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THE DILUTED TRI-DIMENSIONAL SPIN-ONE ISING MODEL  
WITH CRYSTAL FIELD INTERACTIONS \*

M. Saber \*\*

International Centre for Theoretical Physics, Trieste, Italy  
and  
Dipartimento di Fisica, Università di Napoli,  
Mostra d'Oltremare, Pad. 19, Napoli, Italy.

ABSTRACT

3D spin-one Ising models with nearest-neighbour ferromagnetic interactions with crystal-field exhibit tricritical behaviour. A new method that applies to a wide class of random systems is used to study the influence of site and bond dilution on this behaviour. We have calculated temperature-crystal-field-concentration phase diagrams and determined, in particular, the influence of dilution on the zero temperature tricritical temperature.

MIRAMARE - TRIESTE  
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\*\* Permanent address: Laboratoire de Magnétisme, Département de Physique, Faculté des Sciences, B.P. 1014, Rabat, Morocco and Département de Physique, Faculté des Sciences, B.P. 4050, Meknes, Morocco.

1. INTRODUCTION

The magnetic properties of amorphous and disordered materials have been the object of much interest both from the experimental and from the theoretical point of view. We wish to point out in this paper the relevance of a simple formalism, the finite-cluster approximation (FCA), introduced recently by Boccara <sup>1)</sup>, for the determination of the phase diagrams of such materials.

Indeed, where the interest of the investigation lies more on the determination of non-universal properties like the phase diagram, it pays to approach the problem with methods (like FCA) that appear as a systematic improvement over mean-field theory <sup>2)</sup>, instead of applying the admittedly more sophisticated, but clumsier, methods like the real-space renormalization group (RSRG).

In particular, site-dilution (which is physically more relevant than bond-dilution) is much easier to study within FCA. Another advantage is that it is not necessary to introduce ad hoc approximations for the renormalized probability distribution of the interactions, not to choose in a more or less arbitrary way the "right" random variable over which to average <sup>3)-5)</sup>.

We discuss in this paper the application of FCA to the diluted spin-one Ising model on the simple cubic lattice. The presence of the crystal-field interactions gives a richer phase diagram.

To make the paper self-contained we review in Sec. 2 the application of FCA to the pure spin-one half Ising model. The pure spin-one Ising model is introduced and treated in Sec. 3. The diluted model is discussed in Sec. 4. Sec. 5 contains a brief discussion of the results.

2. PURE SPIN-ONE HALF ISING MODEL

Let us describe the application of FCA to a pure spin-one half Ising model with nearest-neighbour interactions. The Hamiltonian is:

$$H = -J \sum_{(i,j)} \sigma_i \sigma_j \quad (2.1)$$

where  $J > 0$ ,  $\sigma_i = \pm 1$  and the summation runs over all pairs of nearest neighbours.

If  $\langle \sigma_0 \rangle_c$  denotes the same value of  $\sigma_0$  for a given configuration  $c$  for all other spins, i.e. when all other spins  $\sigma_i$  ( $i \neq 0$ ) have fixed values we have:

$$\langle \sigma_0 \rangle_c = \left( \frac{\text{Tr}_{\sigma_0} \sigma_0 \exp(-\beta H)}{\text{Tr}_{\sigma_0} \exp(-\beta H)} \right) = \tanh \left( K \sum_{i=1}^z \sigma_i \right) \quad (2.2)$$

where  $K = \beta J$  and the summation is extended over the  $z$  nearest neighbours  $\sigma_i$  ( $i = 1, 2, \dots, z$ ) of  $\sigma_0$ . The  $\sigma_0$  appearing under "Tr" indicates that the trace is performed over  $\sigma_0$  only. Relation (2.2) is exact and the magnetization per site which is the thermal average  $m$  of  $\sigma_0$  is obtained by averaging  $\tanh \left( K \sum_{i=1}^z \sigma_i \right)$  over all configurations. This is a formidable task and the mean-field approximation corresponds to the very crude estimate

$$\left\langle \tanh \left( K \sum_{i=1}^z \sigma_i \right) \right\rangle = \tanh(zK m)$$

which corresponds to the probability distribution:

$$P_{MF}(\{\sigma_i\}) = \prod_i \delta(\sigma_i - m)$$

As the random variables  $\sigma_i$  take the values  $-1$  and  $+1$ , a better choice is:

$$P_{FCA}(\{\sigma_i\}) = \prod_i \left( \frac{1+m}{2} \delta(\sigma_i - 1) + \frac{1-m}{2} \delta(\sigma_i + 1) \right) \quad (2.3)$$

which still neglects correlations between different spins but takes exactly into account relations like  $\sigma_i^2 = 1$ .

To average  $\tanh \left( K \sum_{i=1}^z \sigma_i \right)$  when the  $\sigma_i$  are distributed according to this approximate probability law, it is easier to use the following theorem: the set of all bounded real functions of  $\sigma_1, \sigma_2, \dots, \sigma_z$  is a  $2^z$ -dimensional Euclidean space. The set  $\{1, \sigma_1, \dots, \sigma_z, \sigma_1 \sigma_2, \dots, \sigma_1 \sigma_2 \dots \sigma_z\}$ , which contains all the product of different spins, is an orthonormal basis for the inner product defined by

$$\langle \beta_1 | \beta_2 \rangle = \frac{1}{2^z} \text{Tr}_{\sigma_1, \dots, \sigma_z} \beta_1(\sigma_1, \dots, \sigma_z) \beta_2(\sigma_1, \dots, \sigma_z) \quad (2.4)$$

If, for instance  $z = 4$  (square lattice) we have:

$$\begin{aligned} \tanh[K(\sigma_1 + \sigma_2 + \sigma_3 + \sigma_4)] &= \frac{1}{8} (\tanh 4K + 2 \tanh 2K) (\sigma_1 + \sigma_2 + \sigma_3 + \sigma_4) + \\ &+ \frac{1}{8} (\tanh 4K - 2 \tanh 2K) (\sigma_3 \sigma_4 + \sigma_2 \sigma_3 + \sigma_1 \sigma_3 + \sigma_1 \sigma_2 \sigma_3) \end{aligned} \quad (2.5)$$

and when we average the right-hand side of (2.5) with (2.3), we obtain the equation of state:

$$m = \frac{1}{2} (\tanh 4K + 2 \tanh 2K) m + \frac{1}{2} (\tanh 4K - 2 \tanh 2K) m^3 \quad (2.6)$$

which determines  $m$  over the whole temperature range. Within this approximation the critical temperature is the solution of:

$$1 = \frac{1}{2} (\tanh 4K + 2 \tanh 2K) \quad (2.7)$$

That is,  $T_c = K_c^{-1} = 3.09$ , which is to be compared with the mean-field result  $T_c = 4$  and with the exact Onsager value  $T_c = 2.27$ . Eq.(2.6) has been obtained within the zeroth-order approximation. We define the first-order approximation for  $\langle \sigma_0 \rangle_c$  performing the traces over  $\sigma_0$  and its first neighbour  $\sigma_1, \sigma_2, \sigma_3$  and  $\sigma_4$ , all other spins of the lattice having fixed values. It is clear that the expression for  $\langle \sigma_0 \rangle_c$  in this case will depend only on the spins  $\sigma_5, \sigma_6, \dots, \sigma_{12}$  (Fig. 1) which are the external first neighbours of the spins belonging to the border of the cluster  $\{\sigma_0, \sigma_1, \sigma_2, \sigma_3, \sigma_4\}$ . Taking into account the theorem given above,  $\langle \sigma_0 \rangle_c$  can be written in the form of a polynomial and then averaged as we did for the zeroth-order approximation. We shall not write down explicitly the equation of state  $m = f(K, m)$  which is rather complicated. The second-order approximation for  $\langle \sigma_0 \rangle_c$  is defined with traces performed over the spins belonging to the cluster  $\{\sigma_0, \sigma_1, \dots, \sigma_{12}\}$  and more generally the  $n^{\text{th}}$ -order approximation is defined, in an obvious way, by traces performed over all the spins of a cluster centred on  $\sigma_0$  containing  $1 + 4 + 8 + \dots + 4n = 1 + 4n(n+1)/2$  spins, all the spins of the lattice not belonging to this cluster having fixed values. The expression for

