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GENERALIZED PERCOLATION AND RENORMALIZATION GROUP TREATMENT OF THE RANDOM ISING MODEL IN SQUARE LATTICE

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by

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ABSTRACT

Within a framework which combines the Reynolds-Klein-Stanley real space Renormalization Group ideas (for bond percolation) with those contained in a recent Generalized Percolation formalism, we calculate the transition line in the T-p space for the random $\frac{1}{2}$ spin first-neighbour ferromagnetic Ising model in a square lattice. We obtain, within the smallest-order approximation, the exact limit and assymptotic behaviour for $T \to 0$ (bond percolation limit) and very satisfactory results in the limit $p \to 1$ (pure case limit).

RÉSUMÉ

Dans un cadre combinant les idées introduites par Reynolds, Klein et Stanley pour un Groupe de Rénormalisation dans l'espace réel pour la percolation de liaisons, avec celles contenues dans un récent formalisme de Percolation Généralisée, nous calculons la ligne de transition dans l'espace T-p d'un modèle d'Ising aléatoire avec des interactions ferromagnétiques entre spins $\frac{1}{2}$ premiers voisins dans un réseau carré. Nous obtenous, dans l'approximation de plus bas ordre, la limite et le comportement assymptotique exacts pour $T \to 0$ (limite de percolation de liaisons), ainsi que des résultats trés satisfaisants pour $p \to 1$ (limite du cas pur).

I - INTRODUCTION

In last years the site and bond percolation problems (for a review see Shante and Kirkpatrick (1971) and Essam (1972)) as well as the thermal random models (Syozi and Miyazima (1966), Mc Coy and Wu (1971), Harris and Lubensky (1974), Stinchcombe and Watson (1976), Toulouse (1977), Vannimenus and Toulouse (1977), Bergstresser (1977), Plischke and Zobin (1977), Fisch (1978) and Villain (1978)) have received great attention because of their wide application in a great variety of physical situations (dilute magnetism, spin glass, isolator-conductor transition, macromolecules, etc). Different theoretical approaches have been attempted, the most frequent being the Renormalization Group (RG) treatments (for a review see Wilson and Kogut (1974), Niemejer and Van Leeuwen (1974) and Wallace and Zia (1978)). Reynolds, Klein and Stanley (1977, RKS) have introduced a simple and performing real space RG treatment of the occupancy probability in the site and bond percolation problems. We have recently analyzed some aspects of this treatment in the square lattice (Tsallis and Schwachheim (1978) for site, and Magalhães, Schwachheim and Tsallis (1978, MST) for bond percolation). Plischke and Zobin (1978) discussed the behaviour of an Ising spin glass and a dilute Ising thermal models.

Very recently we have introduced (Tsallis (1978)) a formalism that generalizes the concept of bond percolation and contains the body of Statistical Mechanics as a particular case (we shall from now on refer to it as Generalized Percolation (GP)). Within this framework appears the central concept of fidelity a of a bond ($0 \leq a \leq 1$), which basically measures how well the bond transmits information. The present paper contains the first non trivial physical application of the GP formalism: the calculation of the transition line in the temperature T-bond concentration p space for a random $\frac{1}{2}$ spin first-neighbour ferromagnetic Ising model in a square lattice.

In Section II we obtain the fidelity of a H-shaped cluster or graph which plays a central role for bond percolation in square lattice (see RKS and MST); in Section III we establish a RG which leads (within this H-graph approximation) to the analytical relation between the probability or bond concentration p and the critical fidelity a_c (above which ferromagnetism appears); in Section IV we take advantage from the knowledge of the temperature dependence of the fidelity a (GP formalism) and present the transition line in the T-p space.

