Revista Brasileira de Física, Vol. 18, nº 3, 1988

Influence of Bond Dilution on the Free Surface and Interface Potts Ferromagnetism

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Recebido em 14 de janeiro de 1988

Abstract Within a simple real space renormalization group framework, we discuss the phase diagram of a q-state Potts ferromagnetic system constituted by two semi-infinite bulks separated by a planar interface. Quenched bond dilution has been assumed in the bulks as well as along the interface. The system exhibits percolation-like phenomena which generalize the standard ones occurring in $d=2$ and 3. Also competition between bulk dilution and interface dilution (which respectively enhances and depresses surface magnetisation with respect that in the bulk) is observed.

1. INTRODUCTION

Surface magnetism is a subject which presents great richness, from the theoretical and experimental standpoints as well as due to its important applications such as catalysis and corrosion; see Binder[1], Tsallis[2] and Diehl[3] for recent reviews. Situations such as the free surface problem (semi-infinite bulk) and that of an interface or defect (surface between two semi-infinite bulks, which generalizes the free surface case) have been theoretically considered. The former has received most of the attention through various theoretical approaches such as mean field approximation[4-5], series expansion[6-7], renormalization group[8-17], effective field theory[18-20], Bethe approximation[21] and Monte Carlo studies[22-23]. In spite of its technical difficulties, some experimental work has also been performed[24-27]. On the other hand, almost no attempts are available in the literature concerning the more general problem, namely that of interfaces[28]. Although several models have been assumed, (e.g., spin 1/2 Ising, q-state Potts, spin 1/2 anisotropic

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Heinsenberg, mixed ones), pure systems (that is, non diluted) have been almost exclusively considered. The first attempt (to the best of our knowledge) concerning the effects of (bulk) dilution was due to Ferchmin and Maciejewski[29]. Very recently, real space renormalization group (RG) work has addressed this type of effects: bulk dilution for the free surface spin 1/2 Ising model[31], and surface dilution for the interface Potts model[31], within Migdal-Kadanoff RG frameworks (see Tsallis and Sarmento[16]), and free surface dilution for the spin 1/2 Ising model within a RG which uses a sophisticated cluster and yields quite accurate results[32].

In the present paper we focus on the general interface problem (with semi-infinite bulks which are not necessarily equal) for the q-state Potts simple cubic ferromagnet ($q=1$ and $q=2$ recover the bond percolation and Ising problems respectively) assuming quenched bond arbitrary dilutions in both bulks as well as along the (0,0,1) surface between them. We discuss mainly the phase diagram, although the various critical universality classes associated with the problem emerge as well. Interesting bond-percolation-like phenomena are observed, as well as competition between bulk dilution and interface dilution (which respectively enhances and depresses surface magnetisation with respect to that in the bulk).

In section 2 we introduce the model and the formalism, and in section 3 we present the main results, concluding in section 4.

2. MODEL AND FORMALISM

We consider the following Potts Hamiltonian

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

where J_{ij} equals J_s ($J_s \geq 0$) ig both i and j sites are first neighbours belonging to the (0,0,1) interface of a simple cubic lattice, and J_{ij} equals $J_1 \geq 0$ ($J_2 \geq 0$) if at least one of the first neighbours i and j belongs to the bulk-1 (bulk-2). Furthermore, the coupling constants J_{ij} are assumed to be random variables satisfying the following probability laws:

$$P_s(J_s) = (1-p_s)\delta(J_s) + p_s\delta(J_s-J_s^0) \tag{2.a}$$

$$P_r(J_r) = (1-p_r)\delta(J_r) + p_r\delta(J_r-J_r^0) \quad (r=1,2) \tag{2.b}$$

with

$$0 \leqslant p_s,\ p_1,\ p_2 \leqslant 1$$

and

$$J_s^0,\ J_1^0,\ J_2^0 \geqslant 0 \ .$$

The *pure* case corresponds to

$$p_s = p_1 = p_2 = 1\ ,\ \forall(J_s^0, J_1^0, J_2^0)\ .$$

The *free surface* case corresponds to, say,

$$J_2^0 = 0\ ,\quad \forall(p_s,\ p_1,\ p_2,\ J_s^0,\ J_1^0)$$

or

$$p_2 = 0,\quad \forall(p_s,\ p_1,\ J_s^0,\ J_1^0,\ J_2^0)\ .$$

Before going on, let us introduce a convenient variable (*thermal transmissivity*: see Tsallis and Levy[33])

