambda_2 + K - \omega)^2}{4\lambda_2(\lambda_2 + K)}\,e^{-K-2\lambda_2} + \sum_{i=1}^{3}\left(\frac{b_i-1}{x_i}\right)^2 e^{E_i} \tag{A.12}$$

$$F_3 = \frac{\lambda_3 - \omega - K}{2\lambda_3}\,e^{-\omega+\lambda_3} + \frac{\lambda_3 + \omega + K}{2\lambda_3}\,e^{-\omega-\lambda_3} + \frac{\lambda_1 + \omega - K}{2\lambda_1}\,e^{\omega+\lambda_1} +$$

$$\frac{\lambda_1 - \omega + K}{2\lambda_1}\,e^{\omega-\lambda_1} + \frac{e^{-K}}{2} + \sum_{i=1}^{3}\left(\frac{a_i}{x_i}\right)^2 e^{E_i} \tag{A.13}$$

with

$$\omega \equiv K(1 - \eta) \tag{A.14}$$

$$\lambda_1 = \Big[(K - \omega)^2 + 4\omega^2\Big]^{1/2} \tag{A.15}$$

$$\lambda_2 = \Big[K^2 + \omega^2\Big]^{1/2} \tag{A.16}$$

$$\lambda_3 = \left[(K+\omega)^2 + 4\omega^2\right]^{1/2} \tag{A.17}$$

$$a_i = 2\left(\frac{E_i - K}{E_i + K}\right) \qquad (i = 1,2,3) \tag{A-18}$$

$$b_i = \frac{E_i - K}{2\omega} \qquad (i = 1,2,3) \tag{A.19}$$

$$x_i = \left[2(1 + a_i^2 + b_i^2)\right]^{1/2} \quad (i = 1,2,3) \tag{A.20}$$

where the E_i's are the roots of a cubic equation and are given by

$$E_1 = \alpha \cos\frac{\phi}{3} - K \tag{A.21}$$

$$E_2 = -\alpha \cos\frac{\phi+\pi}{3} - K \tag{A.22}$$

$$E_3 = -\alpha \cos\frac{\phi-\pi}{3} - K \tag{A.23}$$

with

$$\alpha \equiv 4\left[(K^2 - 5\omega^2)/3\right]^{1/2} \tag{A.24}$$

and

$$\phi \equiv \arccos\left[\frac{-2 \times 3^{3/2} K\omega^2}{(K^2 + 5\omega^2)^{3/2}}\right] \tag{A.25}$$

CAPTION FOR FIGURES

Fig. 1 - Semi-infinite simple cubic lattice. The dashed (full) lines represent the surface (bulk) bonds associated with (J_S, η) (with $(J_B, 1)$).

Fig. 2 - RG cell transformation: (a) for the bulk ($K_B \equiv J_B/k_BT$); (b) for the free surface ($K_S \equiv J_S/k_BT$). o and ● respectively represent the terminal and internal (being decimated) nodes.

Fig. 3 - RG flux diagram and critical surface: (a) in the (t_B, t_S, η) space ($t_r \equiv \tanh K_r$ $(r = B, S)$); (b) for the $\eta = 1$ subspace (purely Ising problem). ■ denotes trivial (fully stable) fixed points; ● denotes critical (semi-stable) fixed points; o denotes the multicritical (fully-unstable) fixed point. P, SF and BF respectively denote the para-, surface ferro- and bulk ferromagnetic phases. Dashed lines are indicative.

Fig. 4 - Fixed η cuts of the critical surface in the Δ-T space ($\Delta \equiv J_S/J_B - 1$).

Fig. 5 - η dependence of Δ_c.

Fig. 6 - RG transformation for a series array of three bonds.