II - THE H-FIDELITY

II.1 - Generalities

The central purpose of this Section is to find the fidelity a_H of the H-graph (see Fig. 1), which will correspond (see RKS and MST), within the RG framework we shall introduce later, to "vertical" first-neighbour bond percolation in the square lattice (the difficulty arrives from the fact that the H-graph is not reducible in series-parallel terms). Let us one and for all point out that for vertical percolation (let us say through the H-graph in the sense down-up), where we admit entry (exit) of the information through any of the bottom (top) bonds, we can join (see Tsallis (1978)) all the bottom (top) bonds into a terminal node which we shall call the "input (output) node" (hence graphs (a) and (b) of Fig. 1 are equivalent for our purposes). Unfortunately we have not succeeded in elaborating a rigorous reasoning to obtain the functional dependence of a_H on its five single fidelities. However we present next three heuristic arguments (namely the dual graph, the bounds and the probabilities arguments) which will finally lead to an analytic expression for a_H which leaves no doubt about its correctness.

II.2 - The dual graph argument

In analogy with the concepts introduced in Linear Circuits Theory (as well as in the review by Syozi (1971)) we shall define the duality between two planar graphs G and G* by saying that they are superimposable in such a way that each bond of a graph crosses one and only one bond of the other and also that each internal (non terminal) node of one graph is sorrounded by an elementary mesh of the other (several examples are given in Fig. 2). Whenever a graph equals its dual (G = G*) we shall call it "self-dual" (examples (a) and (e) of Fig. 2). If a graph is reducible in series - parallel terms (examples (b), (c) and (d) of Fig. 2), then and only then the same happens with its dual. We may "decorate" a graph G with a set of fidelities $\{a_i\}$ (like in Fig. 1 or Fig. 2 (c)), and for this eventuality we shall use the notation $G\{a_i\}$. Furthermore, we introduce the notation $G^*\{1-a_i\}$ to mean that we have decorated the dual graph G* by attributing the "dual" fidelity $(1-a_i)$ to the bond which crosses the one whose fidelity is a_i in the original graph G (see the example (c) of Fig. 2).

We shall now state (without proof) the following property for the fidelity $a(G\{a_i\})$ of any decorated graph:

$$a(G\{a_i\}) + a(G^*\{1 - a_i\}) = 1 \qquad (1)$$

or, in compact words, "the fidelity of the dual equals the dual of the fidelity". This property is straightforwardly verifiable for any graph which may be reduced in series - parallel combinations of single bonds. As a corollary of (1) we obtain, for self-dual graphs, that

$$a(G\{a_i\}) + a(G\{1 - a_i\}) = 1 \qquad (1')$$

This expression leads, for the H-graph we are interested in (see Fig. 1), to

$$a_H(a_1, a_2, a_3, a_4, a_5) + a_H(1-a_3, 1-a_1, 1-a_4, 1-a_2, 1-a_5) = 1 \qquad (1'')$$

In the particular case $a_i = a \ \forall i$ we obtain, by introducing the compact notation $a_H(a)$,

$$a_H(a) + a_H(1 - a) = 1 \qquad (1''')$$

in others words, the graphical representation a_H vs a is centrosymmetric with respect to the point $(\frac{1}{2}, \frac{1}{2})$, and in particular $a_H(1/2) = 1/2$.

This is a good opportunity for writing down other two expected (symmetry) properties:

$$a_H(a_1, a_2, a_3, a_4, a_5) = a_H(a_3, a_4, a_1, a_2, a_5) \qquad (3.a)$$

$$= a_H(a_2, a_1, a_4, a_3, a_5) \qquad (3.b)$$

II.3 - The bounds argument

The fidelity of any graph is a monotonically increasing function with respect to each one of its single fidelities. This fact allows us to tighten a_H between an upper bound (noted a_M and obtained by decorating the central bond of the H-graph with an unitary fidelity instead of a_5, an operation which leads to the right graph of Fig. 2 (d)) and a lower bound (noted a_m and obtained by decorating the central bond with a vanishing fidelity, an operation which leads to the left graph of Fig. 2 (d)) whose fidelities are respectively given by (see Tsallis (1978)):