$\langle \sigma_0 \rangle_c$ , which is exact, depend only on the external first neighbours of the spins of the border of the cluster considered. Here again, after having written  $\langle \sigma_0 \rangle_c$ , in polynomial form, we average this last expression neglecting correlations between different spins.

### 3. THE PURE SPIN-ONE ISING MODEL

We consider in this section the spin-one Ising model with crystal-field interactions, defined by the Hamiltonian:

$$H = -J \sum_{(i,j)} S_i S_j + \Delta \sum_i S_i^2$$

where  $J > 0$ ,  $\Delta > 0$ ,  $S_i = -1, 0, +1$  and the first summation runs over all nearest-neighbour pairs.

This model exhibits a tricritical point in the  $T-\Delta$  phase diagram <sup>6)-9)</sup>. The influence of bond and site dilution on the tricritical behaviour for the bidimensional case has been studied using a RSRG technique <sup>5)</sup> for bond dilution and the FCA for both bond and site dilution <sup>10)</sup>.

In this paper we study the influence of site and bond dilution on the tricritical behaviour for the tridimensional case within the framework of the FCA. This method, which leads to systematic successive approximations <sup>2)</sup>, is much less sophisticated than RSRG and applies to a wide class of disordered systems.

If we put the spins on a simple cubic-lattice, the zeroth-order FCA (the only one we shall make here) leads to the following equations (we use the notations  $K = \beta J$ ,  $L = \beta \Delta$ ):

$$\langle S_0 \rangle_c = \frac{\sinh [K(S_1 + S_2 + S_3 + S_4 + S_5 + S_6)]}{\cosh [K(S_1 + S_2 + S_3 + S_4 + S_5 + S_6)] + (\exp(L))/2} \quad (3.1)$$

$$\langle S_0^2 \rangle_c = \frac{\cosh [K(S_1 + S_2 + S_3 + S_4 + S_5 + S_6)]}{\cosh [K(S_1 + S_2 + S_3 + S_4 + S_5 + S_6)] + (\exp(L))/2} \quad (3.2)$$

The theorem quoted previously concerns functions of spins  $\frac{1}{2}$ . It can be easily extended to functions of spins 1. Note that for a single spin,  $\{1, S, S^2\}$  is not an orthogonal basis. Eqs.(3.1) and (3.2) take the forms:

$$\begin{aligned} \langle S_0 \rangle_c = & A_1 \sum_{i \in G} S_i + A_2 \sum_{i \neq j} S_i^2 S_j^2 + \\ & + \sum_{i \neq j \neq k} (A_3 S_i S_j S_k + A_4 S_i^2 S_j^2 S_k) + \\ & + \sum_{i \neq j \neq k \neq l} (A_5 S_i S_j S_k S_l + A_6 S_i^2 S_j^2 S_k^2 S_l) + \\ & + \sum_{i \neq j \neq k \neq l \neq m} (A_7 S_i S_j S_k S_l S_m + A_8 S_i^2 S_j^2 S_k^2 S_l S_m + A_9 S_i^2 S_j^2 S_k^2 S_l^2 S_m) + \\ & + \sum_{i \neq j \neq k \neq l \neq m \neq n} (A_{10} S_i S_j S_k S_l S_m S_n + A_{11} S_i^2 S_j^2 S_k^2 S_l S_m S_n + A_{12} S_i^2 S_j^2 S_k^2 S_l^2 S_m S_n) \end{aligned} \quad (3.3)$$

$$\langle S_0^2 \rangle_c = B_0 + B_1 \sum_{i \in G} S_i^2 + \sum_{i \neq j} (B_2 S_i S_j + B_3 S_i^2 S_j^2) +$$

$$+ \sum_{\substack{i+j+k \\ 1 \leq i,j,k \leq 6}} (B_4 S_i^2 S_j^2 S_k^2 + B_5 S_i^2 S_j^2 S_k^2) +$$

$$+ \sum_{\substack{i+j+k+l \\ 1 \leq i,j,k,l \leq 6}} (B_6 S_i^2 S_j^2 S_k^2 S_l^2 + B_7 S_i^2 S_j^2 S_k^2 S_l^2 + B_8 S_i^2 S_j^2 S_k^2 S_l^2) +$$

$$+ \sum_{\substack{i+j+k+l+m \\ 1 \leq i,j,k,l,m \leq 6}} (B_9 S_i^2 S_j^2 S_k^2 S_l^2 S_m^2 + B_{10} S_i^2 S_j^2 S_k^2 S_l^2 S_m^2 + B_{11} S_i^2 S_j^2 S_k^2 S_l^2 S_m^2) +$$

$$+ \sum_{\substack{i+j+k+l+m+n \\ 1 \leq i,j,k,l,m,n \leq 6}} (B_{12} S_i^2 S_j^2 S_k^2 S_l^2 S_m^2 S_n^2 + B_{13} S_i^2 S_j^2 S_k^2 S_l^2 S_m^2 S_n^2 + B_{14} S_i^2 S_j^2 S_k^2 S_l^2 S_m^2 S_n^2 + B_{15} S_i^2 S_j^2 S_k^2 S_l^2 S_m^2 S_n^2) \quad (3.4)$$

The coefficients are functions of  $K$  and  $L$ . They are given in the Appendix. The averages of (3.3) and (3.4) over all configurations give:

$$m = 6A_1 m + 30A_2 m x + 80A_3 m^2 + 60A_4 m x^2 + 60A_5 m^2 x + 60A_6 m x^3 + 6A_7 m^5 + 60A_8 m^3 x^3 + 30A_9 m x^4 + 6A_{10} m^5 x + 20A_{11} m^3 x^3 + 6A_{12} m x^5 \quad (3.5)$$

$$x = B_0 + 6B_1 x + 15B_2 m^2 + 15B_3 x^2 + 60B_4 m^2 x + 20B_5 x^3 + 15B_6 m^4 + 30B_7 m^2 x^2 + 15B_8 x^4 + 30B_9 m^4 x + 60B_{10} m^2 x^3 + 6B_{11} x^5 + B_{12} m^6 + 15B_{13} m^4 x^4 + 15B_{14} m^2 x^4 + B_{15} x^6 \quad (3.6)$$

where  $\langle S \rangle = m$  and  $\langle S^2 \rangle = x$ .