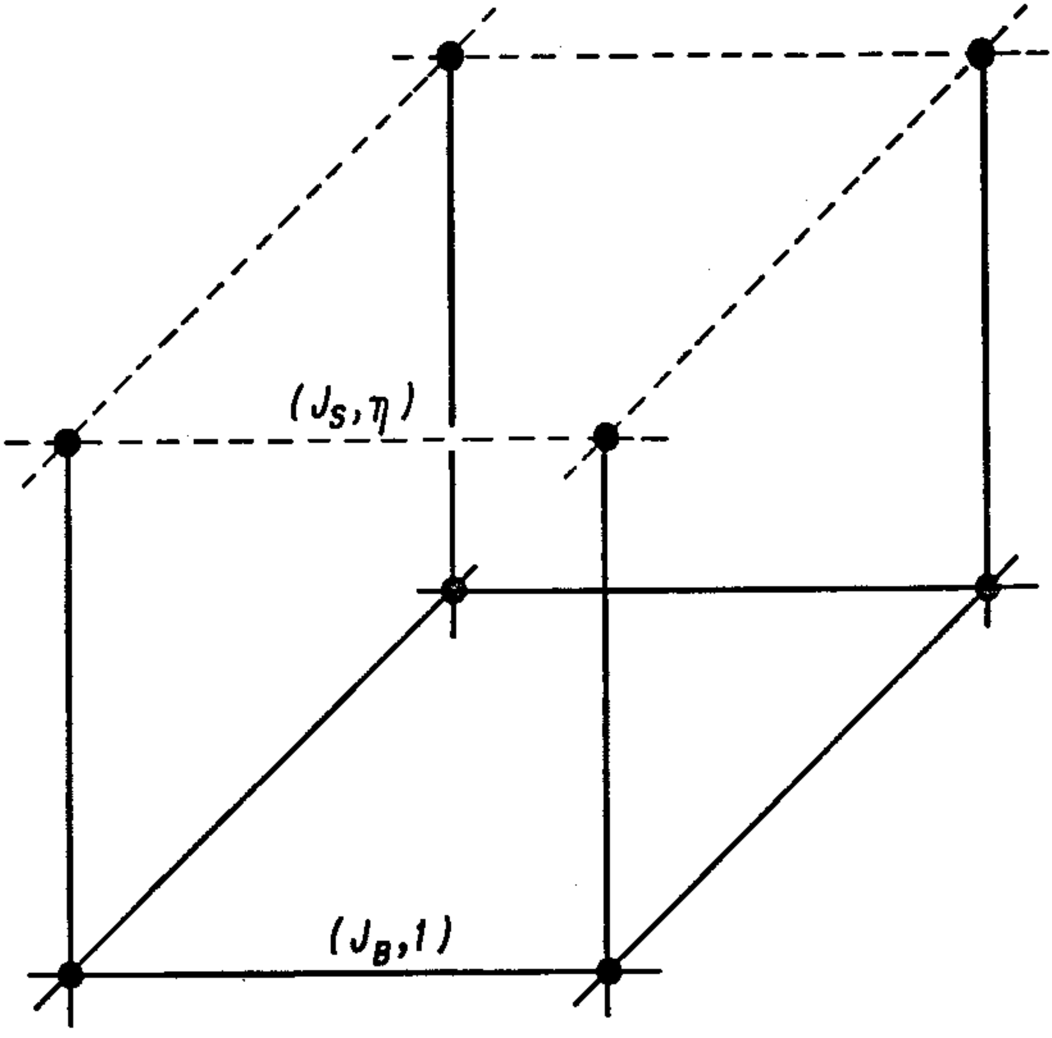

FIG.1

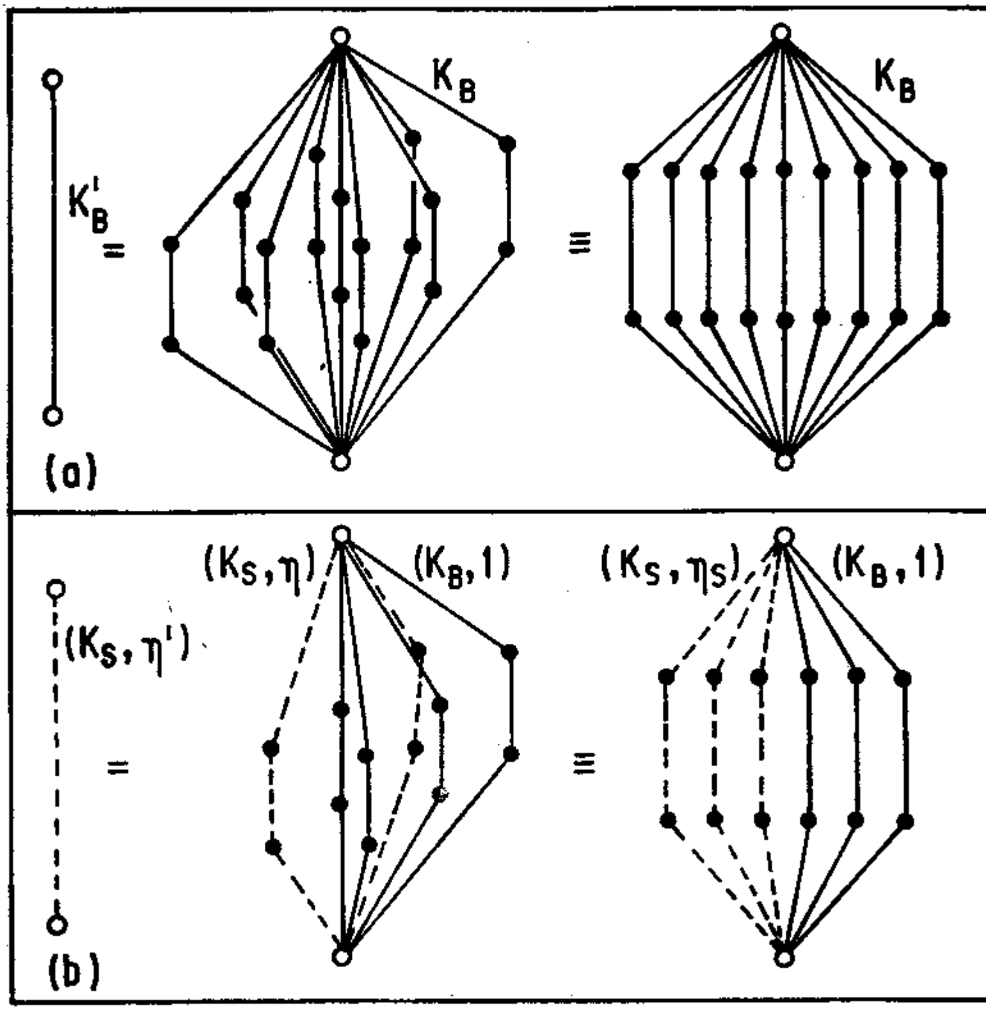