$$a_M = a_1 a_2 + a_2 a_3 + a_3 a_4 + a_4 a_1 - a_1 a_2 a_3 - a_2 a_3 a_4 - a_1 a_3 a_4 - a_1 a_2 a_4 + a_1 a_2 a_3 a_4 \qquad (3.a)$$

$$a_m = a_1 a_2 + a_3 a_4 - a_1 a_2 a_3 a_4 \qquad (3.b)$$

and the inequality states

$$a_m \leq a_H \leq a_M \qquad (4)$$

We may verify that expressions (3.a) and (3.b) verify the property (1), which, in the particular case where $a_i = a \ \forall \ i$, becomes

$$a_M(a) + a_m(1 - a) = 1 \qquad \text{(see Fig. 3)}$$

. with

$$a_M = 4a^2 - 4a^3 + a^4$$

$$a_m = 2a^2 - a^4$$

Furthermore, if we take into account the fact that the two percolation paths which include the central bond of the H-graph, give minor contributions into the percolation process, we have that

$$a_H(a) \sim a_M(a) \sim 1 - 2\,(1-a)^2 \qquad \text{if } a \to 1 \qquad (5.a)$$

$$a_H(a) \sim a_m(a) \sim 2a^2 \qquad \text{if } a \to 0 \qquad (5.b)$$

II.4 - The probabilities argument

In many aspects we do not intend to analyze here, the fidelities present a probabilistic mathematical structure. Let us exhibit this fact with the left graph of Fig . 2(c): its total fidelity a_G is given by (see Tsallis (1978))

$$a_G = a_1\, a_3 + a_2\, a_3 - a_1\, a_2\, a_3 \;;$$

on the other hand, if we make a standard reasoning (see RKS and MST) to calculate the probability p_G for this graph to percolate, we obtain

$$p_G = p_3\, p_1\, (1 - p_2) + p_3\, p_2\, (1 - p_1) + p_1\, p_2\, p_3$$

$$= p_1\, p_3 + p_2\, p_3 - p_1\, p_2\, p_3$$

Therefore we see that $a_G(a_1, a_2, a_3)$ and $p_G(p_1, p_2, p_3)$ have the same functional form. It is straightforward to verify this property for any graph reducible in series-parallel terms, and we shall assume that this is true for any graph. This leads to the end of our research, namely

$$a_H = a_1\,a_2(1-a_3)(1-a_4)(1-a_5) + a_3\,a_4(1-a_1)(1-a_2)(1-a_5)$$

$$+ a_1\,a_2\,a_5(1-a_3)(1-a_4) + a_1\,a_2\,a_4(1-a_5)(1-a_3)$$

$$+ a_1\,a_2\,a_3(1-a_5)(1-a_4) + a_3\,a_4\,a_5(1-a_1)(1-a_2)$$

$$+ a_3\,a_4\,a_2(1-a_5)(1-a_1) + a_3\,a_4\,a_1(1-a_5)(1-a_2)$$

$$+ a_1\,a_5\,a_4(1-a_2)(1-a_3) + a_3\,a_5\,a_2(1-a_1)(1-a_4)$$

$$+ a_1\,a_2\,a_3\,a_4(1-a_5) + a_1\,a_2\,a_3\,a_5(1-a_4) + a_1\,a_2\,a_4\,a_5(1-a_3)$$

$$+ a_1\,a_3\,a_4\,a_5(1-a_2) + a_2\,a_3\,a_4\,a_5(1-a_1) + a_1\,a_2\,a_3\,a_4\,a_5$$

$$= (1-a_5)\,a_m + a_5\,a_M \qquad (6)$$

This expression satisfies properties (1''), (2.a), (2.b) and becomes, in the particular case where $a_i = a \;\forall\, i$,

$$a_H(a) = 2a^2 + 2a^3 - 5a^4 + 2a^5 \qquad (6')$$

Naturally this expression satisfies (1''') and its assymptotic behaviours (for $a \to 1$ and $a \to 0$) are indeed those indicated in (5.a) and (5.b).

