INTERNATIONAL ATOMIC ENERGY AGENCY

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IC/95/338

INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS

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ABSTRACT

The effect of the transverse magnetic field on the phase diagrams structures of the Ising model in a random longitudinal magnetic field with a trimodal symmetric distribution is investigated within a finite cluster approximation. We find that a small magnetizations ordered phase (small ordered phase) disappears completely for a sufficiently large value of the transverse field or/and large value of the concentration of the disorder of the magnetic field. Multicritical behaviour and reentrant phenomena are discussed. The regions where the tricritical, reentrant phenomena and the small ordered phase persist are delimited as a function of the transverse field and the concentration p. Longitudinal magnetizations are also presented.

MIRAMARE – TRIESTE
July 1996

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I. Introduction

Since de Gennes introduced the transverse Ising model to explain the phase transition of hydrogen-bonded ferroelectrics such as KH_2PO_4 in the order-disorder phenomena with tunnelling effects[1], it has been successfully used for the study of cooperative Jahan Teller transition ($DyVO_4$ and $TbVO_4$) and a number of problems of phase transitions associated with order-disorder phenomena in other systems (a more detailed application has been reviewed in ref. [2]). The model is described by the Ising Hamiltonian to which is added a term which represents the effects of the transverse field part.

Recently, some authors have studied the effects of longitudinal random fields on the phase diagrams as well as the tricritical behaviour in a quantum transverse spin-1/2 Ising model[3-9]. However experimental[10] and theoretical[11,12] studies of Ising systems subjected to random magnetic field have concentrated mainly on the question of what is the lower critical dimension. Hence the lower critical dimension above which long-range order can be established, is two[11-13]. Theoretically, the random field Ising model (RFIM) has been widely investigated by the use of various techniques, including the mean field approximation, effective field theories[14-16], finite cluster approximation[17-20], renormalization calculations[11,21] and Monte-Carlo simulations[22,23]. It is well known that the critical behaviour of the RFIM depends on the distribution of the random fields. For instance , the transition is always of second order for a gaussian distribution of random fields, but a tricritical point appears for a bimodal distribution[21]. by using a trimodal distribution for the RFIM, Mattis[24] has shown within a mean-field approach, that the critical behaviour depends on the degree of dilution of the random field. Kaufman, Kluzinger and Khurana[25] have performed a detailed study of the phase diagram of the RFIM with the trimodal distribution of random field. They show that a rich variety of multicritical points appears as a function of the field dilution p. They also show that the trimodal distribution is relevant to the experimental study of diluted antiferromagnets[1,24,26], as, for *instance*, $Fe_xZn_{1-x}F_2$, *in a uniform* magnetic field. In this case, the concentration of the iron ions could be related with p values of the trimodal distributions. For the bimodal and the trimodal distribution, the existence of the tricritical and the reentrant phenomena are due to the competition between the quantum fluctuation and randomness; the quantum fluctuation is induced by the transverse field and the randomness is caused by the random distributions of longitudinal field. However, the two effects do not operate in the same manner when the temperature decreases. When the temperature is reduced, quantum fluctuations dominate and the transition from the disordered phase to the ordered phase is more characteristic of a quantum spin transition. If the temperature is decreased further, the random field dominate and a reentrant transition to the disordered phase may take place. On the other hand, Kaufman et al[25] have studied within a mean field approximation the phase diagram of the Ising model with a symmetric three-peak distribution of the random field, they have found that the ordered phase persists for arbitrary large random fields at low temperatures.

Our goal in the present work is to study the effect of a transverse magnetic field on the phase diagram structures, but since for disordered models the mean field approach neglects all spin correlations is not satisfactory, we will use the finite cluster approximation[27-29] within an expansion technique for spin-1/2 cluster identities[30], which still neglects correlations between different spins, but takes into account relations such as $\langle S^2 \rangle = 1$ exactly.

The outline of the present paper is as follows. In section II we give the model and we propose a description of the finite cluster approximation. Section III is reserved for results and discussion. Finally, we draw our conclusion in section IV.