If we replace  $x$  in (3.5) by its expression taken from (3.6) we obtain an equation for  $m$  of the form:

$$m = am + bm^3 + cm^5 + \dots \quad (3.7)$$

The second-order transition line in the  $T$ - $\Delta$  plane is determined by  $1 = a$ , i.e.

$$1 = 6A_1 + 30A_2 x_0 + 60A_4 x_0^2 + 60A_6 x_0^3 + 30A_8 x_0^4 + 6A_{12} x_0^5 \quad (3.8)$$

where  $x_0$  is the solution of

$$x_0 = B_0 + 6B_1 x_0 + 15B_2 x_0^2 + 20B_5 x_0^3 + 15B_8 x_0^4 + 6B_{11} x_0^5 + B_{15} x_0^6 \quad (3.9)$$

In the vicinity of the second-order transition line the magnetization  $m$  is given by:

$$m^2 = \frac{1-a}{b}$$

The right-hand side must be positive. If this is not the case, the transition is of the first-order in the  $T$ - $\Delta$  plane, the point at which  $1 = a$  and  $b = 0$  is the tricritical point. To obtain the expression for  $b$ , one has to solve (3.6) for small  $m$ . The solution is of the form:

$$x = x_0 + x_1 m^2$$

where  $x_1$  is given by:

$$x_1 = 6B_1 x_1 + 15B_6 + 30B_7 x_0 x_1 + 60B_4 x_0 + 60B_5 x_0^2 x_1 + 90B_7 x_0^2 + 60B_8 x_0^3 x_1 + 60B_{10} x_0^3 + 30B_{11} x_0^4 x_1 + 15B_{14} x_0^4 + 6B_{15} x_0^5 x_1$$

i.e.

$$x_1 = \frac{15B_6 + 60B_4 x_0 + 90B_7 x_0^2 + 60B_{10} x_0^3 + 15B_{14} x_0^4}{1 - 6B_1 - 30B_7 x_0 - 60B_5 x_0^2 - 60B_8 x_0^3 - 30B_{11} x_0^4 - 6B_{15} x_0^5} \quad (3.10)$$

This yields:

$$b = 30A_2 x_2 + 20A_3 + 120A_4 x_0 x_2 + 60A_5 x_0 + 180A_6 x_0^2 x_2 + 60A_8 x_0^3 + 120A_9 x_0^3 x_2 + 20A_{10} x_0^3 + 30A_{11} x_0^4 x_2 \quad (3.11)$$

The coordinates of the tricritical point are  $T = 1.667J$ ,  $\Delta = 2.81J$ . The mean-field approximation gives  $T = 2J$ ,  $\Delta = [4 \ln(2)]J \approx 2.77J$ . At  $T=0$  the transition is of first order. The  $\Delta$ -coordinate of the transition point is given by:

$$-3J + \Delta = 0 \quad (3.12)$$

This is obtained by equating the energies of the ferro- and paramagnetic phases. To determine the first order transition line one can, for example proceed as follows: apply an external magnetic field  $h$  and use the FCA to derive the analogues of Eqs.(3.5) and (3.6). Solve for  $x$  to obtain the equation of state  $m(T,h)$ . In the case of a first order transition the isotherms have the typical S shape of the Van der Waals isotherms and as usual the first order transition point in the  $T$ - $h$  plane is determined by the Maxwell rule. Extrapolate  $h = 0$  to obtain the first order transition temperature as function of  $\Delta$ . The phase diagram is represented in Fig. 2.

#### 4. THE DILUTE SYSTEM

Extension of this method to the less trivial case of random models is straightforward. If, for instance, the interactions are random variables, the mean values  $\langle S_0 \rangle_c$  and  $\langle S_0^2 \rangle_c$ , when all other spins  $S_i$  ( $i \neq 0$ ) and all interactions  $K_{ij}$  and fields  $L_i$  have fixed values, are for the simple cubic lattice given by:

$$\langle S_0 \rangle_c = \frac{\sinh(K_{02}S_2 + K_{03}S_3 + K_{04}S_4 + K_{05}S_5 + K_{06}S_6)}{\cosh(K_{02}S_2 + K_{03}S_3 + K_{04}S_4 + K_{05}S_5 + K_{06}S_6) + \frac{\exp(L_0)}{8}} \quad (4.1)$$

$$\langle S_0^2 \rangle_c = \frac{\cosh(K_{02}S_2 + K_{03}S_3 + K_{04}S_4 + K_{05}S_5 + K_{06}S_6)}{\cosh(K_{02}S_2 + K_{03}S_3 + K_{04}S_4 + K_{05}S_5 + K_{06}S_6) + \frac{\exp(L_0)}{8}} \quad (4.2)$$

The theorem from which we obtained (3.3) and (3.4) from (3.1) and (3.2) can be used here. It gives:

$$\begin{aligned} \langle S_0 \rangle_c = & \sum_{1 \leq i \leq 6} A_1(i) S_i + \sum_{\substack{i \neq j \\ 1 \leq i, j \leq 6}} A_2(i, j) S_i^2 S_j + \\ & + \sum_{\substack{i \neq j \neq k \\ 1 \leq i, j, k \leq 6}} (A_3(i, j, k) S_i S_j S_k + A_4(i, j, k) S_i^2 S_j^2 S_k) + \\ & + \sum_{\substack{i \neq j \neq k \neq l \\ 1 \leq i, j, k, l \leq 6}} (A_5(i, j, k, l) S_i^2 S_j S_k S_l + A_6(i, j, k, l) S_i^2 S_j^2 S_k^2 S_l) + \\ & + \sum_{\substack{i \neq j \neq k \neq l \neq m \\ 1 \leq i, j, k, l, m \leq 6}} (A_7(i, j, k, l, m) S_i S_j S_k S_l S_m + \\ & + A_8(i, j, k, l, m) S_i^2 S_j^2 S_k S_l S_m + A_9(i, j, k, l, m) S_i^2 S_j^2 S_k^2 S_l S_m) + \\ & + \sum_{\substack{i \neq j \neq k \neq l \neq m \neq n \\ 1 \leq i, j, k, l, m, n \leq 6}} (A_{10}(i, j, k, l, m, n) S_i S_j S_k S_l S_m S_n + \\ & + A_{11}(i, j, k, l, m, n) S_i^2 S_j^2 S_k^2 S_l S_m S_n + A_{12}(i, j, k, l, m, n) S_i^2 S_j^2 S_k^2 S_l^2 S_m S_n) \end{aligned} \quad (4.3)$$

$$\begin{aligned} \langle S_0^2 \rangle_c = & B_0(0) + \sum_{1 \leq i \leq 6} B_1(i) S_i^2 + \sum_{\substack{i \neq j \\ 1 \leq i, j \leq 6}} (B_2(i, j) S_i S_j + B_3(i, j) S_i^2 S_j^2) + \\ & + \sum_{\substack{i \neq j \neq k \\ 1 \leq i, j, k \leq 6}} (B_4(i, j, k) S_i^2 S_j S_k + B_5(i, j, k) S_i^2 S_j^2 S_k^2) + \\ & + \sum_{\substack{i \neq j \neq k \neq l \\ 1 \leq i, j, k, l \leq 6}} (B_6(i, j, k, l) S_i S_j S_k S_l + \end{aligned}$$

