IC/87/288
INTERNAL REPORT
(Limited distribution)

International Atomic Energy Agency
and
United Nations Educational Scientific and Cultural Organization

INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS

THE DILUTE RANDOM FIELD ISING MODEL BY FINITE CLUSTER APPROXIMATION *

A. Benyoussef
Laboratoire de Magnétisme, Département de Physique,
Faculté des Sciences, B.P. 1014, Rabat, Morocco.

and

M. Saber **
International Centre for Theoretical Physics, Trieste, Italy.

ABSTRACT

Using the finite cluster approximation, phase diagrams of bond and site diluted three-dimensional simple cubic Ising models with a random field have been determined. The resulting phase diagrams have the same general features for both bond and site dilution.

MIRAMARE - TRIESTE
September 1987

* To be submitted for publication.

** Permanent address: Laboratoire de Magnétisme, Département de Physique, Faculté des Sciences, B.P. 1014, Rabat, Morocco.

1. INTRODUCTION

During recent years, much effort has been directed towards the study of quenched random magnetic systems. For such systems, the free energy and its derivatives must be first calculated for a given configuration of the random variables and then averaged over the probability distribution function of these random variables. The resulting phase diagram depends on the form of the distribution function.

In an Ising system with random fields, on the other hand, Aharony [1)] has suggested that the second order region in the phase diagram may be separated from the first order region by a tricritical point, provided that the symmetric distribution function of the random field has a minimum (or maximum) at zero field. Later, some authors [2)] have examined the conditions of the random field distribution function for the appearance of a tricritical point within mean field theory. Moreover, the value of dimensionality under which weak random fields will destroy long range order has been investigated. It is now believed that the lower critical dimensionality d_ℓ is 2, although some discrepancies still exist about the interpretation of various experimental data [3)].

In this work, we shall study, within the framework of the finite cluster approximation proposed recently by Boccara [4)], bond and site three dimensional random field Ising model which exhibits only second order transition according to an appropriate probability distribution of these random variables. This method is much less sophisticated than real space renormalization group and applies to a wide class of disordered systems. In particular, site-dilution (which is physically more relevant than bond-dilution) is much easier to study within finite cluster approxiation. Another advantage is that it is not necessary to introduce ad hoc approximations for the renormalized probability distribution of the interactions, nor to choose in a more or less arbitrary way the "right" random variable over which to average [5)-7)].

2. PURE SYSTEM

Consider an infinite simple cubic ferromagnetic Ising model in a random field described by the following Hamiltonian:

$$-\beta H = K\sum_{(i,j)} \sigma_i\sigma_j + \sum_i L_i\sigma_i \qquad (1)$$

where $K = \beta J$ is the reduced coupling constant between neighbouring spins and L_i is the reduced random field according to the probability distribution:

$$P(L_i) = \begin{cases} 1/2L & \text{if } -L < L_i < L \\ 0 & \text{otherwise} \end{cases} \qquad (2)$$

In the plane $(K^{-1}, K^{-1}L)$ its phase diagram, determined within mean field approximation [1], is shown in Fig.1.

In this paper, we shall study the influence of bond and site dilution on this system using finite cluster approximation.

Consider a particular site 0 and denote by $<\sigma_0>_c$ the mean value of σ_0 for a given configuration c of all other spins, i.e. when all other spins σ_i $(i \neq 0)$ have fixed values. We have:

$$\langle\sigma_0\rangle_c = \frac{\operatorname{Tr}_{\sigma_0} \sigma_0 \exp(-\beta H)}{\operatorname{Tr}_{\sigma_0} \exp(-\beta H)} \qquad (3)$$

where $\operatorname{Tr}_{\sigma_0}$ means that the trace is performed over σ_0 only. This gives:

$$\langle\sigma_0\rangle_c = \frac{1}{2L} \ln\left\{\frac{\cosh(K\sum_{i=1}^{z}\sigma_i + L)}{\cosh(K\sum_{i=1}^{z}\sigma_i - L)}\right\} \qquad (4)$$

where the summation is extended over the z nearest neighbours σ_i $(i = 1, 2, \ldots, z)$ of σ_0. Relation (4) is exact and the magnetization per site, which is the thermal average m of σ_0, is obtained by averaging the right-hand side of (4) over all configurations. This is a formidable task and the mean field approximation corresponds to the very crude estimate:

$$\left\langle \frac{1}{2L} \ln\left\{\frac{\cosh(K\sum_{i=1}^{z}\sigma_i + L)}{\cosh(K\sum_{i=1}^{z}\sigma_i - L)}\right\}\right\rangle = \frac{1}{2L}\ln\left\{\frac{\cosh(zKm+L)}{\cosh(zKm-L)}\right\}$$

which corresponds to the probability distribution:

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

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

$$P_{FCA}(\{\sigma_i\}) = \prod_i \left(\frac{1+m}{2}\,\delta(\sigma_i - 1) + \frac{1-m}{2}\,\delta(\sigma_i + 1)\right) \qquad (5)$$

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

To average the right-hand side of (4) when the σ_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 $\sigma_1, \sigma_2, \ldots, \sigma_z$ is a 2^z dimensional Euclidean space. The set $\{1, \sigma_1 \ldots, \sigma_z, \sigma_1\sigma_2, \ldots, \sigma_1\sigma_2 \ldots \sigma_z\}$, which contains all the products of different spins, is an orthonormal basis for the inner product defined by:

$$\langle f_1|f_2\rangle = \frac{1}{2^z} \operatorname{Tr}_{\sigma_1,\ldots,\sigma_z} f_1(\sigma_1,\ldots,\sigma_z)\, f_2(\sigma_1,\ldots,\sigma_z)$$

For the simple cubic lattice, we have:

$$\frac{1}{2L}\ln\left\{\frac{\cosh(K\sum_{i=1}^{z}\sigma_i + L)}{\cosh(K\sum_{i=1}^{z}\sigma_i - L)}\right\} = A\sum_{i=1}^{6}\sigma_i + B\sum_{\substack{i,j,k\\ i\neq j\neq k}}\sigma_i\sigma_j\sigma_k + C\sum_{\substack{i,j,k,l,m\\ i\neq j\neq k\neq l\neq m}}\sigma_i\sigma_j\sigma_k\sigma_l\sigma_m \qquad (6)$$

and when we average the right-hand side of (6) approximating $<\sigma_i\sigma_j\sigma_k>$ by m^3 and $<\sigma_i\sigma_j\sigma_k\sigma_\ell\sigma_m>$ by m^5, we obtain:

$$m = 6Am + 20Bm^3 + 6Cm^5 \tag{7}$$

which determines m for the whole temperature range. The coefficients A, B, C are functions of K and L and they are given in the Appendix.

Within this approximation the second order transition line is given by:

$$1 = 6A(K,L) \tag{8}$$

The critical temperature is the solution of:

$$1 = 6A(K_c, L=0)$$

i.e. $T_c = 5.09J$, which is to be compared with the mean field result $T_c = 6J$.

We show in Fig.2 the variation of K^{-1} as a function of $K^{-1}L$.

3. 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 value $<\sigma_0>_c$ when all other spins σ_i $(i \neq 0)$ and all interactions K_{ij} have fixed values, is for the simple cubic lattice

$$\langle\sigma_0\rangle_c = \frac{1}{2L}\ln\left\{\frac{\cosh(K_{01}\sigma_1+K_{02}\sigma_2+K_{03}\sigma_3+K_{04}\sigma_4+K_{05}\sigma_5+K_{06}\sigma_6+L)}{\cosh(K_{01}\sigma_1+K_{02}\sigma_2+K_{03}\sigma_3+K_{04}\sigma_4+K_{05}\sigma_5+K_{06}\sigma_6-L)}\right\} \tag{9}$$

The theorem from which we obtained (6) can be used here. It gives:

$$\langle\sigma_0\rangle_c = \sum_{i=1}^{6} A_{1i}\sigma_i + \sum_{i,j,k} B_{ijk}\sigma_i\sigma_j\sigma_k + \sum_{i,j,k,\ell,m} C_{ijk\ell m}\sigma_i\sigma_j\sigma_k\sigma_\ell\sigma_m \tag{10}$$

For a bond dilute system $K_{0i} = Kn_i$ where n_i is the occupation number of bond $0i$. The coefficients of the polynomial (10) are functions of the discrete random variables n_1, n_2, n_3, n_4, n_5 and n_6.

