BR8612523
ISSN 0029-3865

CNPq

CBPF
CENTRO BRASILEIRO DE PESQUISAS FÍSICAS

Notas de Física

CBPF-NF-060/85

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RIO DE JANEIRO
1985

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Área de Publicações
Rua Dr. Xavier Sigaud, 150 - 4º andar
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BRASIL

ISSN 0029 - 3865

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by

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ABSTRACT

Within a renormalization group scheme, ~~we discuss~~ the phase diagram of a semi-infinite simple cubic Ising ferromagnet is discussed, with arbitrary surface and bulk coupling constants, and including possible dilution of the bulk bonds. It is ~~We~~ obtained that dilution makes easier the appearance of surface magnetism in the absence of bulk magnetism. (Author)

Key-words: Surface magnetism; Phase diagram; Random magnetism; Renormalization group.

I INTRODUCTION

Surface magnetism is an interesting problem which, during recent years, has received both theoretical and experimental attention; see Ref. [1] for a review. A very simple model to study is the spin 1/2 Ising ferromagnet in a semi-infinite simple cubic lattice with a (1,0,0) free surface. The surface and bulk coupling constants (respectively J_S and J_B) are not necessarily equal; furthermore a (quenched) concentration $(1-p_B)$ of the bulk bonds might be absent. The reason for including bulk bond dilution it that, as already remarked some time ago [2], it enhances surface magnetism. To be more explicit, the phase diagram (in the $(k_BT/J_B, J_S/J_B, p_B)$ space for instance) presents three phases, namely the *paramagnetic* (P), *bulk ferromagnetic* (BF; both bulk and surface non-vanishing magnetizations) and *surface ferromagnetic* (SF; finite surface but vanishing bulk magnetizations) ones. All three phases join at a multicritical line. We intend to (qualitatively) show, within a simple Migdal-Kadanoff-like real-space renormalization-group (RG) framework which extends a recently developed one [3], that the location of this multicritical line is such that the appearance (*and therefore the experimental observation*) of surface magnetism is made easier through bulk bond dilution (i.e., decrease of p_B).

II MODEL AND FORMALISM

We consider the following Ising Hamiltonian:

$$\mathcal{H} = - \sum_{i,j} J_{ij} \sigma_i \sigma_j \quad (\sigma_i = \pm 1, \forall i) \tag{1}$$

where (i,j) run over all pairs of first-neighbouring sites on a semi-infinite simple cubic lattice with a (1,0,0) free surface. J_{ij} equals $J_S \geq 0$ when *both* sites belong to the surface, and obeys, otherwise, the following distribution law:

$$P_B(J_{ij}) = (1-p_B)\delta(J_{ij}) + p_B\delta(J_{ij} - J_B) \tag{2}$$

with $J_B > 0$ and $0 \leq p_B \leq 1$. Let us introduce a convenient variable ([4] and references therein), namely $t_{ij} \equiv \tanh(J_{ij}/k_BT)$, T being the temperature. Consequently the model probability laws can be rewritten as follows:

$$P_S(t_{ij}) = \delta(t_{ij} - t_S) \tag{3}$$

and

$$P_B(t_{ij}) = (1 - p_B)\delta(t_{ij}) + p_B\delta(t_{ij} - t_B) \tag{4}$$

where t_S and t_B respectively correspond to J_S and J_B.

To construct the RG recursive relations (in the (t_B, t_S, p_B) space) we follow along the lines of Ref. [3] and renormalize the clusters indicated in Fig. 1 into single (surface and bulk) bonds. The terminal nodes of the surface cluster (Fig.1(a)) lay on the free surface. The probability laws corresponding to series arrays of 3 surface and 3 bulk bonds respectively are $\delta(t_{ij}-t_S^3)$ and $(1-p_B^3)\delta(t_{ij})+p_B^3\delta(t_{ij}-t_B^3)$, where we have used the series algorithm $t_{series} = t_1 t_2$ [4], t_1 and t_2 being arbitrary values. By also using the parallel algorithm $t_{parallel} = (t_1 + t_2) / (1 + t_1 t_2)$ [4], we obtain the probability laws $\overline{P_S}$ and $\overline{P_B}$ respectively associated with the cluster of Fig. 1(a) and that of Fig. 1(b). They are given by