$$\begin{aligned}
& + B_7(i,j,k,l) S_i^+ S_j^+ S_k^+ S_l^+ + B_8(i,j,k,l) S_i^+ S_j^+ S_k^+ S_l^+ \\
& + \sum_{\substack{i+j+k+l=m \\ 1 \leq i,j,k,l,m \leq 6}} (B_9(i,j,k,l,m) S_i^+ S_j^+ S_k^+ S_l^+ S_m^+ + \\
& + B_{10}(i,j,k,l,m) S_i^+ S_j^+ S_k^+ S_l^+ S_m^+ + B_{11}(i,j,k,l,m) S_i^+ S_j^+ S_k^+ S_l^+ S_m^+) + \\
& + \sum_{\substack{i+j+k+l+m+n \\ 1 \leq i,j,k,l,m,n \leq 6}} (B_{12}(i,j,k,l,m,n) S_i^+ S_j^+ S_k^+ S_l^+ S_m^+ S_n^+ + B_{13}(i,j,k,l,m,n) S_i^+ S_j^+ S_k^+ S_l^+ S_m^+ S_n^+ + \\
& + B_{14}(i,j,k,l,m,n) S_i^+ S_j^+ S_k^+ S_l^+ S_m^+ S_n^+ + B_{15}(i,j,k,l,m,n) S_i^+ S_j^+ S_k^+ S_l^+ S_m^+ S_n^+) \quad (4.4)
\end{aligned}$$

For a bond-diluted system  $K_{01} = Kn_1$  and  $L_0 = L$ , where  $n_1$  is the occupation number of bond 0t. The coefficients of the polynomials (4.3) and (4.4) are functions of the discrete random variables  $n_1, n_2, n_3, n_4, n_5$  and  $n_6$ .

To average first over all spin configurations and then over disorder, we use the same theorem, writing all functions of  $n_1, n_2, n_3, n_4, n_5$  and  $n_6$  in polynomial forms. This leads to the following equations:

$$\begin{aligned}
m &= 6\bar{A}_1 m + 30\bar{A}_2 m x + 60\bar{A}_3 m^2 + 60\bar{A}_4 m x^2 + 60\bar{A}_5 m^3 x + \\
& + 60\bar{A}_6 m x^3 + 6\bar{A}_7 m^5 + 60\bar{A}_8 m^3 x^2 + 30\bar{A}_9 m x^4 + \\
& + 6\bar{A}_{10} m^5 x + 20\bar{A}_{11} m^3 x^3 + 6\bar{A}_{12} m x^5 \quad (4.5)
\end{aligned}$$

$$\begin{aligned}
x &= \bar{B}_0 + 6\bar{B}_1 x + 15\bar{B}_2 m^2 + 15\bar{B}_3 x^2 + 60\bar{B}_4 m^2 x + \\
& + 20\bar{B}_5 x^3 + 15\bar{B}_6 m^4 + 90\bar{B}_7 m^2 x^2 + 15\bar{B}_8 x^4 + \\
& + 30\bar{B}_9 m^4 x + 60\bar{B}_{10} m^2 x^3 + 6\bar{B}_{11} x^5 + \bar{B}_{12} m^6 + \\
& + 15\bar{B}_{13} m^4 x^2 + 15\bar{B}_{14} m^2 x^4 + \bar{B}_{15} x^6 \quad (4.6)
\end{aligned}$$

where, whatever value  $i$  takes  $\bar{A}_i(i) = \bar{A}_i$ , etc. The bars over the coefficients indicate that they have been averaged over disorder. These coefficients are functions of  $K, L$  and  $\langle n \rangle = p$  and they are given in the Appendix.

To obtain the  $T$ - $\Delta$ - $p$  phase diagram (Fig. 3) we proceed as in the previous section. Eqs.(4.5) and (4.6) are similar to Eqs.(3.5) and (3.6) except that in (4.5) and (4.6) the coefficients are not functions of only  $T$  and  $\Delta$  but depend also on  $p$ .

The phase diagram we obtained within the FCA for the tridimensional case has exactly the same qualitative features as the phase diagrams, derived from Benayed et al. and Dickinson et al. for the bidimensional case: the same variation of the tricritical point as a function of  $p$  (Fig. 5).

For a site diluted system  $K_{01} = Kn_0 n_1$  where  $n_0$  and  $n_1$  are the occupation numbers of sites 0 and 1. A simple calculation shows that  $m$  and  $x$  are given by Eqs. (4.5) and (4.6) where the coefficients are functions of  $K, L$  and  $p$ . Their dependences of these variables are the same as for the bond problem except that they are all multiplied by an extra factor  $p$  and that on the right-hand side of Eq.(4.6) an extra term of the form  $\frac{2}{3}(1-p)$  has to be added.

The corresponding phase diagrams are given respectively in Figs. 6, 7 and 8 for the  $T$ - $\Delta$ - $p$  phase diagram, the variation of  $\Delta$  as a function of  $p$  for  $T=0$  and the variation of the tricritical point as a function of  $p$ .

## 5. CONCLUSION

FCA has allowed us to recover by means of a comparatively simple calculation phase diagrams for the diluted tridimensional spin one Ising model with crystal field interactions which has the same qualitative features of the ones obtained from FCA and RSRG for the bidimensional case. FCA allows one to treat as easily site percolation as bond percolation and appears to be a rather powerful method to calculate non-critical properties.

One should however remark a few short-comings of the method: one is common to all mean-field-like methods, namely that is necessary to identify the order parameter beforehand and it is essential for the approximation to work that the spins have a finite number of states each, in order to provide a finite algebra; and the number of terms in the approximate increases rapidly as the number of states of each spin is increased.

ACKNOWLEDGMENTS

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APPENDIX

We put:

$$f(n) = \frac{\sinh(nK)}{\cosh(nK) + \frac{\exp(L)}{2}}, \quad g(n) = \frac{\cosh(nK)}{\cosh(nK) + \frac{\exp(L)}{2}}$$

where  $K = \beta J$ ,  $L = \beta \Delta$  and  $n$  an integer number.