III - RENORMALIZATION GROUP

In this Section we shall atribute, to each single bond of a square lattice, a probability distribution (see Tsallis (1978))

$$P(a) = (1-p)\;\delta(a) + p\;\delta(a-a_0) \qquad (7)$$

for the aleatory fidelity a, with $0 \leq a_0 \leq 1$. The particular case $a_0 = 1$ corresponds to the traditional bond percolation problem. The distribution immediately leads to

$$\langle a \rangle_P \equiv \int_0^1 da\; P(a) = pa_0 \qquad (7')$$

The probability distribution P_H of the H-graph will then be given (see Table 1) by

$$\begin{aligned} P_H(a) = {} & (1-2p^2-2p^3+5p^4-2p^5)\ \delta(a) \\ & +2p^2(1-p)^2(1+2p)\ \delta(a-a_o^2) \\ & +2p^3(1-p)^2\ \delta(a-a_o^3) \\ & +p^4(1-p)\ \delta(a-2a_o^2+a_o^4) \\ & +4p^4(1-p)\ \delta(a-a_o^2-a_o^3+a_o^4) \\ & +p^5\ \delta(a-2a_o^2-2a_o^3+5a_o^4-2a_o^5) \end{aligned} \tag{8}$$

hence

$$\langle a \rangle_{P_H} = p^2 a_o^2 (2+2pa_o-5p^2a_o^2+2p^3a_o^3) \tag{8'}$$

Now, within the RG framework, we shall consider the H-graph as a renormalized "vertical" bond whose probability distribution P'(a) is given by

$$P'(a) = (1-p')\ \delta(a) + p'\ \delta(a-a_o') \tag{9}$$

hence

$$\langle a \rangle_{P'} = p'a_o' \tag{9'}$$

The group transformation is given by

$$\langle a \rangle_{P'} = \langle a \rangle_{P_H} \tag{10}$$

a relation which reproduces the RKS result in the particular case $a_o' = a_o = 1$. The fixed point of transformation (10) satisfies, by using (8') and (9') and after elimination of the trivial solution $pa_c = 0$,

$$pa_c(2+2pa_c-5p^2a_c^2+2p^3a_c^3) = 1$$

hence (by eliminating the other trivial solution: $pa_c = 1$)

$$pa_c = 1/2 \tag{11}$$

IV - THE RANDOM ISING MODEL

Though we have not said it explicitely, we have been working all the time under the assumption that the input (therefore the output) to each bond is a binary aleatory variable (see Tsallis (1978)). This is exactly the case of the $\frac{1}{2}$ spin Ising model, whose Hamiltonian may be written as follows

$$\mathcal{H} = -J \sum_{i,j} S_i^z S_j^z \qquad (J>0;\ S_i^z = \pm 1\ \forall i)$$

where (ij) are first neighbours in a square lattice. If we assume this system to be in thermodynamical equilibrium at temperature T, the fidelity of each bond is given by (Tsallis (1978))

$$a_o = \text{th}\,\frac{J}{k_B T} \tag{12}$$

The random model consists in that only a concentration p of bonds are (partially) activated, the rest being completely blocked (in other words, absent). The use of relations (11) and (12) leads to the transition line in the T-p space:

$$\frac{k_B T_c}{J} = \frac{1}{\text{argth}\ \frac{1}{2p}} \qquad \text{(see Fig. 4)}$$

In the limit $T \to 0$ we have

$$\frac{k_B T_c}{J} \sim - \frac{2}{\ln\,(p - \frac{1}{2})}$$

which leads not only to the exact value $p_c = \frac{1}{2}$ (see RKS and Shante and Kirkpatrick (1971)) for the critical probability for bond percolation, but also to the exact assymptotic behaviour (see Bergstresser (1977), Essam (1972),

Plischke and Zobin (1977) and Fisch (1978)).