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

Eqs. (2) can be rewritten as follows:

$$P_s(t_s) = (1-p_s)\delta(t_s) + p_s\delta(t_s-t_s^0) \tag{4.a}$$

$$P_r(t_r) = (1-p_r)\delta(t_r) + p_r\delta(t_r-t_r^0) \quad (r=1,2) \tag{4.b}$$

To treat the model defined by eqs. (1) and (2) we shall use the RG approach indicated in fig.1 with the renormalized probability laws

$$P_s'(t_s) = (1-p_s')\delta(t_s) + p_s'\delta(t_s-t_s^{0\prime}) \tag{5.a}$$

$$P_r'(t_r) = (1-p_r')\delta(t_r) + p_r'\delta(t_r-t_r^{0\prime}) \quad (r=1,2) \tag{5.b}$$

where $(p_s',\ p_1',\ p_2',\ t_s^{0\prime},\ t_1^{0\prime},\ t_2^{0\prime})$ are parameters to be determined.

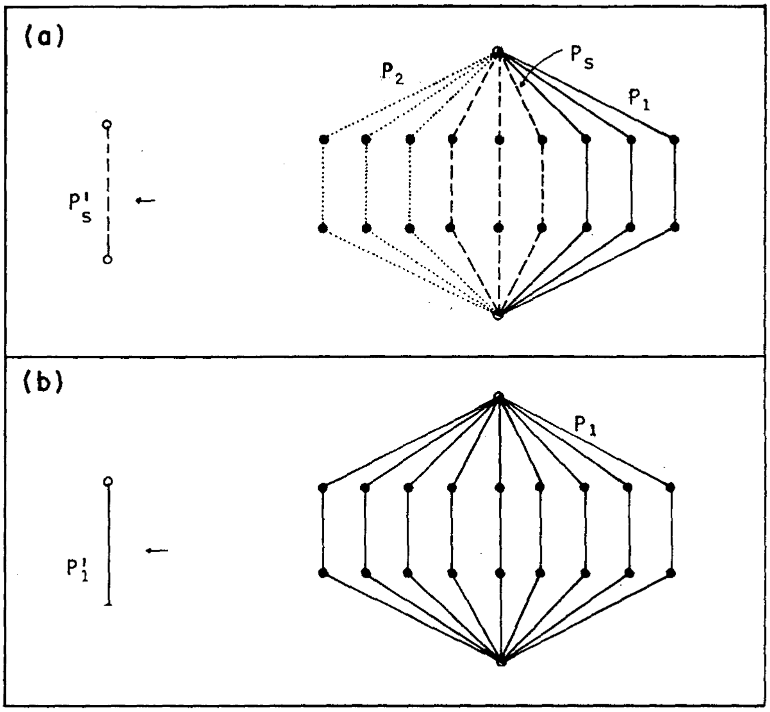

Fig. 1 - RG transformation (the large cluster are renormalized into the small ones); o and ● respectively denote terminal and internal sites. (a) interface RG transformation; (b) bulk-1 RG transformation (that of bulk-2 is completely analogous).

The probability law $\bar{P}_s$ associated with the large cluster of fig. 1(a) is given by

$$\bar{P}_s(t_s) = \sum_{n_s=0}^{3} \sum_{n_1=0}^{3} \sum_{n_2=0}^{3} \binom{3}{n_s} \binom{3}{n_1} \binom{3}{n_2} \times (1-p_s^3)^{3-n_s} p_s^{3n_s} (1-p_1^3)^{3-n_1} p_1^{3n_1} (1-p_2^3)^{3-n_2} p_2^{3n_2} \times \delta(t_s - t^{(n_s,n_1,n_2)}) \tag{6}$$