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

$$m = 6\bar{A}m + 20\bar{B}m^3 + 6\bar{C}m^5 \tag{11}$$

where the coefficients, which are averaged over disorder, are functions of K, L and $<n> = p$. We have put:

$$\bar{A} = \bar{A}_i \;,\; \bar{B} = \bar{B}_{ijk} \;,\; \bar{C} = \bar{C}_{ijk\ell m}$$

where $i = 1, 2, ..., 6$ and $i \neq j \neq k \neq \ell \neq m$. These coefficients are given in the Appendix. To obtain the $(K^{-1}, K^{-1}L, p)$ phase diagram (Fig.3) we proceed as in the previous section.

For a site dilute system $K_{0i} = Kn_0n_i$ and $L = Ln_0$ where n_0 and n_i are the occupation numbers of sites 0 and i. A simple calculation shows that m is given by Eq.(11) where the coefficients are functions of K, L and the site concentration p. Their dependences on these variables are the same as for the bond problem except that they are all multiplied by an extra factor p.

The corresponding phase diagram is given in Fig.4. It has the same general features as the one we obtained for bond dilution.

4. CONCLUSION

Phase diagrams of bond and site diluted three dimensional random field Ising model with ferromagnetic exchange interactions have been determined within the framework of the finite cluster approximation. It is also shown that the dilution does not affect this behaviour.

ACKNOWLEDGEMENTS

The authors would like to thank Professor R.B. Stinchcombe for some comments and a critical reading of the manuscript. One of the authors (M.S.) would like to thank Professor Abdus Salam, the International Atomic Energy Agency and UNESCO for hospitality at the International Centre for Theoretical Physics, Trieste. He also acknowledges the financial support given by the International Centre for Theoretical Physics, Trieste.

APPENDIX

Coefficients of Eq.(7):

$$A = \frac{1}{64L}\left\{ \ln\left[\frac{\cosh(6K+L)}{\cosh(6K-L)}\right] + 4\ln\left[\frac{\cosh(4K+L)}{\cosh(4K-L)}\right] + 5\ln\left[\frac{\cosh(2K+L)}{\cosh(2K-L)}\right]\right\}$$

$$B = \frac{1}{64L}\left\{ \ln\left[\frac{\cosh(6K+L)}{\cosh(6K-L)}\right] - 3\ln\left[\frac{\cosh(2K+L)}{\cosh(2K-L)}\right]\right\}$$

$$C = \frac{1}{64L}\left\{ \ln\left[\frac{\cosh(6K+L)}{\cosh(6K-L)}\right] - 4\ln\left[\frac{\cosh(4K+L)}{\cosh(4K-L)}\right] + 5\ln\left[\frac{\cosh(2K+L)}{\cosh(2K-L)}\right]\right\}$$

Coefficients of Eq.(11):

$$\begin{aligned}
\bar{A} = \frac{1}{64L}\Big\{ & p^6 \ln\left[\frac{\cosh(6K+L)}{\cosh(6K-L)}\right] + (10p^5 - 10p^6)\ln\left[\frac{\cosh(5K+L)}{\cosh(5K-L)}\right] \\
& + (40p^4 - 80p^5 + 44p^6)\ln\left[\frac{\cosh(4K+L)}{\cosh(4K-L)}\right] \\
& + (80p^3 - 240p^4 + 270p^5 - 110p^6)\ln\left[\frac{\cosh(3K+L)}{\cosh(3K-L)}\right] \\
& + (80p^2 - 320p^3 + 560p^4 - 480p^5 + 165p^6)\ln\left[\frac{\cosh(2K+L)}{\cosh(2K-L)}\right] \\
& + (32p - 160p^2 + 400p^3 - 560p^4 + 480p^5 - 132p^6)\ln\left[\frac{\cosh(K+L)}{\cosh(K-L)}\right]\Big\}
\end{aligned}$$

$$\bar{B} = \frac{1}{64L}\Big\{ p^6 \ln\left[\frac{\cosh(6K+L)}{\cosh(6K-L)}\right] + (6p^5 - 6p^6)\ln\left[\frac{\cosh(5K+L)}{\cosh(5K-L)}\right]$$