$$\overline{P_S}\,(t_{ij}) = \sum_{m=0}^{3} \binom{3}{m} (1-p_B^3)^{3-m} p_B^{3m} \delta(t_{ij}-t_S^{(m)}) \tag{5}$$

with

$$t_S^{(m)} \equiv \frac{1 - \left[\dfrac{1-t_S^3}{1+t_S^3}\right]\left[\dfrac{1-t_B^3}{1+t_B^3}\right]^m}{1 + \left[\dfrac{1-t_S^3}{1+t_S^3}\right]\left[\dfrac{1-t_B^3}{1+t_B^3}\right]^m} \quad (m = 0,1,2,3) \tag{6}$$

and

$$\overline{P_B}\,(t_{ij}) = \sum_{n=0}^{9} \binom{9}{n} (1-p_B^3)^{9-n} p_B^{3n} \delta(t_{ij}-t_B^{(n)}) \tag{7}$$

with

$$t_B^{(n)} \equiv \frac{1 - \left[\dfrac{1-t_B^3}{1+t_B^3}\right]^n}{1 + \left[\dfrac{1-t_B^3}{1+t_B^3}\right]^n} \quad (n = 0,1,2,\dots,9) \tag{8}$$

As we see, none of $\overline{P_S}$ and $\overline{P_B}$ is binary, and they become more and more complex through successive renormalizations. We can either follow the distributions until arrival to invariant forms, or more simply (and without appreciable loose of efficiency, as already quite well known), approximate them by renormalized binary laws, namely.

$$P'_S(t_{ij}) = \delta(t_{ij} - t'_S) \tag{9}$$

and

$$P'_B(t_{ij}) = (1-p'_B)\delta(t_{ij}) + p'_B\delta(t_{ij} - t'_B) \tag{10}$$

where t'_B, t'_S and p'_B are to be found. To determine them, we impose preservation of the first momenta, more precisely

$$< t_{ij} >_{P'_S} = <t_{ij}>_{\overline{P_S}} \tag{11}$$

$$< t_{ij} >_{P'_B} = <t_{ij}>_{\overline{P_B}} \tag{12}$$

and

$$< t^2_{ij} >_{P'_B} = <t^2_{ij}>_{\overline{P_B}} \tag{13}$$

These equations immediately yield explicit RG recursive relations, i.e. (t'_B, t'_S, p'_B) as function of (t_B, t_S, p_B). The corresponding flow diagram determines the criticality of the model.

III RESULTS AND CONCLUSION

The RG flow determined by Eqs. (11)-(13) exhibits 3 trivial (fully stable) fixed points, namely $(t_B, t_S, p_B) = (0,0,0), (1,1,1)$ and $(0,1,1)$, respectively characterizing the P, BF and SP phases. Several unstable fixed points are also present. Typical cuts of the phase diagram are indicated in Figs. 2 [(t_B, t_S, p_B) space] and 3 [$(k_BT/J_B, J_S/J_B, p_B)$ space]. Also we have represented in Fig. 4 the p_B -dependence of J_S^*/J_B, value which corresponds to the multicritical point where all three phases join, i.e. the value of J_S/J_B above which magnetically ordered surface is possible even if the bulk is disordered. J_S^*/J_B monotonously decreases when p_B decreases and vanishes for p_B^*, the simple cubic lattice bond percolation critical concentration. In other words, as already announced, *bulk dilution indeed enhances surface magnetism*; the effect is quite abrupt while approaching, by above, the bulk percolation threshold.

One of us (C.T.) acknowledges warm hospitality received at the CRTBT/CNRS, where the present work was concluded.

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CAPTION FOR FIGURES

Fig. 1: RG cluster transformations for the surface (a) and bulk (b) bonds. • and O respectively represent internal and terminal nodes.
The RG linear expansion factor equals 3.

Fig. 2: (a) RG flow diagram for $p_B = 1$. P, BF and SF respectively represent the para-, bulk ferro-, and surface ferromagnetic phases. The dashed lines are indicative. (b) Fixed p_B cuts of the phase diagram (only the $p_B = 1$ case corresponds to an invariant subspace under RG). The BF phase lays at the "right side" of the "vertical" straight line corresponding to the particular value of p_B. The "vertical" straight line attains the $t_B = 1$ axis at the bulk bond percolation threshold ($p_B = p_B^*$).