where

$$t^{(n_s,n_1,n_2)} \equiv \frac{1-\left[\frac{1-t_s^{0\,3}}{1+(q-1)t_s^{0\,3}}\right]^{n_s}\left[\frac{1-t_1^{0\,3}}{1+(q-1)t_1^{0\,3}}\right]^{n_1}\left[\frac{1-t_2^{0\,3}}{1+(q-1)t_2^{0\,3}}\right]^{n_2}}{1+(q-1)\left[\frac{1-t_s^{0\,3}}{1+(q-1)t_s^{0\,3}}\right]^{n_s}\left[\frac{1-t_1^{0\,3}}{1+(q-1)t_1^{0\,3}}\right]^{n_1}\left[\frac{1-t_2^{0\,3}}{1+(q-1)t_2^{0\,3}}\right]^{n_2}} \tag{7}$$

with $n_s,\ n_1,\ n_2 = 0,1,2,3$. Similarly, the probability law $\bar{P}_1$ associated with the large cluster of fig. 1(b) is given by

$$\bar{P}_1(t_1) = \sum_{n=0}^{9} \binom{9}{n} (1-p_1^3)^{9-n}\, p_1^{3n}\, \delta(t_1-t_1^{(n)}) \tag{8}$$

where

$$t_1^{(n)} \equiv \frac{1-\left[\frac{1-t_1^{0\,3}}{1+(q-1)t_1^{0\,3}}\right]^{n}}{1+(q-1)\left[\frac{1-t_1^{0\,3}}{1+(q-1)t_1^{0\,3}}\right]^{n}} \quad (n=0,1,\ldots,9) \tag{9}$$

The probability law $\bar{P}_2(t_2)$ associated with bulk-2 is completely analogous to $\bar{P}_1(t_1)$.

It is important to stress that the distributions $\bar{P}_s$, $\bar{P}_1$ and $\bar{P}_2$ are much more complex than the corresponding binary ones P'_s, P'_1 and P'_2. Consequently the representations indicated in fig. 1 involve an *approximation*. This (binary) approximation could in principle be avoided by leaving the distributions free to evolve, through successive renormalization steps, towards their fixed Forms. However, it well known[34-35] that the *binary approximation* behaves quite satisfactorily in a great variety of similar systerns. Consequently we shall adopt it for the present discussion. To determine the parameters p'_s, p'_1, p'_2, $t_s^{0\prime}$, $t_1^{0\prime}$ and $t_2^{0\prime}$ we impose the lower momenta to be preserved, more precisely

$$\langle t_s \rangle_{P'_s} = \langle t_s \rangle_{\bar{P}_s} \tag{10}$$

$$\langle t_s^1\rangle_{P'_s} = \langle t_s^2\rangle_{\bar{P}_s} \tag{11}$$

$$\langle t_r\rangle_{P'_r} = \langle t_r\rangle_{\bar{P}_r} \qquad (r=1,2) \tag{12}$$

$$\langle t_r^2\rangle_{P'_r} = \langle t_r^2\rangle_{\bar{P}_r} \qquad (r=1,2) \tag{13}$$

Consequently we have

$$P'_s\, t_s' = \sum_{n_s=0}^{3}\sum_{n_1=0}^{3}\sum_{n_2=0}^{3} \binom{3}{n_s}\binom{3}{n_1}\binom{3}{n_2}$$

$$\times (1-p_s^3)^{3-n_s}\, p_s^{3n_s} (1-p_1^3)^{3-n_1}\, p_1^{3n_1} (1-p_2^3)^{3-n_2}\, p_2^{3n_2}$$

$$\times\, t^{(n_s,n_1,n_2)} \equiv F_s(p_s,p_1,p_2,t_s^0,t_1^0,t_2^0) \tag{14}$$

$$p'_s(t_s')^2 = \sum_{n_s=0}^{3}\sum_{n_1=0}^{3}\sum_{n_2=0}^{3} \binom{3}{n_s}\binom{3}{n_1}\binom{3}{n_2}$$

$$\times (1-p_s^3)^{3-n_s}\, p_s^{3n_s}\, (1-p_1^3)^{3-n_1}\, p_1^{3n_1}\, (1-p_2^3)^{3-n_2}\, p_2^{3n_2}$$

$$\times \left[t^{(n_s,n_1,n_2)}\right]^2 \equiv G_s(p_s,p_1,p_2,t_s^0,t_1^0,t_2^0) \tag{15}$$