FIG. 2

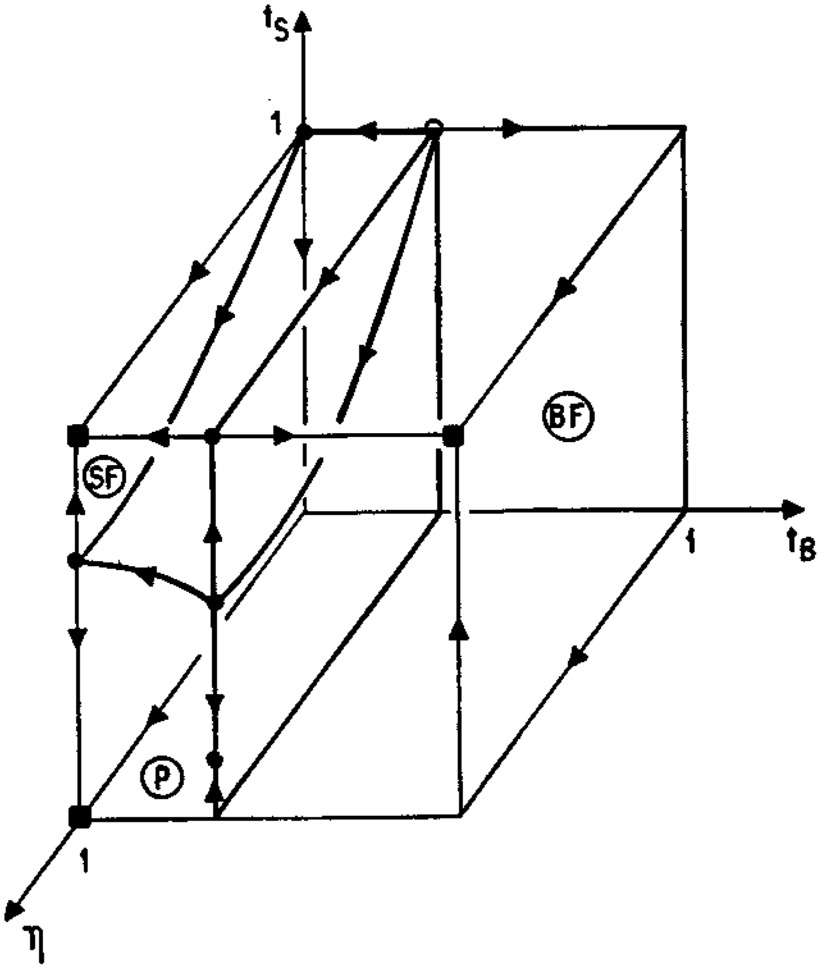

FIG. 3 - a