Fig. 3: p_B-evolution of the phase diagram. $T_c^B(p_B = 1)$ is the simple cubic pure Ising ferromagnet critical temperature.

Fig. 4: p_B dependence of the location of the multicritical point (value of J_S/J_B above which the surface is magnetized while the bulk is paramagnetic).

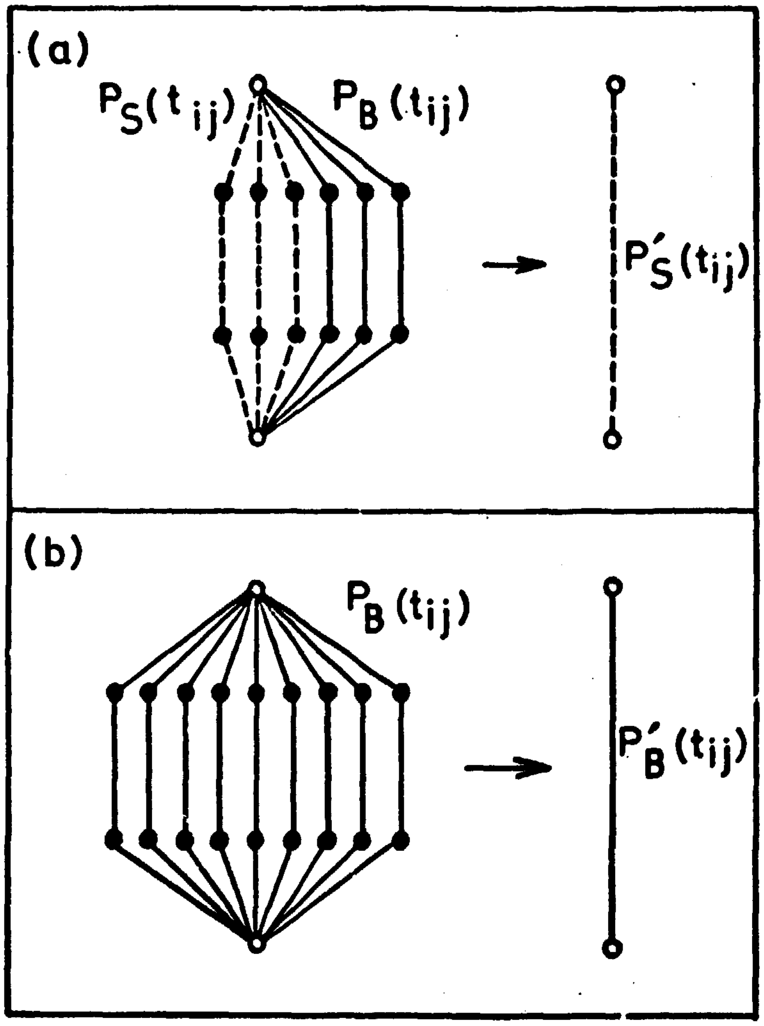

Fig. 1

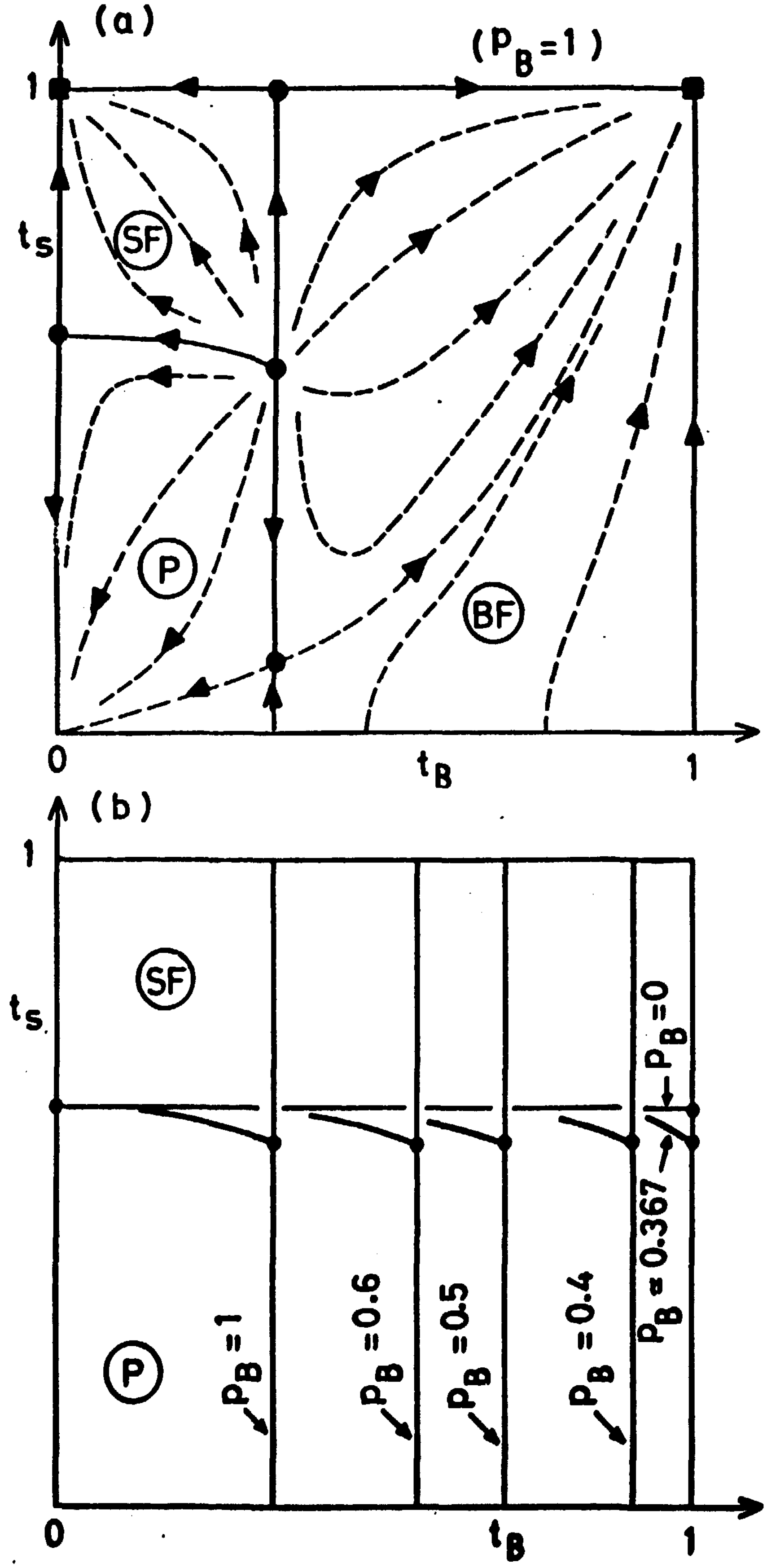
(a)
(p_B=1)
1
t_S
SF
P
BF
0
t_B
1
(b)
1
t_S
SF
P
p_B=1
p_B=0.6
p_B=0.5
p_B=0.4
p_B=0.367
p_B=0
0
t_B
1