II. Model and Method

We consider a spin-1/2 transverse Ising model in a three-peak random field distribution which is described by the following Hamiltonian:

$$H = -J \sum_{<i,j>} S_i^z S_j^z - \Omega \sum_i S_i^x - \sum_i h_i S_i^z \qquad (1)$$

where S_i^x and S_i^z are respectively the x component and the z component of a spin-1/2 operator at site i, Ω is the transverse field, J is the magnetic coupling constant. $\langle i,j \rangle$ runs over all nearest-neighbour pairs of spins and h_i is the applied random longitudinal magnetic field governed by the following three-peak symmetric distribution (P(h) = P(-h)):

$$P(h_i) = \frac{1}{2} p \left[\delta(h_i - h) + \delta(h_i + h) \right] + (1-p)\, \delta(h_i)$$

where $0 \le p \le 1$, $h \ge 0$.

Our calculations are carried out for the simple-cubic structure, with the corresponding coordination number N = 6.

For disordered models the mean field approximation which neglects all spin correlations is not satisfactory. But to compute the average over all spin configurations $\langle\langle S_i \rangle\rangle_D$, where $\langle \ldots \rangle$ indicates the thermal average, and $\langle \ldots \rangle_D$ means the random configurational average, we will use the finite-cluster approximation[27,29] within an expansion technique for spin 1/2 cluster identities[30].

Using a single-site cluster approximation in which attention is focused on a cluster comprising just a single selected spin labelled 0, and the neighbouring spins with which it directly interacts, We get the Hamiltonian containing 0, namely

$$H_0 = (A - h_0)\, S_0^z + B S_0^x \qquad (2)$$

where

$$A = -J\sum_{j=1}^{N} S_j^z \quad \text{and} \quad B = -\Omega \tag{3}$$

N is the coordination number.

The starting point of single-site cluster approximation is a set of formal identities of the type

$$\langle\langle S_0^\alpha\rangle_c\rangle = \left\langle \frac{Tr_0\, S_0^\alpha \exp(-\beta H_0)}{Tr_0 \exp(-\beta H_0)} \right\rangle \tag{4}$$

where $\langle S_0^\alpha\rangle_c$ ($\alpha = z,x$) denotes the average value of the spin 0 for a given configuration c of all other spins, i.e when all other spins S_i $(i \neq 0)$ have fixed values. $\langle ... \rangle$ denotes the average over all spin configurations. $trace_0$ means the trace performed over $S_{0\alpha}$ only. $\beta = \frac{1}{K_B T}$, T is the absolute temperature and K_B is the Boltzmann constant.

To calculate $\langle S_0^\alpha\rangle_c$, one has to effect the inner traces in eq (4) over the configuration of spin 0. hence,

$$\langle S_0^z\rangle_c = \frac{A}{\sqrt{A^2+\Omega^2}} \tanh\left(\frac{1}{k_B T}\sqrt{A^2+\Omega^2}\right) \tag{5}$$

$$\langle S_0^x\rangle_c = \frac{\Omega}{\sqrt{A^2+\Omega^2}} \tanh\left(\frac{1}{k_B T}\sqrt{A^2+\Omega^2}\right) \tag{6}$$

The magnetizations m_Z and m_X are given by:

$$m_x = \langle\langle f_x(A)\rangle_\Omega\rangle \tag{7}$$

$$m_z = \langle\langle f_z(A)\rangle_\Omega\rangle \tag{8}$$

with

$$f_x(A) = \langle S_0^x \rangle_c$$

$$f_z(A) = \langle S_0^z \rangle_c$$

where $\langle ... \rangle$ denotes the average over all configurations of the other spins $S_j\,(j\neq 0)$ and $\langle ... \rangle_D$ denotes the average over all configurations of the disorder of the longitudinal magnetic field. Using the distribution of h_i mentioned above, the average over the disorder of h_i of $\langle S_0^\alpha \rangle_c$ $(\alpha = z,x)$ is given by:

$$\langle\langle S_0^\alpha \rangle\rangle_D = \int \langle S_0^\alpha \rangle_c P(h)\, dh$$
$$= \frac{p}{2}\left(\langle S_0^\alpha \rangle_c^+ + \langle S_0^\alpha \rangle_c^-\right) + (1-p)\langle S_0^\alpha \rangle_c^0 \quad (9)$$

where $\langle S_0^\alpha \rangle_c^\pm$ is the value of $\langle S_0^\alpha \rangle_c$ when $h = \pm h_0$ and $\langle S_0^\alpha \rangle_c^0$ is its value when $h = 0$.