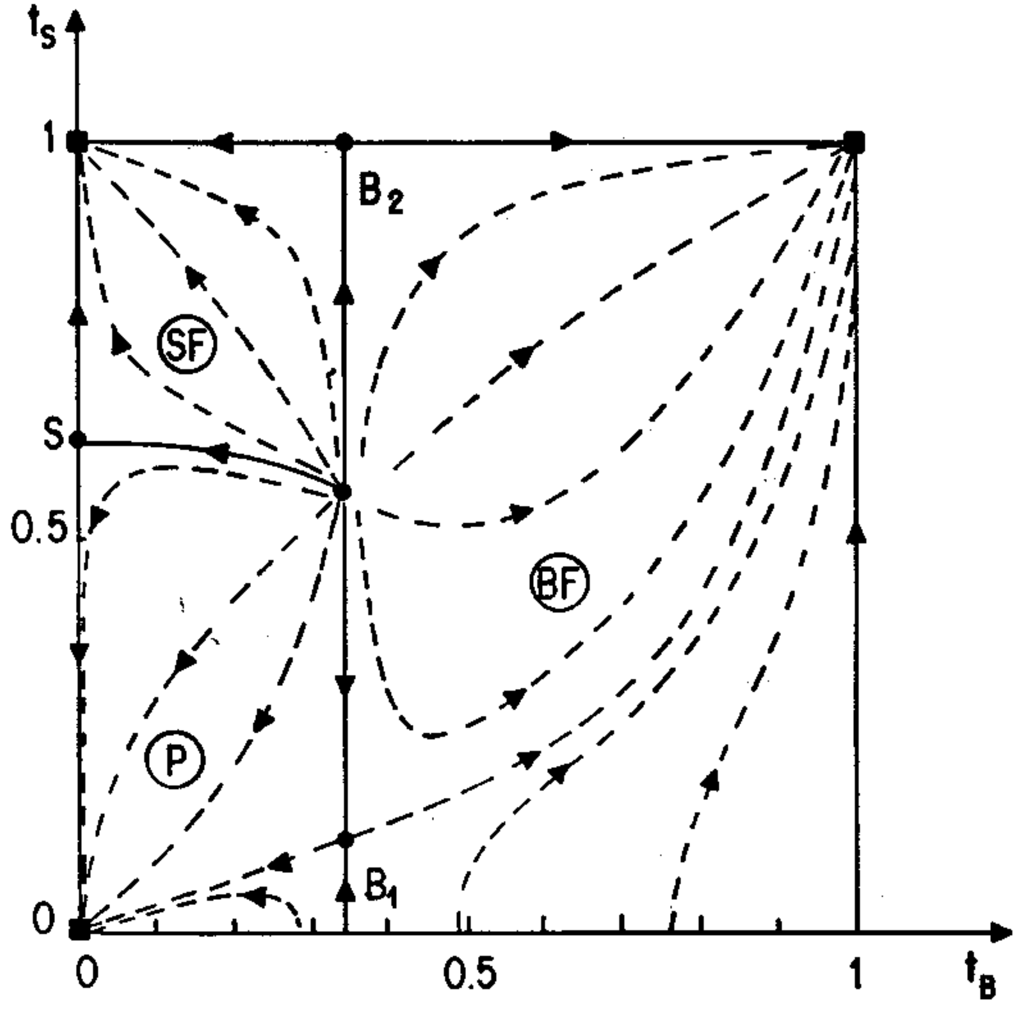

FIG. 3 - b

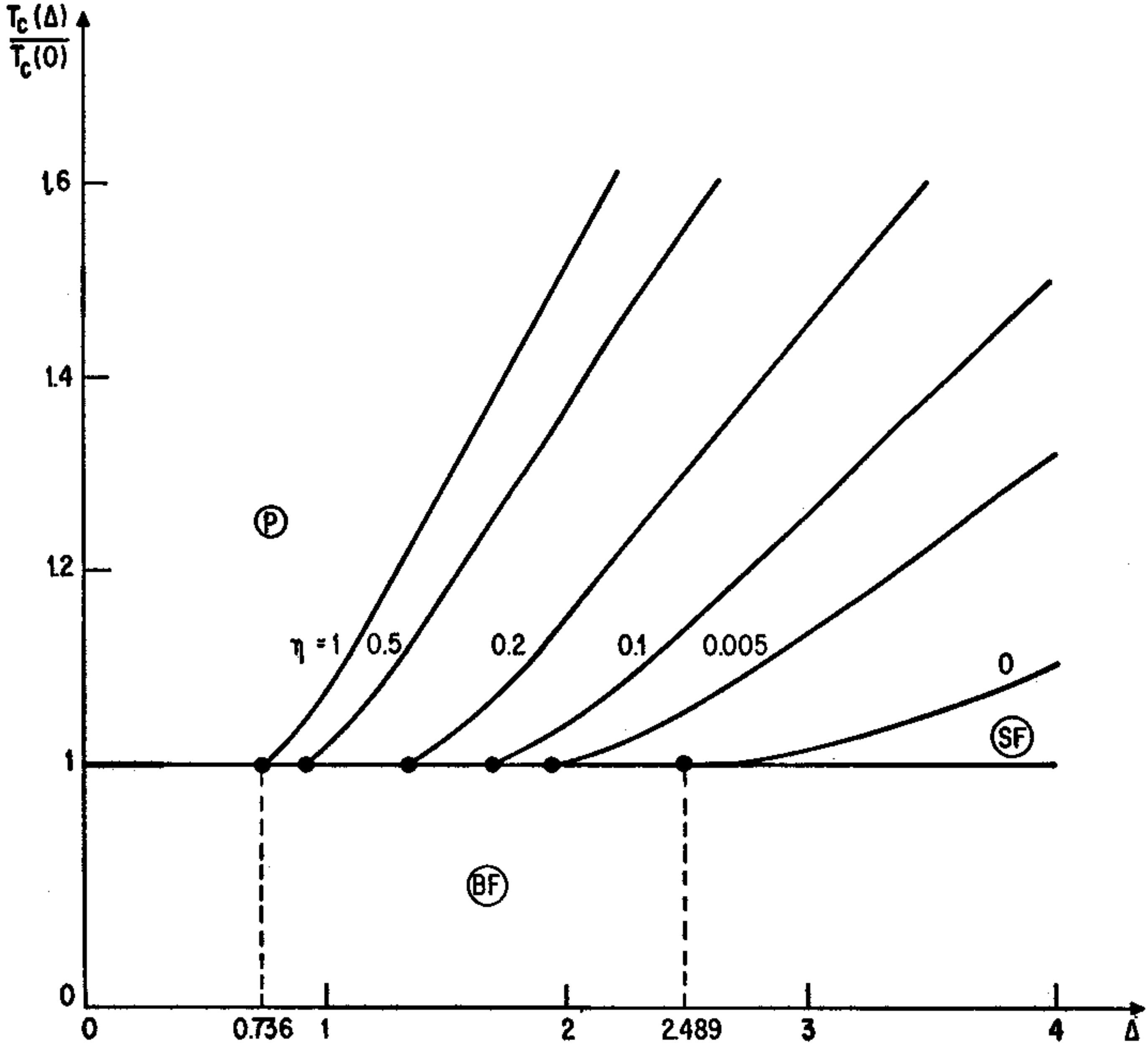
$T_c(\Delta)/T_c(0)$
1.6
1.4
1.2
1
0
P
η = 1
0.5
0.2
0.1
0.005
0
SF
BF
0
0.736
1
2
2.489
3
4
Δ