$$p'_r\, t_r^{0\prime} = \sum_{n=0}^{9} \binom{9}{n} (1-p_r^3)^{9-n}\, p_r^{3n}\, t_r^{(n)} \equiv F_r(p_r,t_r^0) \quad (r=1,2) \tag{16}$$

$$p'_r(t_r^{0\prime})^2 = \sum_{n=0}^{9} \binom{9}{n} (1-p_r^3)^{9-n}\, p_r^{3n}\left[t_r^{(n)}\right]^2 \equiv G_r(p_r,t_r^0) \quad (r=1,2) \tag{17}$$

and finally

$$p'_s = F_s^2/G_s \tag{18}$$

$$t_s^{0\prime} = G_s/F_s \tag{19}$$

$$p_r' = F_r^2/G_r \qquad (r=1,2) \tag{20}$$

$$t_r^{0\,\prime} = G_r/F_r \qquad (r=1,2) \tag{21}$$

Equations (18-21) completely determine the RG recursive relations in the 6-dimensional parameter-space (p_s, p_1, p_2, t_s^0, t_1^0, t_2^0) (or equivalently in the (k_BT/J_1^0, J_s^0/J_1^0, J_2^0/J_1^0, p_s, p_1, p_2) space. The RG flow diagram in this space fully determines the complex phase diagram (hypersurfaces in a 6-dimensional space) as well as the corresponding critical universality classes. In the next section we present convenient cross-sections of this phase diagram and its evolution with q.

3. RESULTS

We have chosen as a prototype the *free surface* (i.e., $p_2=0$ and/or $J_2^0=0$) *pure* (i.e., $p_s=p_1=1$) *Ising model* (i.e., q = 2): its RG flux diagram is indicated in fig.2. It exhibits three phases, namely *bulk ferromagnetic* (BF; both bulk and surface are magnetically ordered), *surface ferromagnetic* (SF; only the surface is magnetically ordered) and *paramagnetic* (P; magnetically fully disordered system). The P-SF critical line belongs to the $d=2$ universality class (characterized by the $t_1^0=0$ semi-stable fixed point); the SF-BF critical line belongs to the $d=3$ universality class (characterized by the $t_s^0=1$ semi-stable fixed point); the P-BF critical line belongs, for the surface magnetization, to a non trivial universality class (characterized the $0<t_s^0$, $t_1^0<1$ semi-stable fixed point) which differs from both $d=2$ and $d=3$ ones; all three critical' lines join at a multicritical point which constitutes by itself a new universality class (characterized by the single fully unstable fixed point). This RG flux diagram evolves smoothly with q. The influence of *bulk dilution* is to shift the *vertical* asymptote to the right, therefore *enhancing* the SF phase; for $p_1=p_c^{3D}$ (d=3 bon percolation threshold) the asymptote merges with the $t_1^0=1$ axis. The influence of *surface dilution* is to shift the *horizontal* asymptote (S-SB line) to higher values of t_s^0, therefore *depressing* the SF phase; for $p_s=p_c^{2D}$ ($d=2$ bond percolation threshold) the $t_1^0=0$ point of the *horizontal* asymptote is on the $t_s^0=1$ axis. Simultaneous bulk and surface

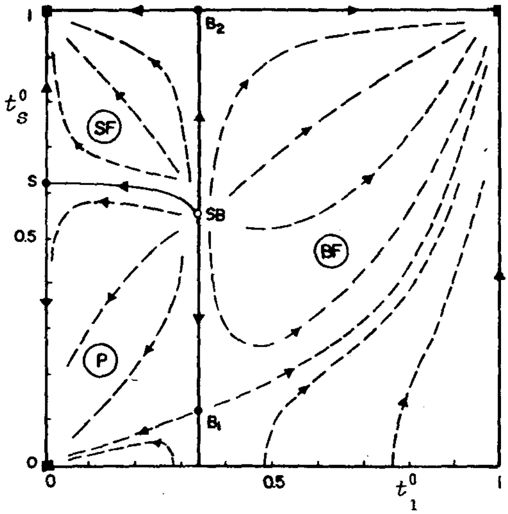

Fig. 2 - Pure ($p_s=p_1=1$) Ising model ($q=2$) for the freesurface case ($p_2=0$ and/or $t_2^0=0$): RG flux diagrarn. ■, ● and o respectively denote the trivial (fully stable), critical (semi-stable) and multicritical (fully unstable) fixed points. P, BF and SF respectively denote the paramagnetic, bulkferrornagneticand surface ferromagnetic phases. t_s^0 and t_1^0 are transmissivities.