$$+ (18p^4 - 24p^5 + 12p^6)\ln\left[\frac{\cosh(4K+L)}{\cosh(4K-L)}\right]$$

$$+ (8p^3 - 24p^4 + 18p^5 - 2p^6)\ln\left[\frac{\cosh(3K+L)}{\cosh(3K-L)}\right]$$

$$+ (-24p^4 + 48p^5 - 27p^6)\ln\left[\frac{\cosh(2K+L)}{\cosh(2K-L)}\right]$$

$$+ (-24p^3 + 72p^4 - 84p^5 + 36p^6)\ln\left[\frac{\cosh(K+L)}{\cosh(K-L)}\right]\Big\}$$

$$\bar{C} = \frac{1}{64L}\Big\{ p^6 \ln\left[\frac{\cosh(6K+L)}{\cosh(6K-L)}\right] + (2p^5 - 2p^6)\ln\left[\frac{\cosh(5K+L)}{\cosh(5K-L)}\right]$$

$$+ (-4p^6)\ln\left[\frac{\cosh(4K+L)}{\cosh(4K-L)}\right] + (-10p^5 + 10p^6)\ln\left[\frac{\cosh(3K+L)}{\cosh(3K-L)}\right]$$

$$+ (5p^6)\ln\left[\frac{\cosh(2K+L)}{\cosh(2K-L)}\right] + (20p^5 - 20p^6)\ln\left[\frac{\cosh(K+L)}{\cosh(K-L)}\right]\Big\}$$

REFERENCES

1) A. Aharony, Phys. Rev. B18 (1978) 3318.

2) D. Andelman, Phys. Rev. B27 (1983) 3079;
S. Galam and J.L. Birman, Phys. Rev. B28 (1983) 5322.

3) Y. Shapir, J. Appl. Phys. 57 (1985) 3279.

4) N. Boccara, Phys. Lett. 94A (1983) 185.

5) A. Benyoussef and N. Boccara, J. Phys. C16 (1983) 1901.

6) R.B. Stinchcombe and B.P. Watson, J. Phys. C9 (1976) 3221.

7) H. Dickinson and J. Yeomans, J. Phys. C16 (1983) L345.

FIGURE CAPTIONS

Fig.1 Mean field theory phase diagram of the three dimensional random field Ising model in the $(K^{-1}, K^{-1}L)$ plane.

Fig.2 Finite cluster approximation phase diagram of the three dimensional random field Ising model in the $(K^{-1}, K^{-1}L)$ plane.

Fig.3 The $(K^{-1}, K^{-1}L, p)$ phase diagram of the bond dilute model.

Fig.4 The $(K^{-1}, K^{-1}L, p)$ phase diagrams of the site dilute model.