On the other hand, in the pure case limit $p \to 1$, we obtain

$$\frac{k_B T_c}{J} \sim \frac{1}{\operatorname{argth} \frac{1}{2}} \left[1 - \frac{2}{3 \operatorname{argth} \frac{1}{2}} (1 - p) \right]$$

which leads to a Curie temperature

$$\frac{k_B T_c(1)}{J} = \frac{1}{\operatorname{argth} \frac{1}{2}} \simeq 1.82$$

to be compared with Onsager's exact solution (see for example Huang (1963)):

$\frac{k_B T_c(1)}{J} = \frac{2}{\operatorname{argsh} 1} \simeq 2.27$. This error may be considered as very acceptable if we remember that the H-cluster is the simplest we could have considered. Furthermore we have that

$$\frac{d}{dp} \left. \frac{T_c(p)}{T_c(1)} \right|_{p=1} = \frac{2}{3 \operatorname{argth} \frac{1}{2}} \simeq 1.21$$

to be compared with Plischke and Zobin's result ($\simeq 1.28$), and also with the result obtained for related (but different) Syozi model ($2(\sqrt{2} - 1)/\operatorname{argsh} 1 \simeq 0.94$; see for example Essam (1972)).

V - CONCLUSION

Let us conclude by saying that the present work exhibits how simple and compact can be the treatment of random thermal models within a framework that combines both the Generalized Percolation and the Renormalization Group ideas. In order to summarize our results, let us say that, in

spite of the fact that we have used the lowest-erder approximation (the H-graph) we have obtained, for the transition line in the T-p space (which separates the ferromagnetic from the paramagnetic regions) of the random $\frac{1}{2}$ spin first-neighbour Ising model in a square lattice, the following satisfactory results:

a) the exact value ($p_c = \frac{1}{2}$) for the critical probability in the limit $T \to 0$;

b) the exact assymptotic behaviour of T_c in the limit $T \to 0$, more precisely

$$\left.\frac{d\ e^{-2J/k_B T_c}}{dp}\right|_{p=\frac{1}{2}} = 1 \quad ;$$

c) a 20% error in the absolute value of the Curie temperature of the pure case (p = 1) (this error should sensibly decrease if higher-order graphs were used);

d) a 6% difference with Plischke and Zobin's result in what concerns the slope of $T_c(p)/T(1)$ in the limit $p \to 1$;

e) a 23% difference if we compare our result for the already mentioned slope, with the result obtained with the related (but different) Syozi model.

It is with pleasure that I aknowledge here fruitful discussions with C.G. Bollini, E.F.M. Curado and G. Schwachheim.

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CAPTION FOR FIGURES AND TABLE

Fig. 1 - The H-graph decorated with fidelities $\{a_i\}$; graphs (a) and (b) are equivalent; open (full) dots denote the terminal (internal) nodes of the graph.

Fig. 2 - Several examples of dual graphs; (a) and (e)-graphs are self-dual; the two (d)-graphs are limiting cases of the (e)-graph; the (c)-graphs are decorated ones; the (e) and (f) graphs are in general not reducible into series-parallel arrangements.

Fig. 3 - Fidelities of the H-graph $a_H(a)$ and of the right-side-(d) graph (a_M (a)) and the left-side-(d) graph ($a_m(a)$) of Fig. 2, as functions of the elementary bond fidelity a (the same for all the bonds); $a \to o$ implies $a_H \sim a_m \sim 2a^2$ and $a_M \sim 4a^2$, and $a \to 1$ implies $a_H \sim a_M \sim 1 - 2(1 - a)^2$ and $a_m \sim 1 - 4(1-a)^2$.

Fig. 4 - The reduced critical temperature as a function of the bond concentration (P and F denote the paramagnetic and ferromagnetic regions respectively).

Table 1- Contributions to $P_H(a)$ associated to each occupancy configuration of the H-graph; only the topologically non equivalent configurations are indicated; occupied bonds are marked with x.