Coefficients of Eqs. (3.5) and (3.6):

$$A_1 = f(1)$$

$$A_2 = \frac{1}{2}[f(2) - 2f(1)]$$

$$A_3 = \frac{1}{4}[f(3) - 3f(1)]$$

$$A_4 = \frac{1}{4}[f(3) - 4f(2) + 5f(1)]$$

$$A_5 = \frac{1}{8}[f(4) - 2f(3) - 2f(2) + 6f(1)]$$

$$A_6 = \frac{1}{8}[f(4) - 6f(3) + 14f(2) - 14f(1)]$$

$$A_7 = \frac{1}{16}[f(5) - 5f(3) + 10f(1)]$$

$$A_8 = \frac{1}{16}[f(5) - 4f(4) + 3f(3) + 8f(2) - 14f(1)]$$

$$A_9 = \frac{1}{16}[f(5) - 8f(4) + 27f(3) - 48f(2) + 42f(1)]$$

$$A_{10} = \frac{1}{32}[f(6) - 2f(5) - 4f(4) + 10f(3) + 5f(2) - 20f(1)]$$

$$A_{11} = \frac{1}{32}[f(6) - 6f(5) + 12f(4) - 2f(3) - 27f(2) + 36f(1)]$$

$$A_{12} = \frac{1}{32}[f(6) - 10f(5) + 44f(4) - 110f(3) + 165f(2) - 132f(1)]$$

REFERENCES

- 1) N. Boccara, Phys. Lett. A94 (1983) 185.
- 2) A. Benyoussef and N. Boccara, J. de Phys. 44 (1983) 1143.
- 3) A. Benyoussef and N. Boccara, J. Phys. C16 (1983) 1901.
- 4) R.B. Stinchcombe and B.P. Watson, J. Phys. C9 (1976) 3224.
- 5) H. Dickinson and J.M. Yeomans, J. Phys. C16 (1983) L345.
- 6) M. Blume, V.J. Emery and R.B. Griffiths, Phys. Rev. A4 (1971) 1074.
- 7) A.N. Berker and M. Wortis, Phys. Rev. B14 (1976) 4946.
- 8) J. Alder, A. Aharony and J. Oitmaa, J. Phys. A11 (1978) 963.
- 9) M. Kaufman, R.B. Griffiths, J.M. Yeomans and M.E. Fisher, Phys. Rev. B23 (1981) 3448.
- 10) N. Benayad, A. Benyoussef and N. Boccara, J. Phys. C18 (1985) 1899.

$$\begin{aligned}
 B_0 &= g(0) \\
 B_1 &= g(1) - g(0) \\
 B_2 &= \frac{1}{2}[g(2) - g(0)] \\
 B_3 &= \frac{1}{2}[g(2) - 4g(1) + 3g(0)] \\
 B_4 &= \frac{1}{4}[g(3) - 2g(2) - g(1) + 2g(0)] \\
 B_5 &= \frac{1}{4}[g(3) - 6g(2) + 15g(1) - 10g(0)] \\
 B_6 &= \frac{1}{8}[g(4) - 4g(2) + 3g(0)] \\
 B_7 &= \frac{1}{8}[g(4) - 4g(3) + 4g(2) + 4g(1) - 5g(0)] \\
 B_8 &= \frac{1}{8}[g(4) - 8g(3) + 28g(2) - 56g(1) + 35g(0)] \\
 B_9 &= \frac{1}{16}[g(5) - 2g(4) - 3g(3) + 8g(2) + 2g(1) - 6g(0)] \\
 B_{10} &= \frac{1}{16}[g(5) - 6g(4) + 13g(3) - 8g(2) - 14g(1) + 14g(0)] \\
 B_{11} &= \frac{1}{16}[g(5) - 10g(4) + 45g(3) - 120g(2) + 210g(1) - 126g(0)] \\
 B_{12} &= \frac{1}{32}[g(6) - 6g(4) + 15g(2) - 10g(0)] \\
 B_{13} &= \frac{1}{32}[g(6) - 4g(5) + 2g(4) + 12g(3) - 17g(2) - 8g(1) + 14g(0)] \\
 B_{14} &= \frac{1}{32}[g(6) - 8g(5) + 26g(4) - 40g(3) + 15g(2) + 48g(1) - 42g(0)] \\
 B_{15} &= \frac{1}{32}[g(6) - 12g(5) + 66g(4) - 220g(3) + 495g(2) - 792g(1) + 462g(0)]
 \end{aligned}$$

Coefficients of Eqs. (4.5) and (4.6):

$$\begin{aligned}
 \bar{A}_1 &= pA_1, \quad \bar{A}_2 = p^2A_2, \quad \bar{A}_3 = p^3A_3, \quad \bar{A}_4 = p^3A_4, \quad \bar{A}_5 = p^4A_5, \quad \bar{A}_6 = p^4A_6, \quad \bar{A}_7 = p^5A_7 \\
 \bar{A}_8 &= p^5A_8, \quad \bar{A}_9 = p^5A_9, \quad \bar{A}_{10} = p^6A_{10}, \quad \bar{A}_{11} = p^6A_{11}, \quad \bar{A}_{12} = p^6A_{12}, \quad \bar{B}_0 = B_0, \\
 \bar{B}_1 &= pB_1, \quad \bar{B}_2 = p^2B_2, \quad \bar{B}_3 = p^2B_3, \quad \bar{B}_4 = p^3B_4, \quad \bar{B}_5 = p^3B_5, \quad \bar{B}_6 = p^4B_6, \\
 \bar{B}_7 &= p^4B_7, \quad \bar{B}_8 = p^4B_8, \quad \bar{B}_9 = p^5B_9, \quad \bar{B}_{10} = p^5B_{10}, \quad \bar{B}_{11} = p^5B_{11}, \quad \bar{B}_{12} = p^6B_{12}, \\
 \bar{B}_{13} &= p^6B_{13}, \quad \bar{B}_{14} = p^6B_{14}, \quad \bar{B}_{15} = p^6B_{15}.
 \end{aligned}$$



FIGURE CAPTIONS

- Fig. 1 First, second and third neighbours of site 0 on a square lattice.
- Fig. 2 The phase diagram in the  $T-\Delta$  plane.
- Fig. 3 The  $T-\Delta-p$  phase diagram of the bond-dilute model.
- Fig. 4 The variation of the zero-temperature critical crystal field with bond dilution.
- Fig. 5 The variation of the tricritical temperature with bond-dilution.
- Fig. 6 The  $T-\Delta-p$  phase diagram of the site-dilute model.
- Fig. 7 The variation of the zero temperature critical crystal field with site dilution.
- Fig. 8 The variation of the tricritical temperature with site-dilution.