To calculate $\langle\langle\langle S_0^\alpha \rangle_c \rangle_D\rangle$ we have used the expansion technique for cluster identities of spin-1/2 Ising systems[30] as follows:

Suppose one considers the general product $\prod_{j=1}^{N} \sum_{k=0}^{1} S_{jz}^k$ which contains 2^N terms. From these terms one may collect together all those terms containing p factors of S_j^z. Such a set is denoted by $\langle S^z \rangle_p$.

Our aim is to expand the function $\langle\langle S_0^\alpha \rangle_c \rangle_D$ of eqs (7,8) in terms of these $\langle S^z \rangle_p$. Thus, *if one* write:

$$\langle\langle S_0^\alpha \rangle_c \rangle_D = \sum_{p=0}^{N} A_{p\alpha} \langle S^z \rangle_p \quad (10)$$

To calculate the coefficients $A_{p\alpha}$ $(\alpha = x,z)$, we use the expansion technique for the cluster identities of the spin-1/2 Ising systems[30], namely.

$$A_{p\alpha} = \frac{1}{2^N C_p^N} \sum_{i=0}^{N} C_i^N \varepsilon_i(N,p)\, f_{i\alpha}(N) \quad (11)$$

with

$$\varepsilon_i(N.p) = \sum_{\mu=0}^{i} (-1)^\mu C_\mu^i C_{p-\mu}^{N-i}$$

where

$$f_{i\alpha}(N) = f_{0\alpha}(N-2i) \qquad (\alpha=x,z)$$

and

$C_n^m = \frac{m!}{n!\,(m-n)!}$ are the binomial coefficients.

Using the simplest approximation of the Zernike decoupling of the type: $\langle S_{iz}S_{jz} \ldots S_{kz} \ldots \rangle = \langle S_{iz}\rangle\langle S_{jz}\rangle \ldots \langle S_{kz}\rangle \ldots$ *for* $i \neq j \neq k \neq \ldots$

and seeing that the number of elements of the set $\{S^z\}_p$ is equal to C_p^N, then the averaged magnetizations $m_\alpha = \langle\langle\langle S_0^\alpha\rangle_c\rangle_D\rangle$ $(\alpha=x,z)$ are given by:

$$m_x = \sum_{p=0}^{N} A_{px}\, C_p^N\, m_z^p \qquad (12)$$

$$m_z = \sum_{p=0}^{N} A_{pz}\, C_p^N\, m_z^p \qquad (13)$$

Let us put $m = m_z = \langle S_z\rangle$. we obtain an equation in powers of m of the form

$$m = A_1\, m + A_3\, m^3 + \ldots\ldots\ldots\ldots \qquad (14)$$

The critical temperature of the second-order transition is determined by $A_1 = 1$. *In the vicinity of the second-order transition the magnetization* m_z is determined by

$$m_z^2 = \frac{1 - A_1}{A_3} \qquad (15)$$

The right-hand side of (15) must be positive. If this is not the case the transition is of first order. The point $A_1 = 1$ and $A_3 = 0$ is the tricritical point. With expressions (12,13) we are able to determine the complete phase diagram in the space (T,h, Ω) for each value of p.

III. Results and Discussion

In this section we present the results of the model (1) in which we improve the phase diagram topologies calculated within mean field approach by Kaufman et al[25], by using the finite cluster approximation which *is superior than the* mean field approach for disordered systems. On the other hand we examine the effect of quantum fluctuations (i.e the effect of the transverse field) on the phase diagrams structures of the model (1). Equations (12,13) are solved by iteration, however the phase diagrams are determined numerically in the plane (T, h), for several values of the transverse field and concentration p of the disordered field. Hence, for $\Omega=0$, and as a function of the concentration p, we find six different phase diagrams topologies instead of three as has been calculated within mean field approach by Kaufman et al[25].

For $p_{c1}<p\leq 1$, $p_{c1} = 0.67$, we obtain a phase diagram (Fig.1a) with a tricritical point C, which is located at T = 2 and $h_0 = 3.39$, for p = 0.8 and $\Omega = 0$. Ferromagnetic ordered and disordered phases, coexist at a line of first order transition at low temperature, while they are separated by a line of critical point at sufficiently high temperature and small value of the magnetic field. In particular, for the case p = 1, we obtain exactly the same diagram as obtained by Yokota and Sugiyama[4].