dilutions move *both* asymptotes, thus giving rise to *competition* concerning the SF phase. For high enough q, surface and bulk dilutionyield new non trivial critical fixed points, thus driving the system into new (*random*) universality classes. This fact is consistent with Harris's[36] criterion; however the main purpose of the present work being the phase diagram, we will not study the details of thys type of crossover.

The effect of surface dilution (with $p_1=1$) in the T vs. J_s^0/J_1^0 representation is illustrated in fig.3 (T_c^{3D} denotes the $d=3$ Ising critical temperature). Let us stress that the SF phase exists even *below* the $d=2$ percolation threshold (i.e., for $p<p_c^{2D}$), a new percolation-like threshold now arising. This effect can be referred to as *bulk-assisted surface percolation.*

The effect of bulk dilution (with $p_s=1$) in the T vs. J_s^0/J_1^0 representation is illustrated in fig. 4. The effect of *simultaneous* surface and bulk dilutions is illustrated in fig. 5. The influence of p_s and p_1 on the phase diagram is conveniently synthetized by looking at the way they shift the location J_s^*/J_1^0 of the multicritical point: this is depicted in figs. 6a, b, c.

We have represented in fig. 7 the q-evolution of the pure case ($p_s=p_1=1$) phase diagrarn. The q-dependence of J_s^*/J_1^0 appears in fig.9 (on the $J_2^0/J_1^0=0$ plane).

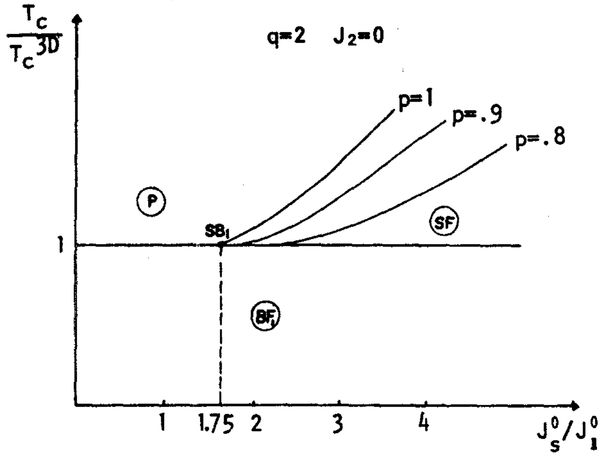

Fig.3 - q=2, p_1=1 phase diagram for p_2= 0 and/or J_2^0=0, and typical values of p_s.

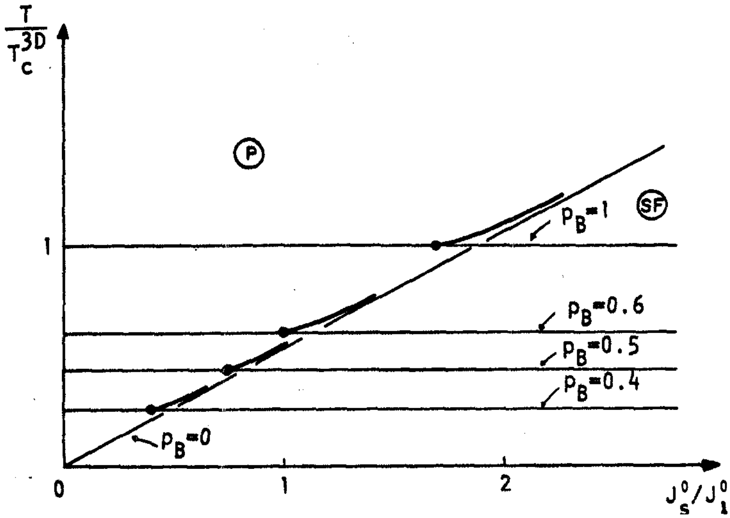

Fig.4 - q=2, p_s=1 phase diagram for p_2=0 and /or J_2^0=0, and typical values of p_1.