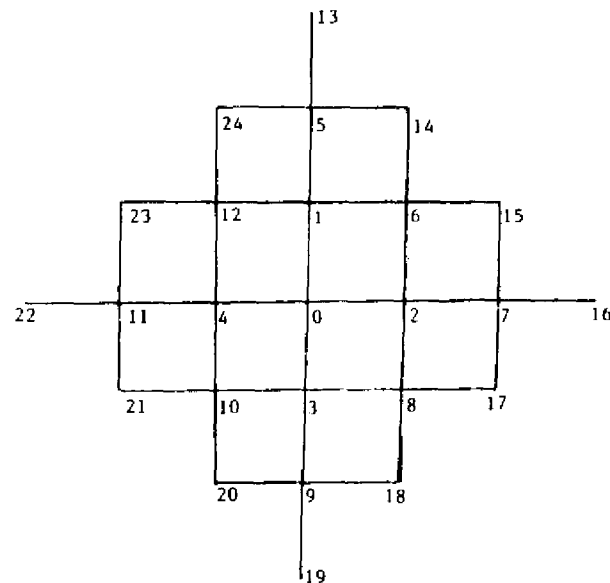


Fig. 1

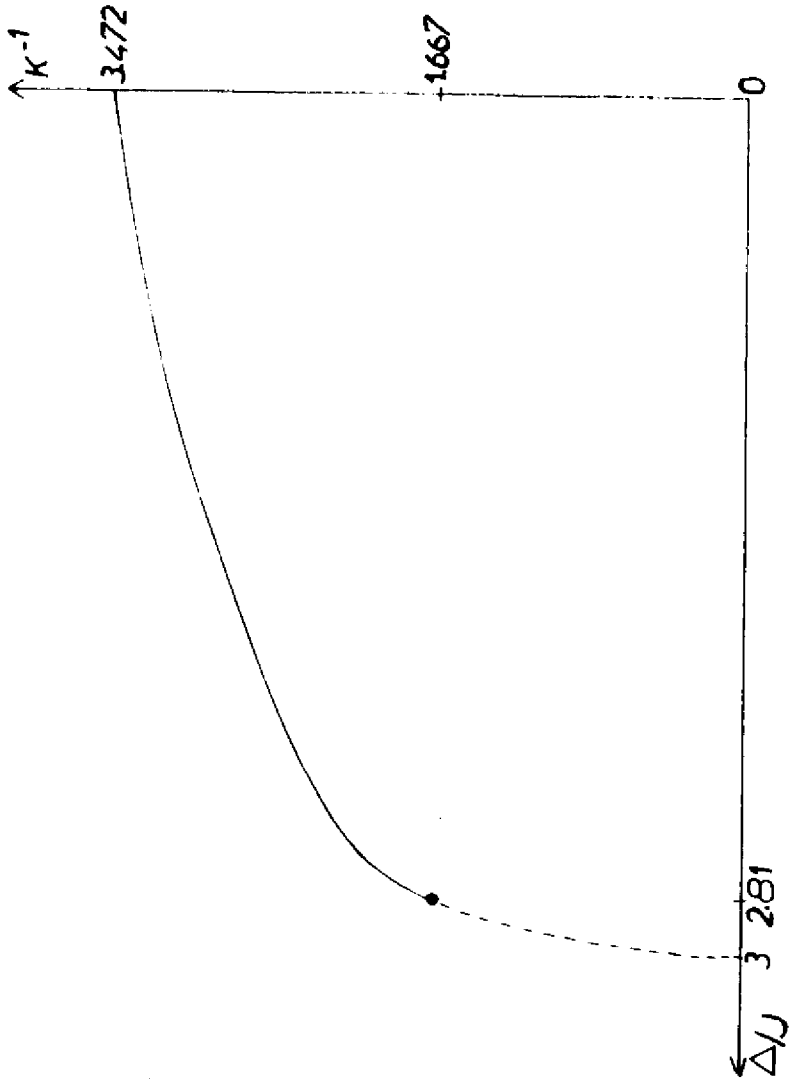


FIG. 2

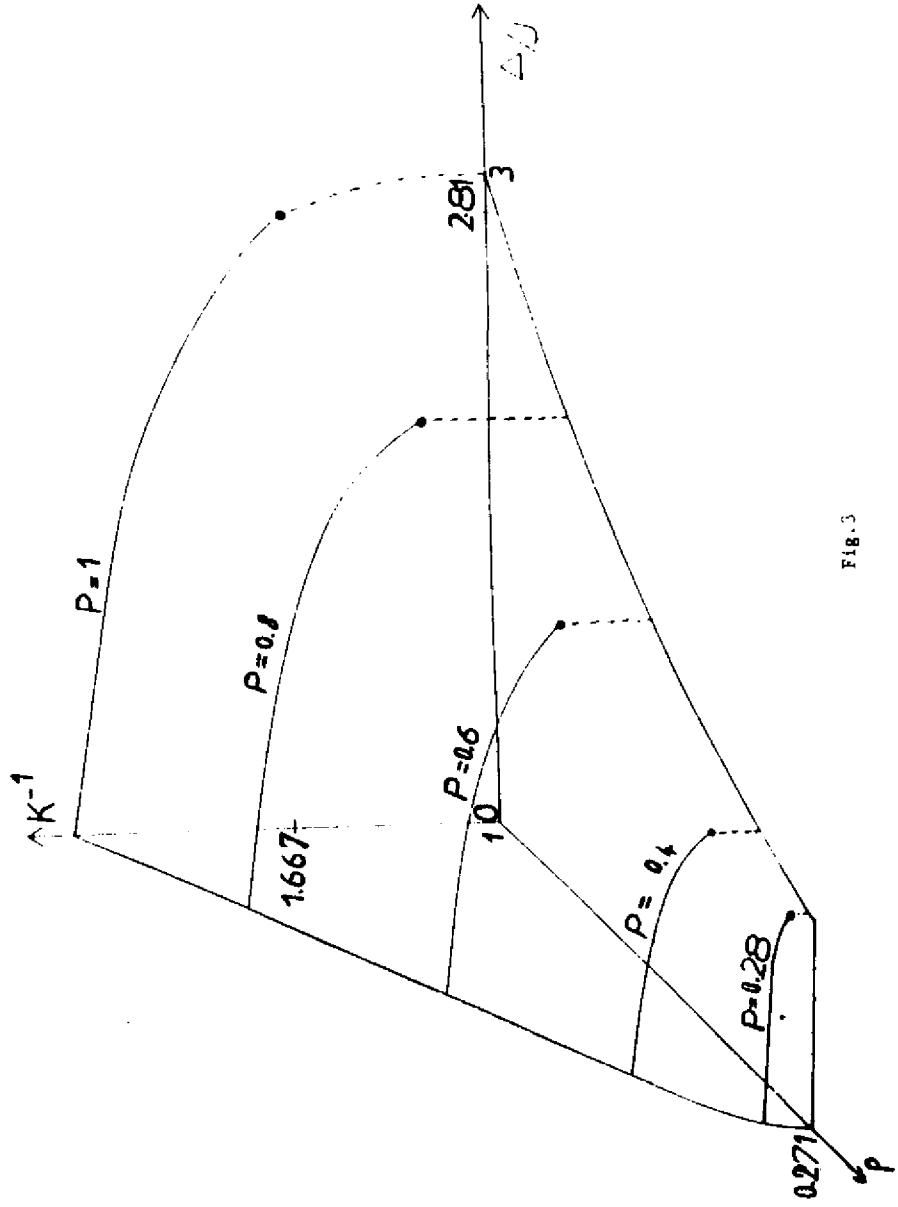