FIG.4

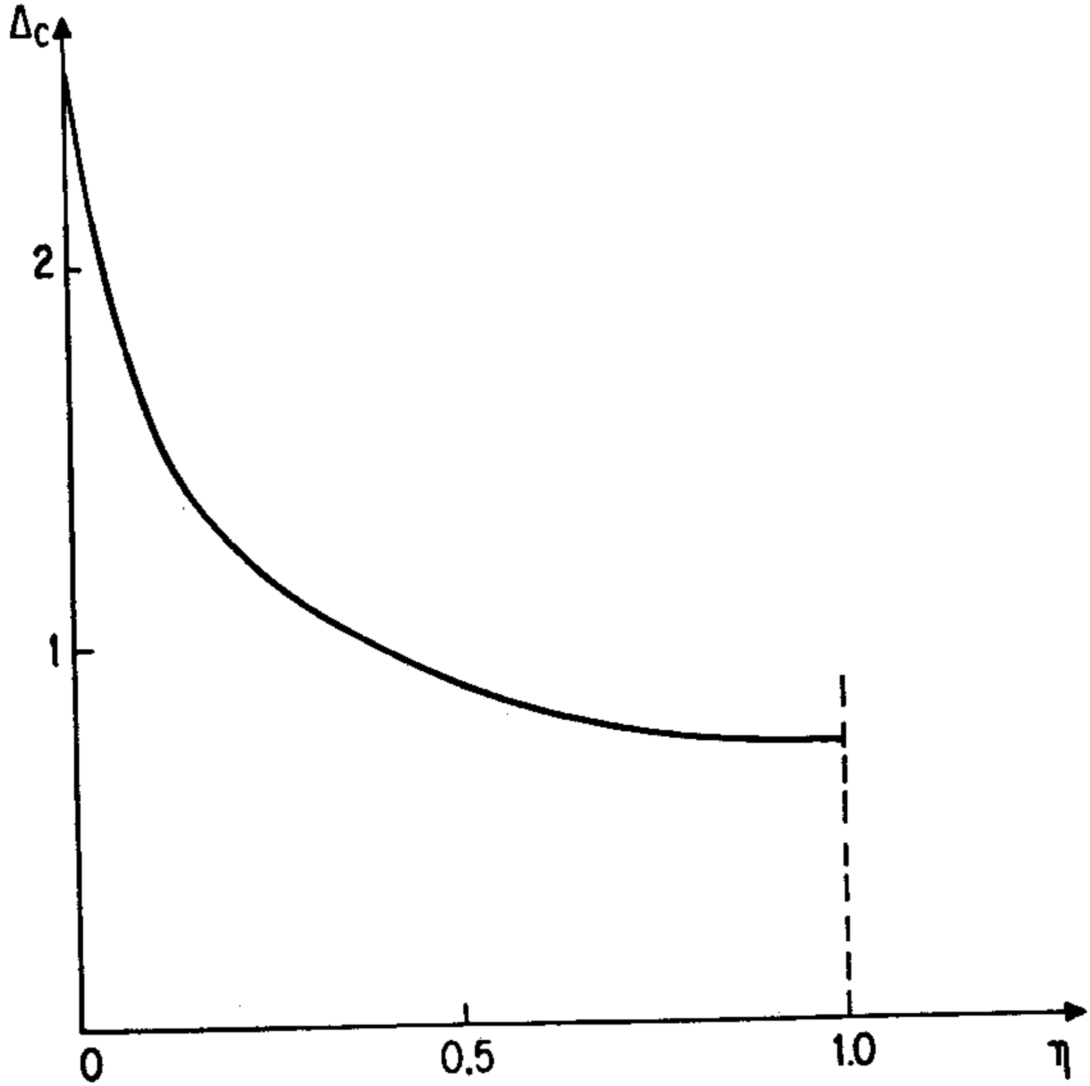

FIG. 5

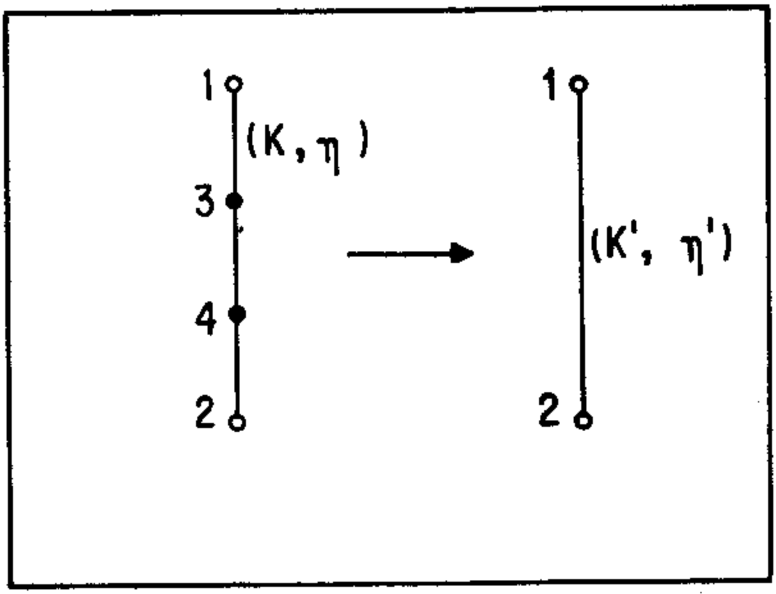

FIG. 6

REFERENCES

1 - K. Binder, "Critical behavior at surfaces" in "Phase transition and Critical Phenomena", ed. C. Domb and J.L. Lebowitz, vol. 8 (Academic Press, 1983)

2 - N.M. Svrakic and M. Wortis, Phys. Rev. B15, 396 (1977)

3 - T.W. Burkhardt and E. Eisenriegler, Phys. Rev. B16 3213 (1977)

4 - N.M. Svrakic, R. Pandit and M. Wortis, Phys. Rev. B22, 1286 (1980)

5 - C. Tsallis and E.F. Sarmento, J. Phys. C 18 (1985; in press)

6 - U.M.S. Costa, C. Tsallis and E.F. Sarmento, J. Phys. C (1985, in press)

7 - A.O. Caride, C. Tsallis and S.I. Zanette, Phys. Rev. Let. 51, 145 (1983) and Phys. Rev. Lett. 51, 616 (1983); A.M. Mariz, C. Tsallis and A.O. Caride, J. Phys. C (1985, in press)

8 - K. Binder and P.C. Hohenberg, Phys. Rev. B6, 3461 (1972) and Phys. Rev. B9, 2194 (1974)

9 - R. Lipowsky, Z. Phys. B. Cond. Matter 45, 229 (1982)

10 - T.W. Burkhardt and E. Eisenriegler: Phys. Rev. B17, 318 (1978)

11 - K. Binder and D.P. Landau, Phys. Rev. Lett. 52, 318 (1984)

12 - L.R. da Silva, U.M.S. Costa and C. Tsallis, preprint (1985)

13 - A.A. Migdal, Zh. Eksp. Teor. Fiz. 69, 1457 (1975) [Sov. Phys. JETP 42, 743 (1975)]

14 - L.P. Kadanoff, Ann. Phys. (N.Y.) 100, 359 (1976)

15 - C. Tsallis and S. Levy, Phys. Rev. Lett. 47, 950 (1981)

16 - S. Selzer and N. Majlis, Phys. Rev. B 27, 544 (1983)

17 - A.N. Berker and S. Ostlund, J. Phys. C12, 4961 (1979)