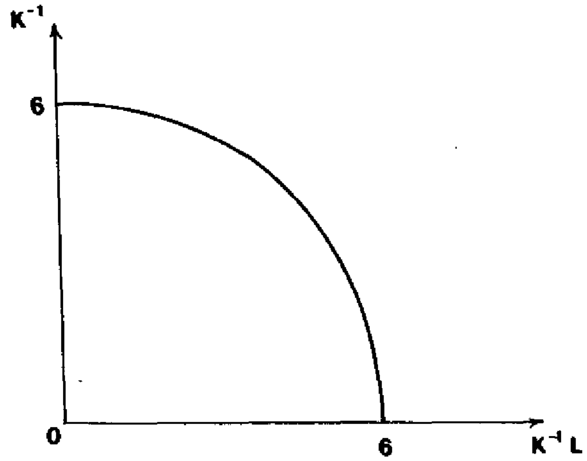

Fig.1

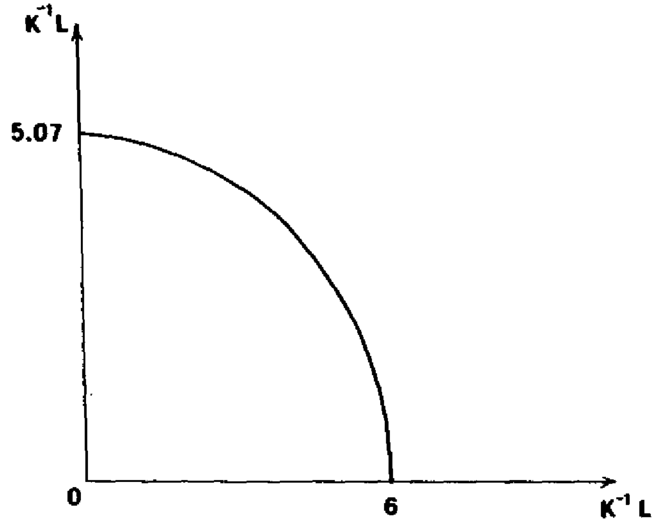

Fig.2

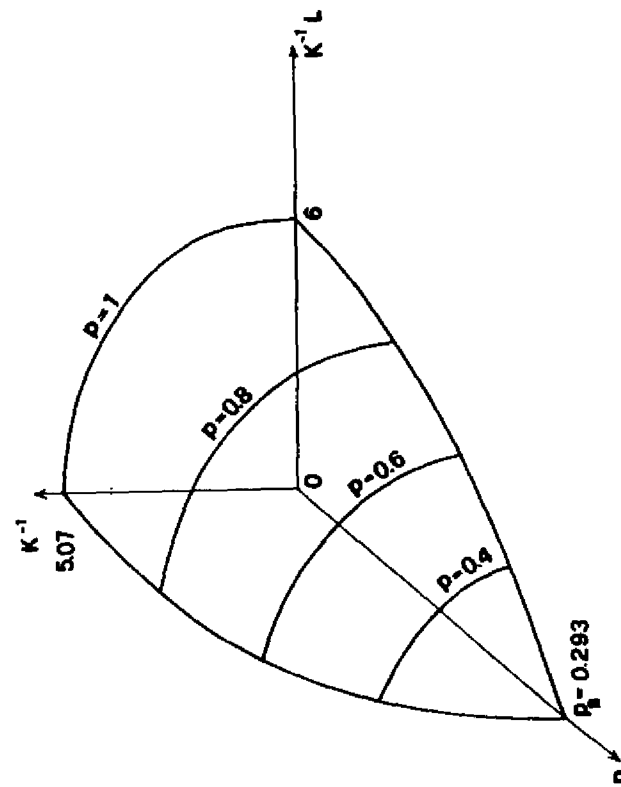

Fig.3

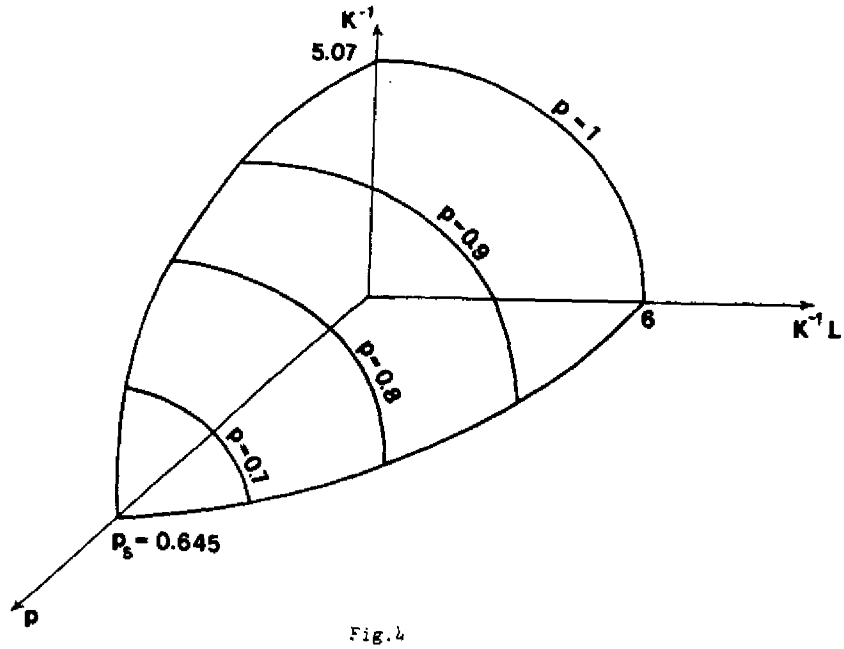

Fig.4