For $p_{c2}<p\leq p_{c1}$, $p_{c2} = 0.58$, the tricritical behaviour persist again, but accompanying with a reentrance of the disordered phase. For p = 0.6 the tricritical point C is located at T = 0.3 and $h_0 = 4.13$ (Fig.1b).

The phase diagram corresponding to the region $p_{c3}<p\leq p_{c2}$, $p_{c3} = 0.51$, is a little more complicated than that of Fig.1b. Furthermore the reentrant phenomena, the phase diagram include an ordered critical point B^2 (*coexistence of two critical* B phases) and a critical end point BA^2 (coexistence of critical point B and ordered A^2 phases) where we used the notations introduced by Griffiths[33], and used in the work for kaufman et

al[25]. For $p = 0.52$ and $\Omega = 0$. B^2 point is given by $T = 0.28$ and $h_0 = 4.16$, while BA^2 point by $T = 0.23$ and $h_0 = 4.62$ (Fig.1c).

If $p_{c4} < p \leq p_{c3}$, $p_{c4} = 0.47$, the figure is similar to our Fig.1c, except that the BA^2 point is shifted to the ($T = 0$, $h_0 = 5.96$) point, while the coordinate of the ordered critical point B^2 depends on the value of the concentration p, hence, for $\Omega = 0$, and $p = 0.49$, B^2 is located at $T = 0.28$ and $h_0 = 4.16$. The reentrant phenomena is still exist (Fig.1d).

Although, reentrant phase transition appear for all values of p in the range $0.47 \leq p \leq 0.67$. For suitable values of p, as the temperature decreases, we observe in the T-h diagram the Para-Ferromagnetic phase transitions and Ferro-Paramagnetic phase transitions successively.

We exhibit in Fig.1e, for $p = 0.42$, a typical phase diagram concerning the région $p_{c5} < p \leq p_{c4}$, $p_{c5} = 0.34$, the BA^2 point and the reentrant phenomena are canceled, but a small ordered phase persist for arbitrary large values of the longitudinal magnetic field. It is characterised by a smaller magnetization than that of the ordered phase at weak magnetic field. The new ordered phase is due to the fact that, for sufficiently small concentration p (i.e $p < 1 - p_c$), where p_c is the site-percolation threshold, there is formation of an infinite cluster of spins subjected to zero magnetic field and then we expect the ordered phase at zero temperature which can persist at sufficiently low temperature for arbitrary large field h_0. The two ordered phases are reperated by a first-order line which is terminated by an ordered critical point B^2 ($T = 0.27$, $h_0 = 4.24$).

For $p_{c5} \leq p \leq 0$, the first-ordered line which separates the two ordered phases is destroyed and there is a continuous passage between the two ordered phases (see Fig.1f). The $p = 1/3$ case may be thought of as a good approximation to the gaussian distribution[31]. Schneider and Pytte has concluded that there is no tricritical point for the Gaussian distribution, contrary to the observations of Houghton et al[32]. On the other hand, the Gaussian distribution phase diagram has no ordered phase for large random fields, while the three-peak distribution exhibits an ordered phase for arbitrary large value of the random magnetic field at low temperatures. Finally, at $p = 0$, the random field disappears, and we have only a line of critical points in the T-h plane.

From the zero transverse field Ω, we conclude that :

(i) the tricritical behaviour persist only at $p > p_{c2}$

(ii) the reentrance of the disordered phases occurs only at $p_{c4} < p < p_{c1}$

(iii) the critical end point BA^2 appears only at $p_{c3} < p < p_{c2}$

(iv) the ordered critical point takes place only at $p_{c5} < p < p_{c2}$

(v) the small ordered phase appears for a sufficiently small concentration $p < p_{c3}$.