FIG. 3

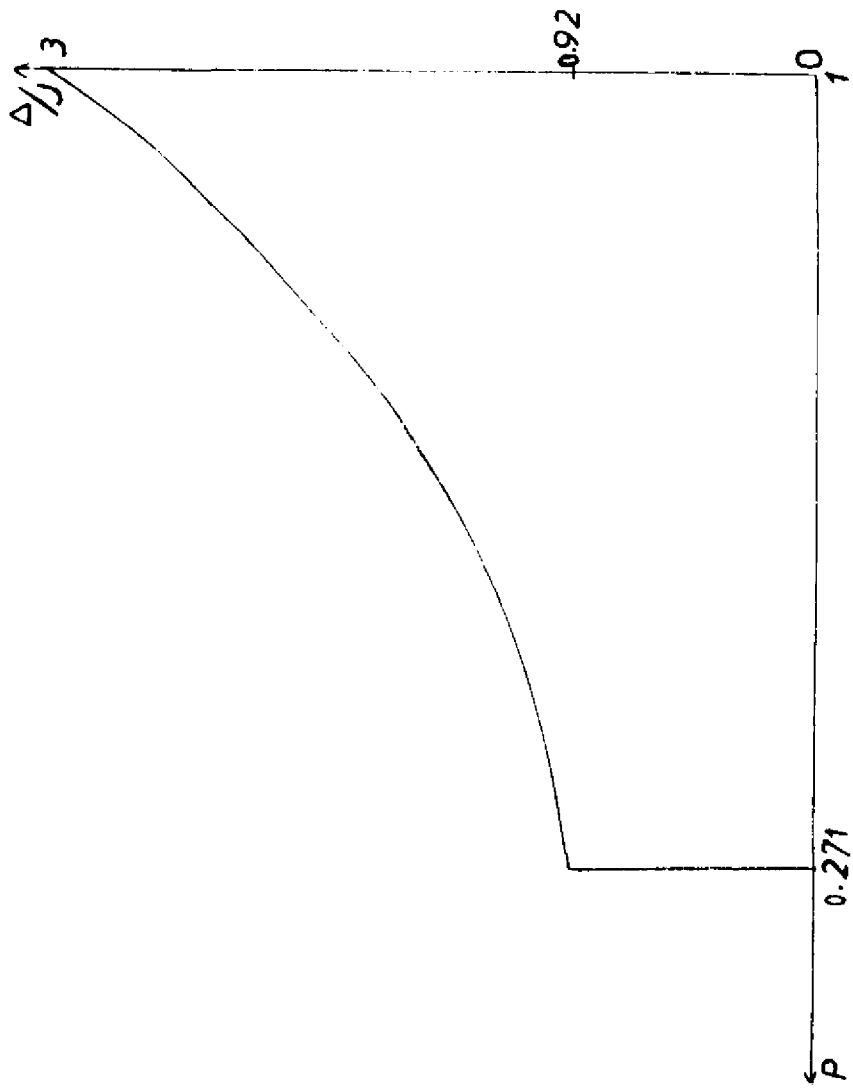


FIG. 4

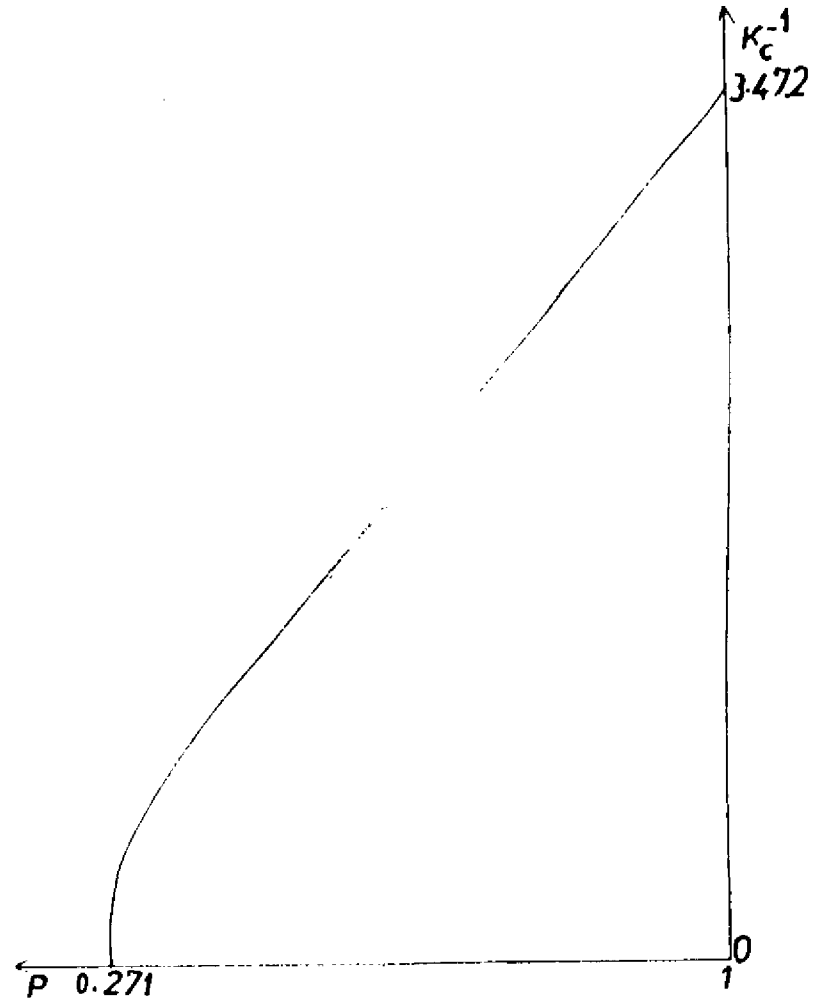


FIG. 5