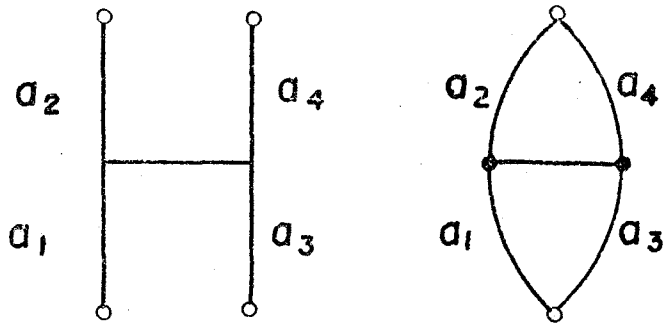


FIG. 1

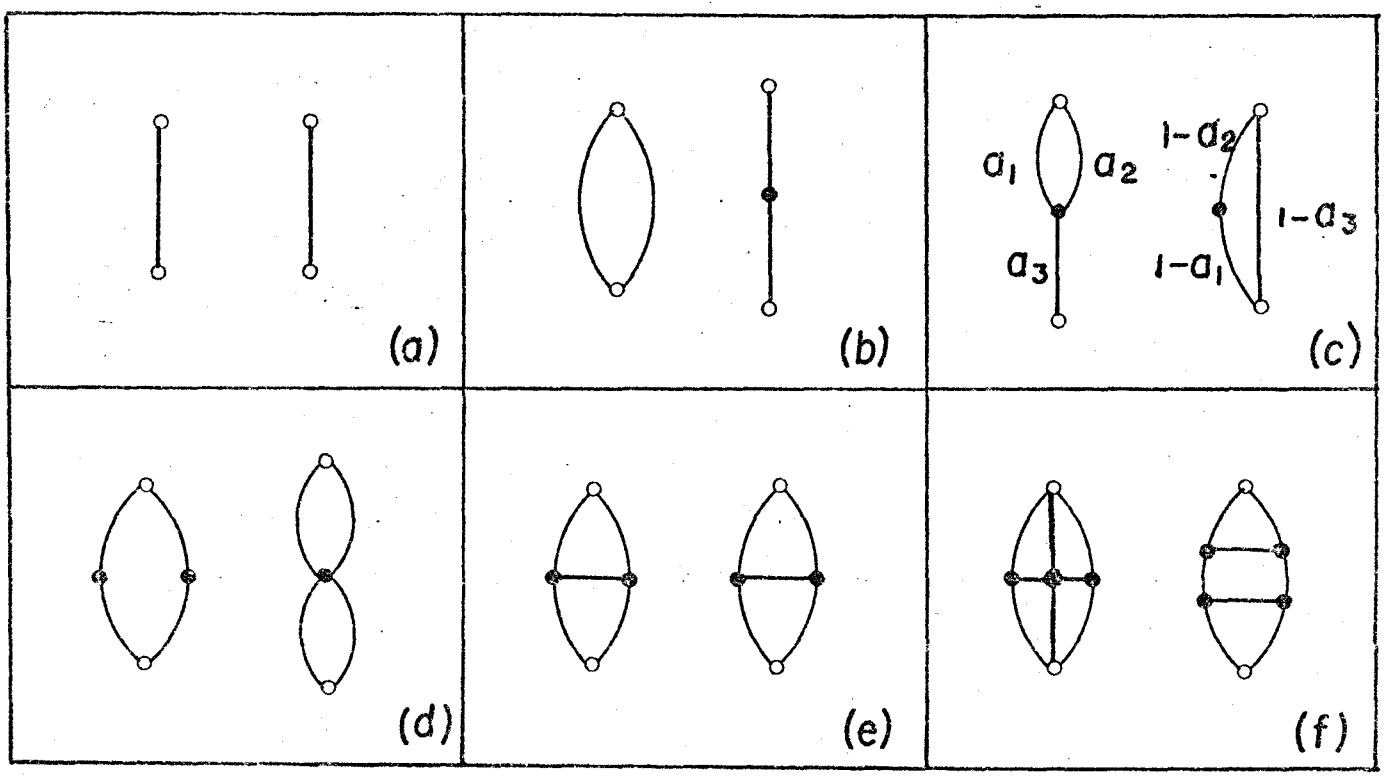


FIG. 2

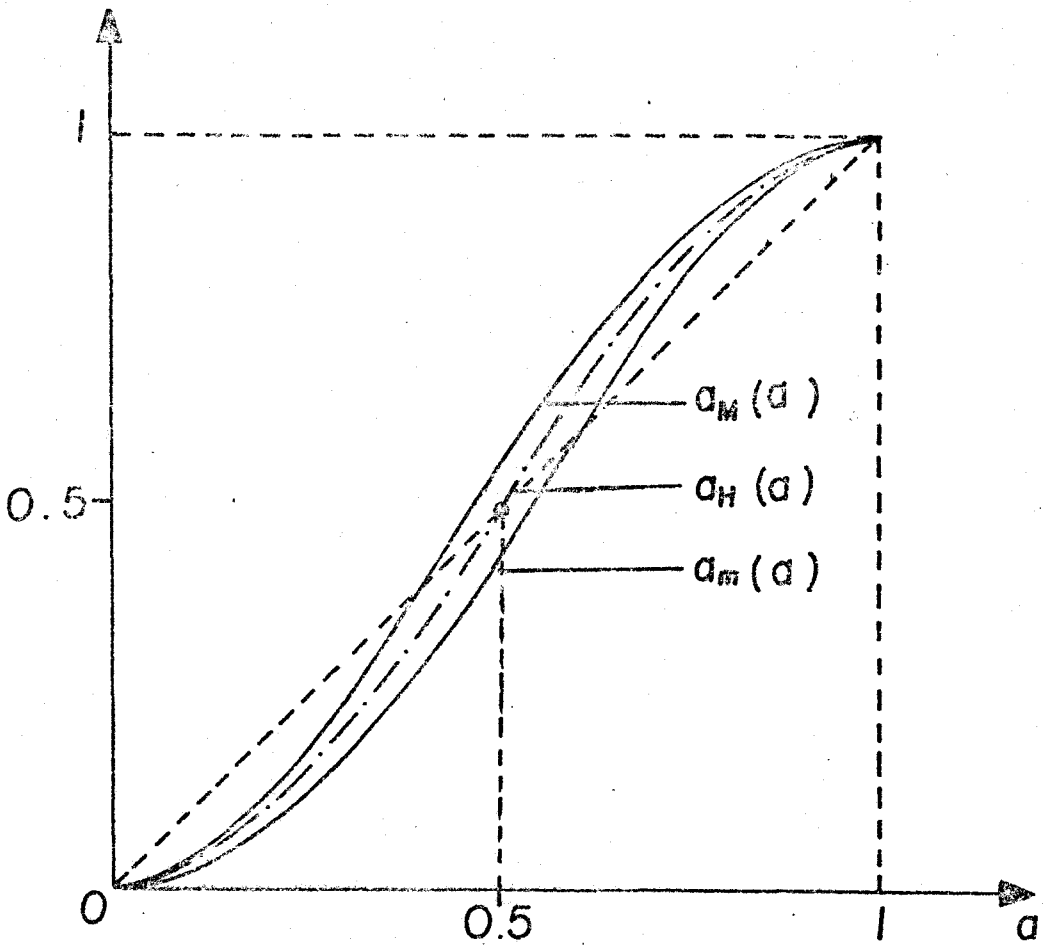


FIG. 3

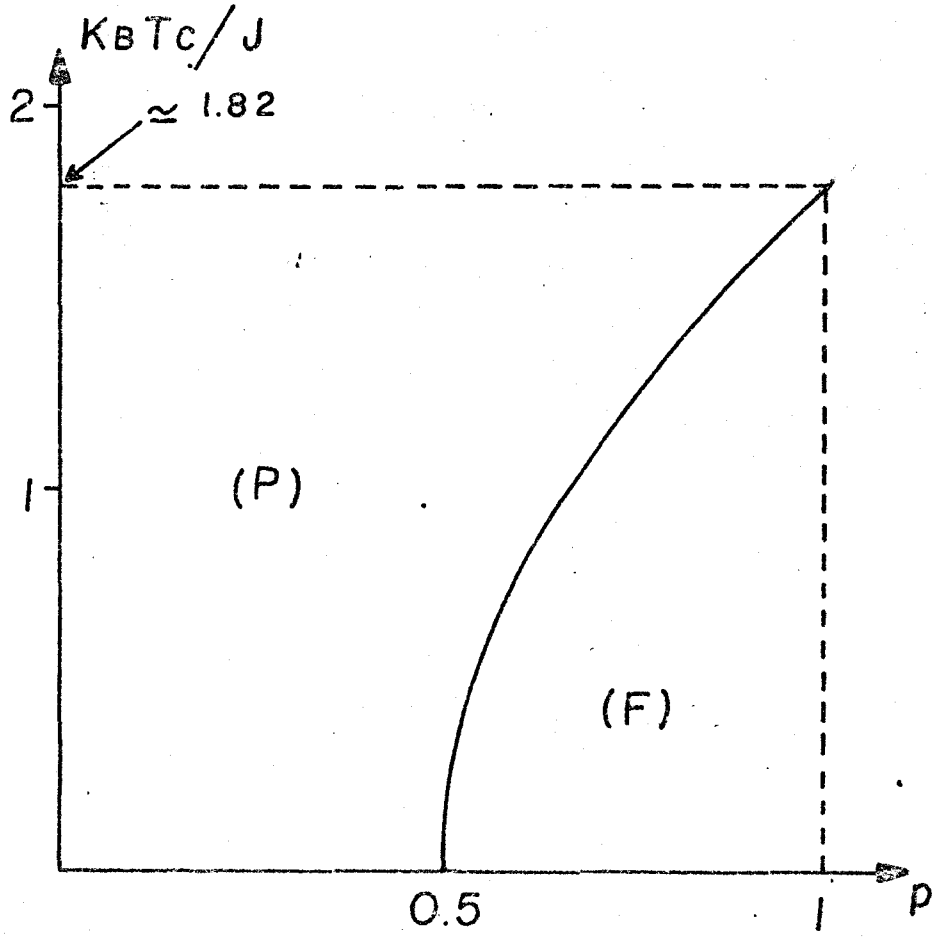
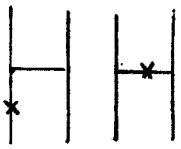
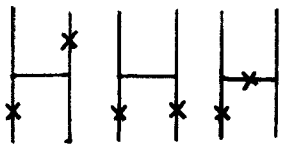
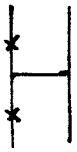
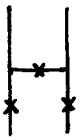
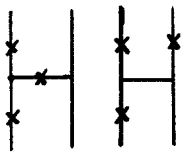
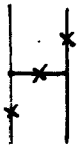
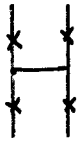
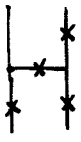
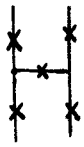


FIG. 4

Table 1

Graph configuration	Contribution
	$(1-p)^5\,\delta(a)$
	$5p(1-p)^4\,\delta(a)$
	$8p^2(1-p)^3\,\delta(a)$
	$2p^2(1-p)^3\,\delta(a-a_o^2)$
	$2p^3(1-p)^2\,\delta(a)$
	$6p^3(1-p)^2\,\delta(a-a_o^3)$
	$2p^3(1-p)^2\,\delta(a-a_o^3)$
	$p^4(1-p)\,\delta(a-2a_o^2+a_o^4)$
	$4p^4(1-p)\,\delta(a-a_o^2-a_o^3+a_o^4)$
	$p^5\,\delta(a-2a_o^2-2a_o^3+5a_o^4-2a_o^5)$