For a transverse field $\Omega \neq 0$ the threshold percolation concentrations p_c (i=1,......5) calculated in the $\Omega = 0$ case, are functions of Ω. Hence we represent in the plane (Ω , p) the variation laws of p_c as a function of Ω for different phenomena observed at $\Omega = 0$. However in Fig.2 we have delimited the regions where tricritical behaviour of the model (1) occurs (i.e) for each transverse field $\Omega < \Omega_t$ (Ω_t is the critical value above which tricritical behaviour can not occurs for any concentration p) there exist a concentration $p_c(\Omega)$ such that for $p > p_c(\Omega)$, the model (1) present a tricritical behaviour while $p < p_c(\Omega)$ such phenomena can not exists. Ω_t is the value of the transverse field corresponding to $p = 1$, hence $\Omega_t = 2.19$. From Fig.3, it is clear that for $\Omega > \Omega_r$, $\Omega_r = 1.90$, the reentrant phenomena can not persist for any concentration p, while for each $\Omega < \Omega_r$, the reentrant phenomena occurs for all concentration $p_{c4}(\Omega) < p < p_{c1}(\Omega)$. Such phenomena are exhibited within appropriate ranges of the transverse field and the random field, indicating possible competition between randomness and quantum fluctuations. When the random field is sufficiently diluted ($p > 0.67$), the quantum effects dominate and the reentrant phenomena disappear. Both the randomness and quantum effects prevent ordering, but the two effects do not affect in the same manner. The transition in which the randomness *dominates has the tendency to be first order.* Quantum effects tend to make it second order. Then, it is easy to see that the appearance of reentrance phenomena and tricritical points is suppressed by either the increasing quantum effects due to the transverse field or the decreased dilution of the random field distribution.

The *region where the ordered* phase persist for arbitrary value of the longitudinal magnetic field in the plane (Ω , p), is given in Fig.4. Contrary to the mean *field* approach *this* order persist *only* for a concentration $p < p_{c4}(\Omega)$ with $p_{c4}(0) = p_{c4} = 0.47$. It appears also for a transverse *magnetic field* $\Omega < \Omega_0 = 4.71$, *for* $p = 0$.

Longitudinal magnetization of the model (1) is determined for $\Omega = 0$ both as a function of the temperature for several values of the longitudinal magnetic field (Fig.5a) and as a function of the longitudinal magnetic field for several values of the temperature (Fig.5b). From these figures it is clear that the longitudinal magnetization undergoes a discontinuity at the first-order transition, while this magnetization vanishes continuously at the second order transition. For h = 5, (Fig.5a) the longitudinal magnetization vanishes twice; this is a characteristic of the reentrant phenomena in agreement with the phase diagram represented in Fig.1c. Longitudinal magnetization for h = 5 is represented as a function of the temperature for several values of the transverse magnetic field (Fig.6). However it is found that the reentrant phenomena is defavoured by increasing the transverse magnetic field Ω.

VI. Conclusion

Using a finite cluster approximation, we have examined the effect of a transverse magnetic field on the phase diagrams topologies of the spin-1/2 Ising model with three-peak random magnetic field distribution. It is found that the small ordered phase persist only at a sufficiently small concentration of the longitudinal disordered field, which depends on the value of the transverse field, contrary to the mean field results. We have studied the multicritical behaviour and reentrant phenomena as a function of the transverse field. However we have delimited the regions where tricritical behaviour, reentrant phenomena and small ordered phases persist as a functions of the transverse field and concentration p.

Acknowledgements:

Two of the authors (A.B.) and (C.E.B.) would like to thank the International Centre for Theoretical Physics, Trieste, for hospitality.

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Figures Captions:

Fig.1 Phase diagram in *T/J- h/J* plane for *Ω/J* = 0

(a) p = 0.8; (b) p = 0.6; (c) p = 0.52; (d) p = 0.49; (e) p = 0.42; (f) p = 0.3; solid line, *critical points*; *dashed* line, first-order transitions. A tricritical point also occurs.

Fig.2 Concentration dependence of the transverse magnetic field, delimiting the region of tricritical behaviour existence.

Fig.3 Concentration dependence of the transverse magnetic field, delimiting the domain of existence of the reentrant phenomena.

Fig.4 Concentration dependence of the transverse magnetic field, delimiting the region where the small ordered phase exist.

Fig.5a The temperature dependence of the longitudinal magnetization for p = 0.52 and $\Omega = 0$. The number accompanying each curve denotes the value of the longitudinal magnetic field.

Fig.5b The longitudinal field dependence of the longitudinal magnetization for p = 0.42 and $\Omega = 0$. The number accompanying each curve denotes the value of the temperature.