Fig. 2

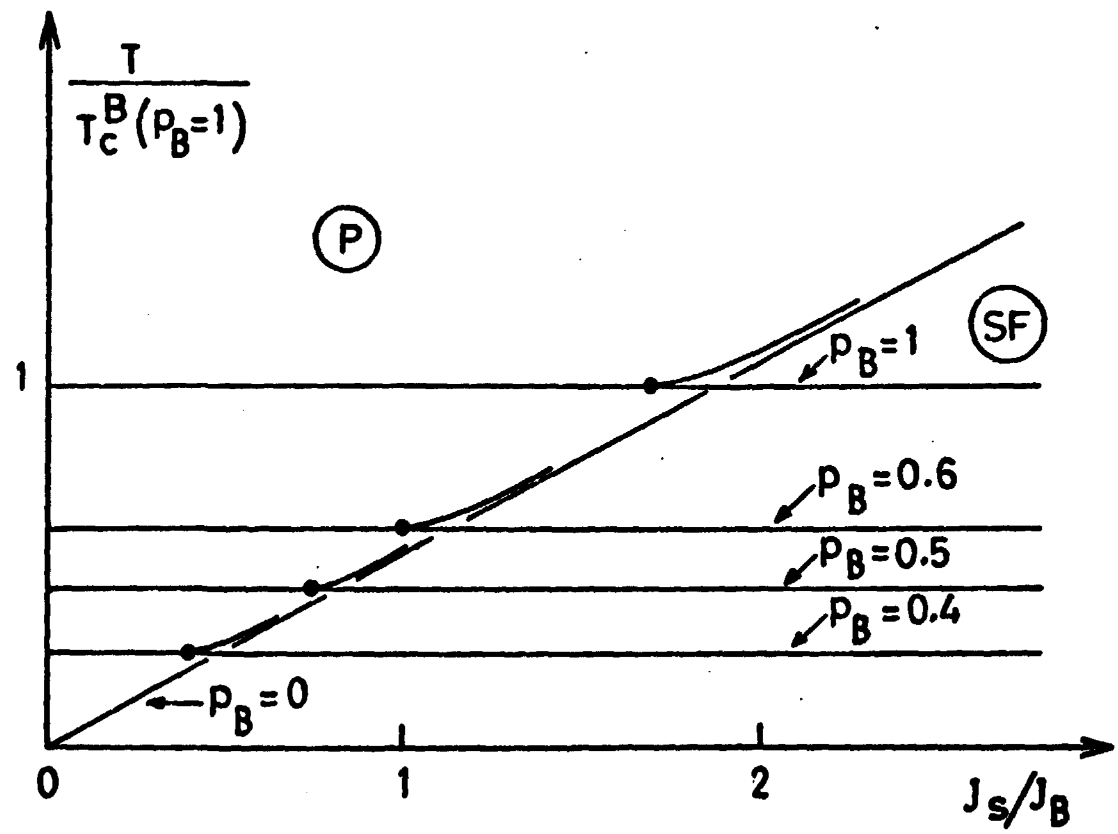

Fig. 3

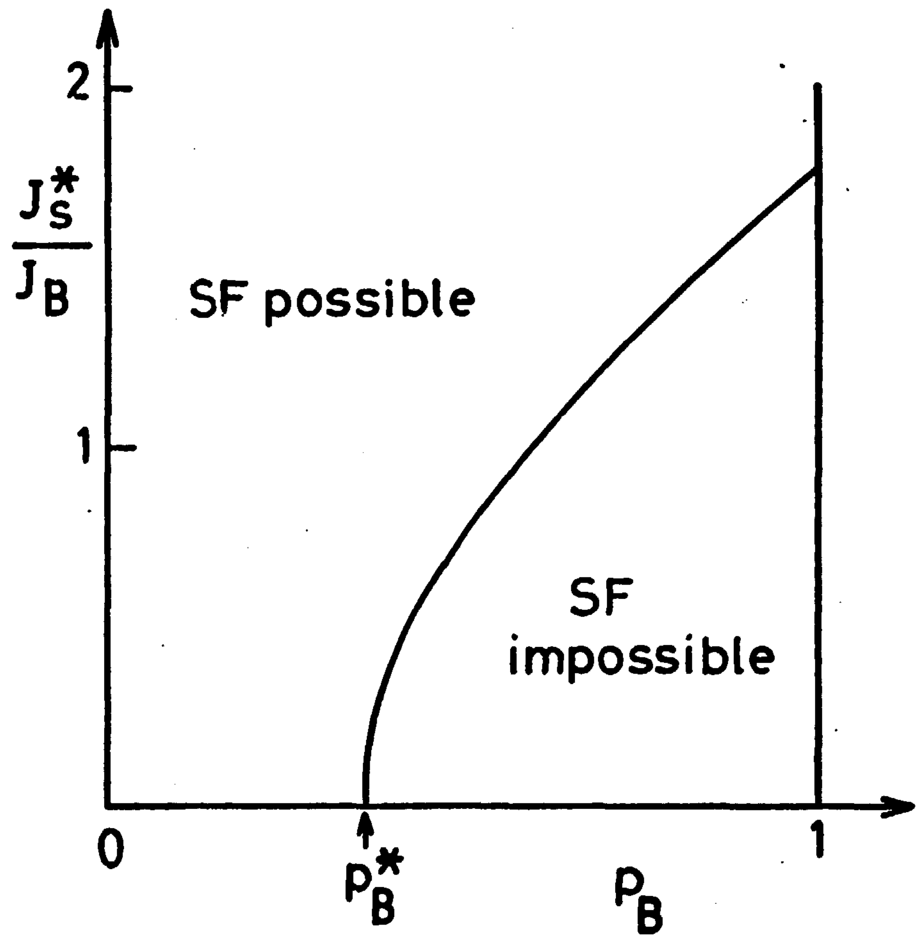

Fig.4