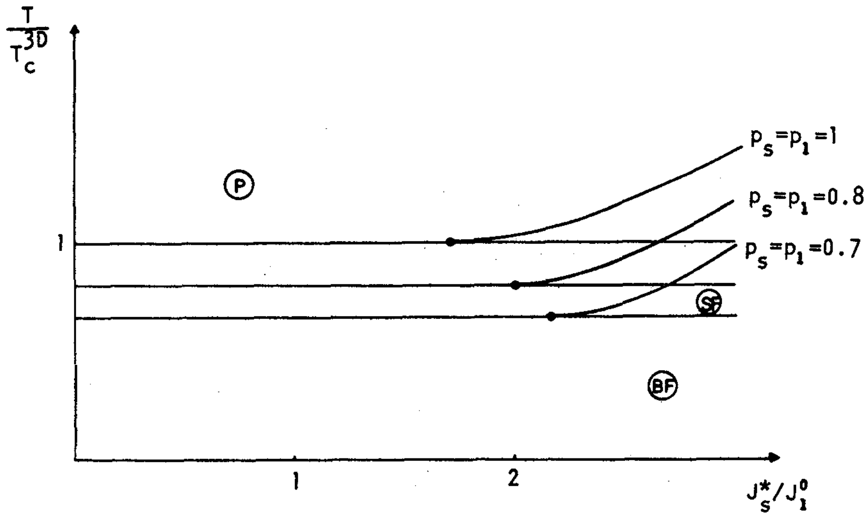

Fig.5 - q=2, phase diagram for p_2=0 and/or J_2^0=0 and typical values of p_s=p_1.

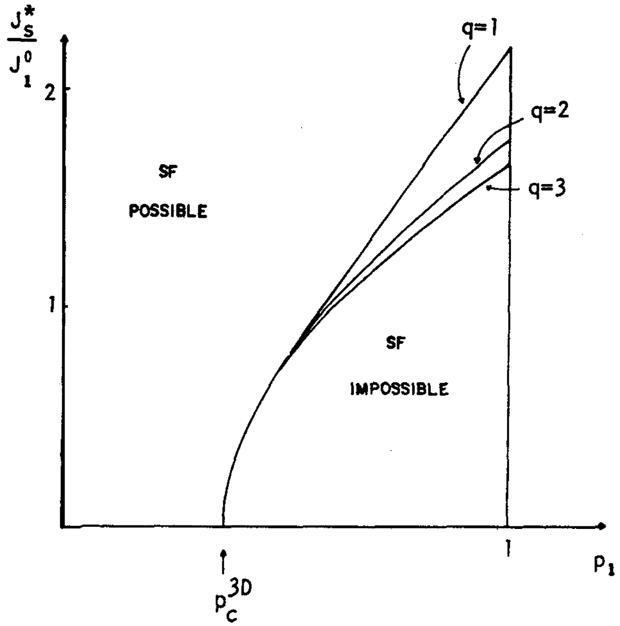

Fig. 6(a)

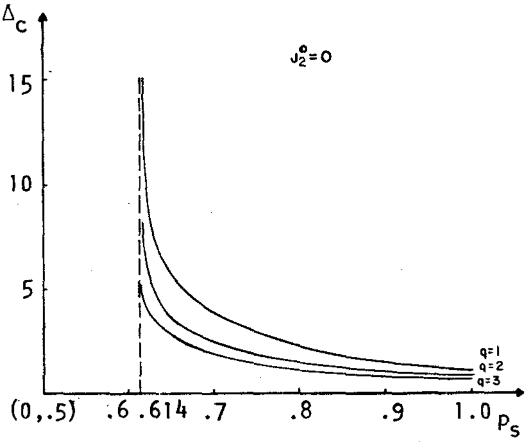

Fig.6(b)