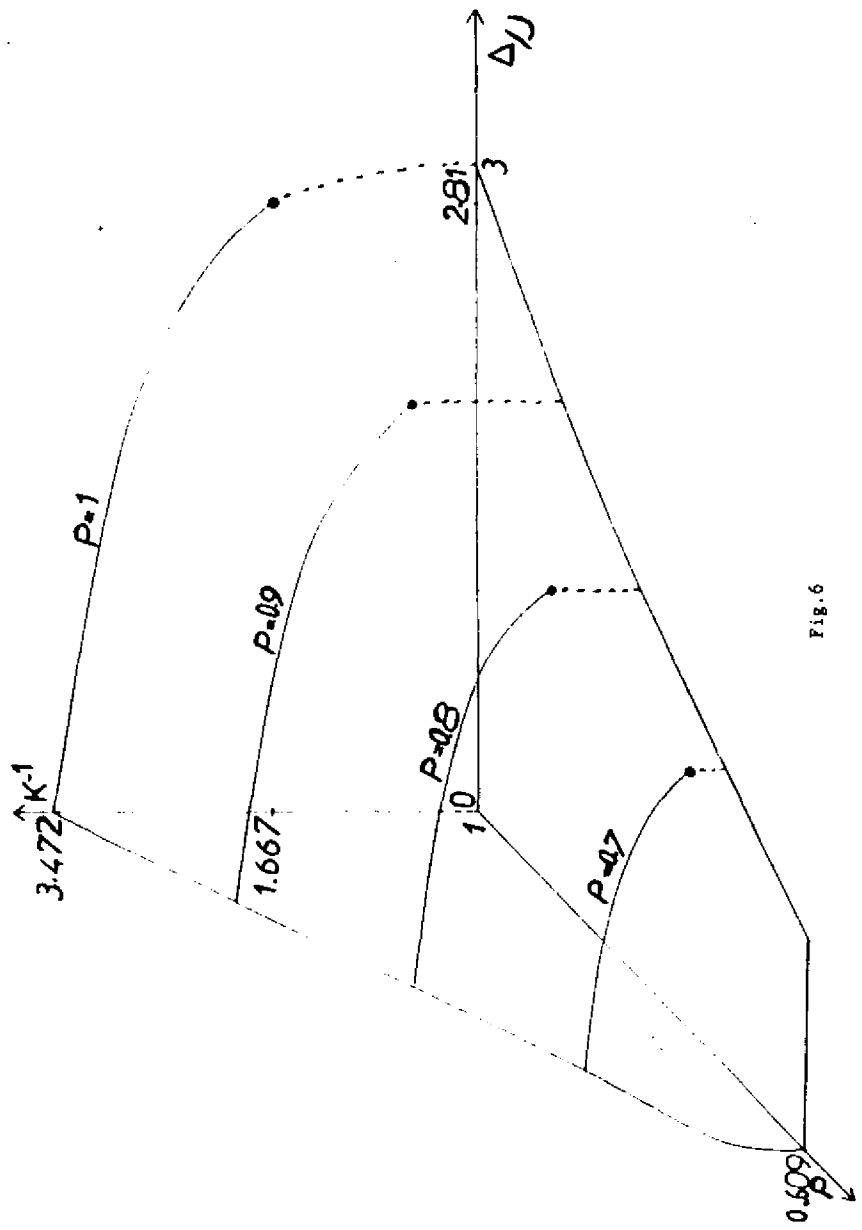


Fig. 6

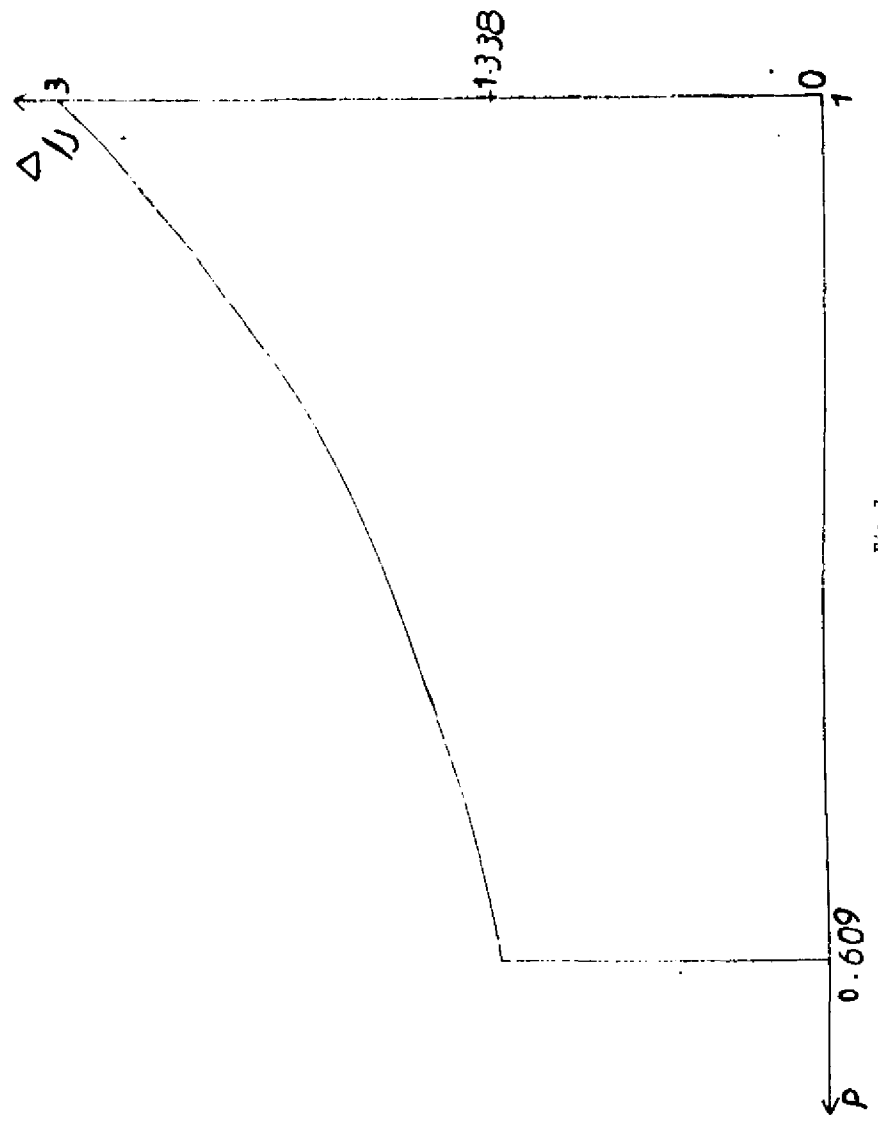


Fig. 7

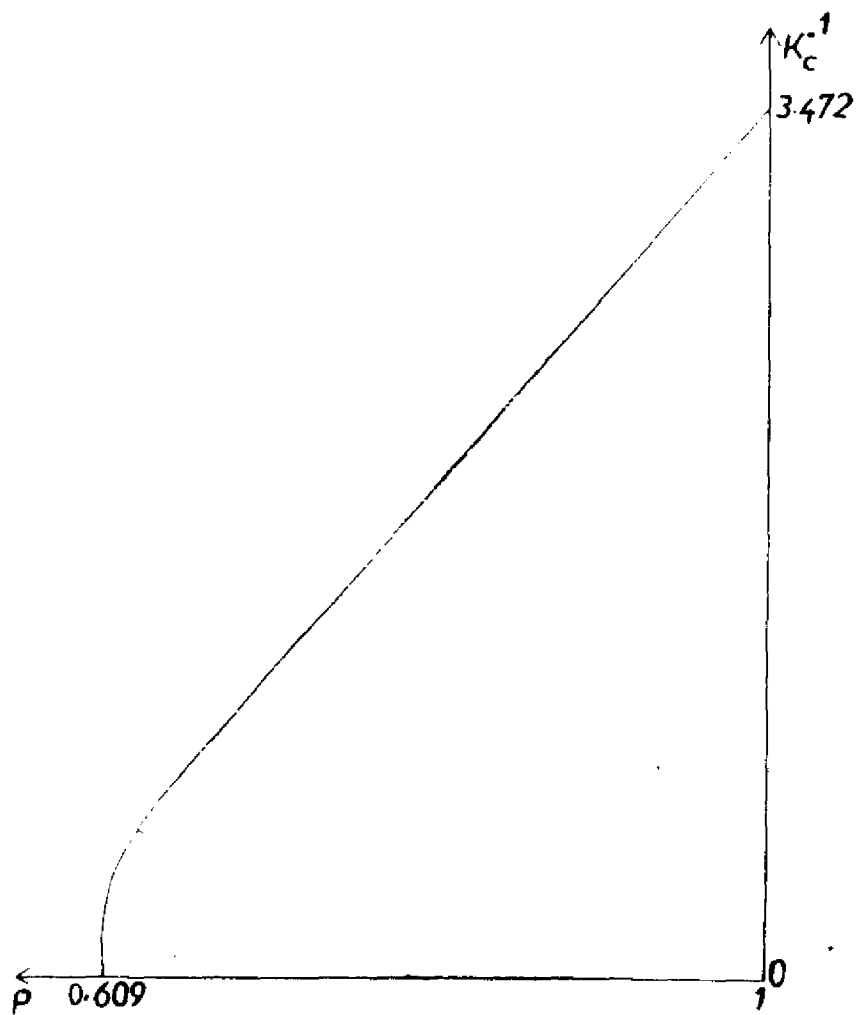


Fig. 8