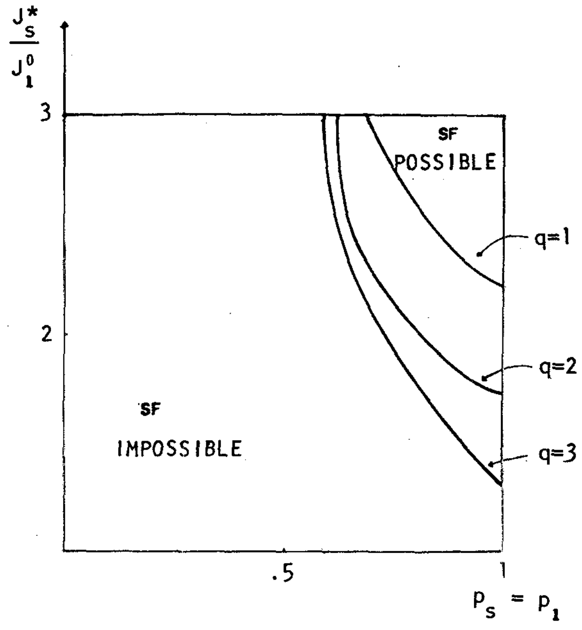

Fig.6(c)

Fig.6 - Concentration-dependence of $J_s^*/J_1^0 \equiv 1+\Delta_c$ (location of the multicritical points (for the $q=2$, $p_2=0$ and/or $J_2^0=0$ model. a) $p_s=1$; $p_1=1$; c) $p_s=p_1$.

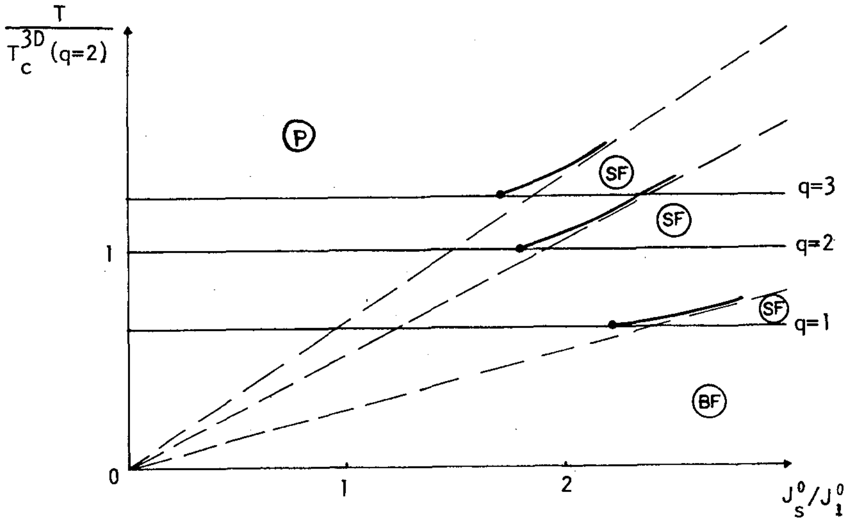

Fig.7 - q-evolution of the pure (p_s=p_1=1) model for the free surface case.

Let us now turn our attention to the *interface* case (both J_1^0 and J_2^0 non vanishing). A typical phase diagram is indicated in fig. 8, where BF_{12} means that *both* bulks as well as the interface are magnetized, and BF_1 refers to the fact that only bulk-1 (and of course the interface) is magnetized, bulk-2 now being paramagnetic. The location of the multicritical points is indicated in fig.9 for the pure case.

4. CONCLUSION

The quenched bond-diluted double-bulk Potts ferromagnet is a quite complex system, whose phase diagram is almost completely unknown. At the $T=0$ limit one recovers the standard $d=2$ and $d=3$ percolation thresholds[37-39] for the simple cubic with (0,0,1) interface values. Within a simple real space renormalization group scheme we have obtained this phase diagram (and also obtained information on its various universality classes). For all values of q, it displays four physically different phases, namely paramagnetic, ferromagnetic single bulk, ferromagnetic double-bulk, and ordered surface. The paramagnetic, single bulk and surface phases join along a multicritical line which can be characterised by the value $\Delta_c = J_s/J_1-1$ above which surface magnetic order can

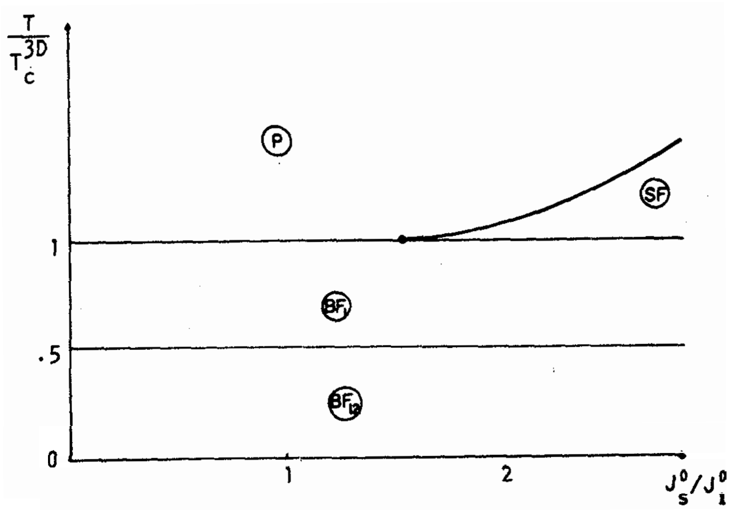

Fig.8 - $q=2$, $p_1=p_2=p_s=1$ diagram for the double - bulk; $J_2^0/J_1^0 = 1/2$ case.

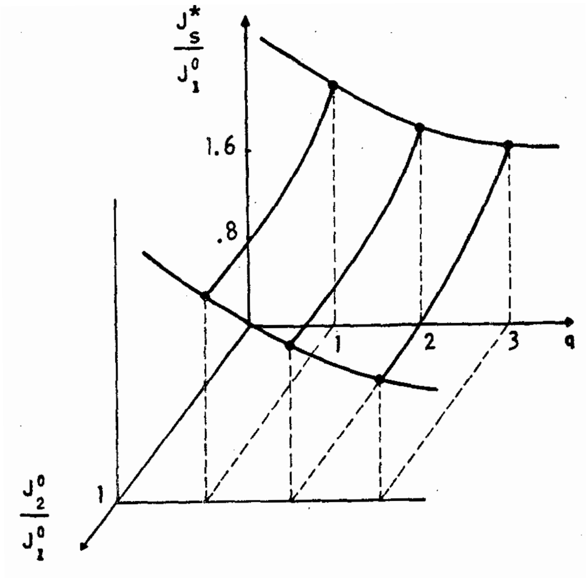

Fig.9 - q-evolution of the location of the multicritical point as a function of J_2^0/J_1^0 for the double-bulk $p_1=p_2=p_s=1$ model.

exist even if it has disappeared from both bulks. In particular, for the pure Ising free-surface model we find $\Delta_c = 0.74$ (to be compared with the series result 0.6 ± 0.1 [7], the Monte Carlo result 0.5 ± 0.03 [23], the MFRG result 0.64 [40] and with the mean field value 0.25 [5]); for the equal bulks case ($J_1=J_2$), we obtain $\Delta \simeq 0.10$, to be compared with the mean field value 0. The q-evolution of the phase diagram has been followed, and various interesting phenomena have been exhibited. The increase of the number of states of the model implies a decrease of the critical value $\Delta_c(p)$. Also, we observe the competitive trends of bulk dilution, which enhances surface magnetism with respect to that in the bulk, and surface dilution which depresses it (see figs. 6a, b, c).

All the results which we have presented in this work are valid for second-order phase transitions (i.e., $q \leq q_c \simeq 3$), the framework not being appropriate for the description of first order ones. We would be very happy if the present work could act as a guide to the choice of convenient real systems, and stimulate further (and quantitatively more precise) theoretical and experimental work on surface magnetism in diluted and/or mixed magnetic substances.

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Resumo

Usando a técnica de grupo de Renormalização no espaço real, são discutidos os diagramas de fase de um sistema ferromagnético de Potts com q estados, constituidos por dois volumes semi-infinitos separados por uma interface planar. Diluição temperada é admitida tanto nos volumes como na interface. O sistema apresenta fenômenos de percolação que generalizam os resultados conhecidos para d=2 e d=3. Efeito de competição entre as diluições nos volumes e na interface (o qual respectivamente aumenta e diminui o magnetismo de superfície comparado ao do volume) é também observado.