Fig.6 The temperature dependence of the longitudinal magnetization for p = 0.52 and h = 5. The number accompanying each curve denotes the value of the transverse magnetic field.

Fig.1

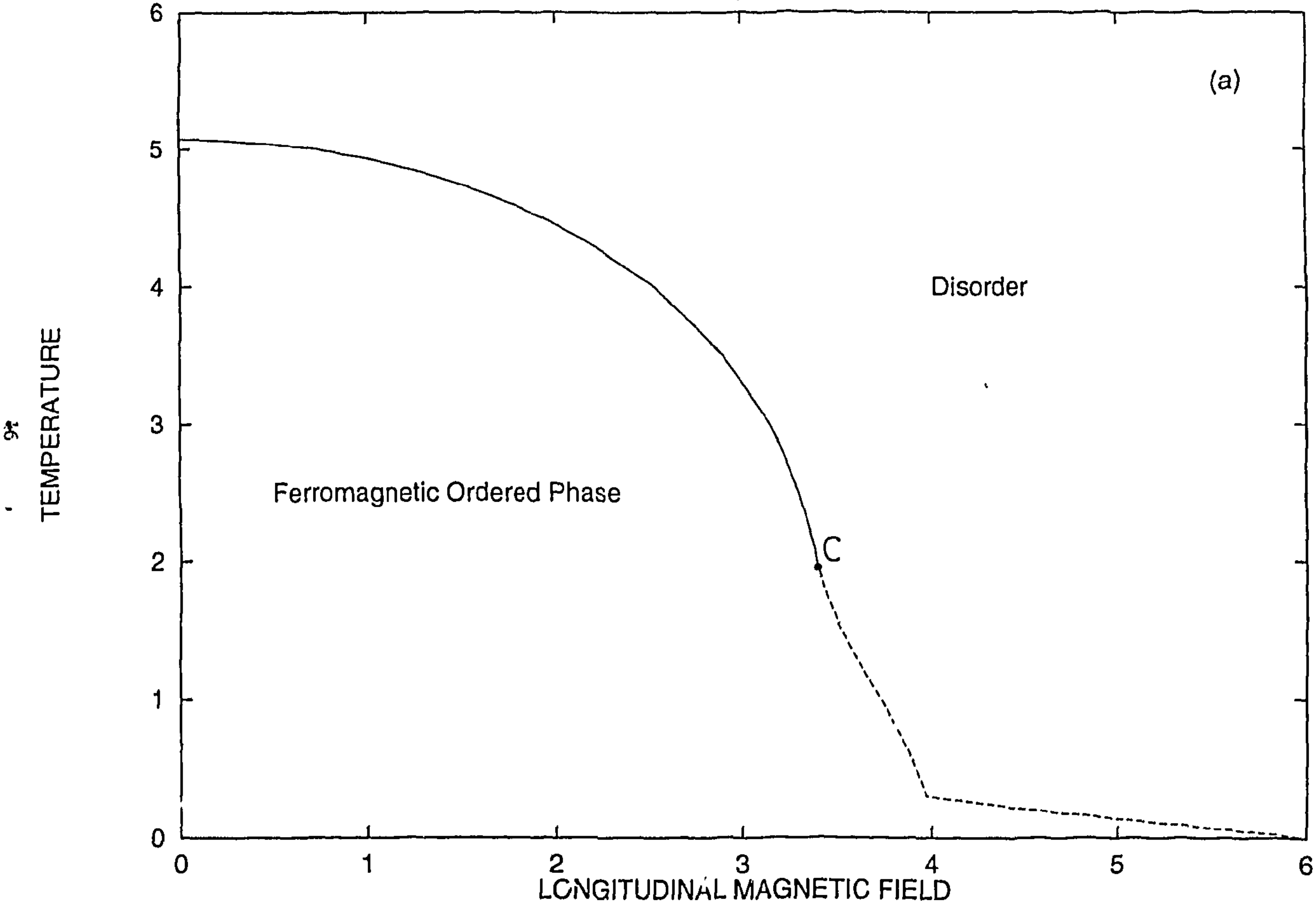

(a)
Disorder
Ferromagnetic Ordered Phase
C
TEMPERATURE
LONGITUDINAL MAGNETIC FIELD
0
1
2
3
4
5
6

Fig.1

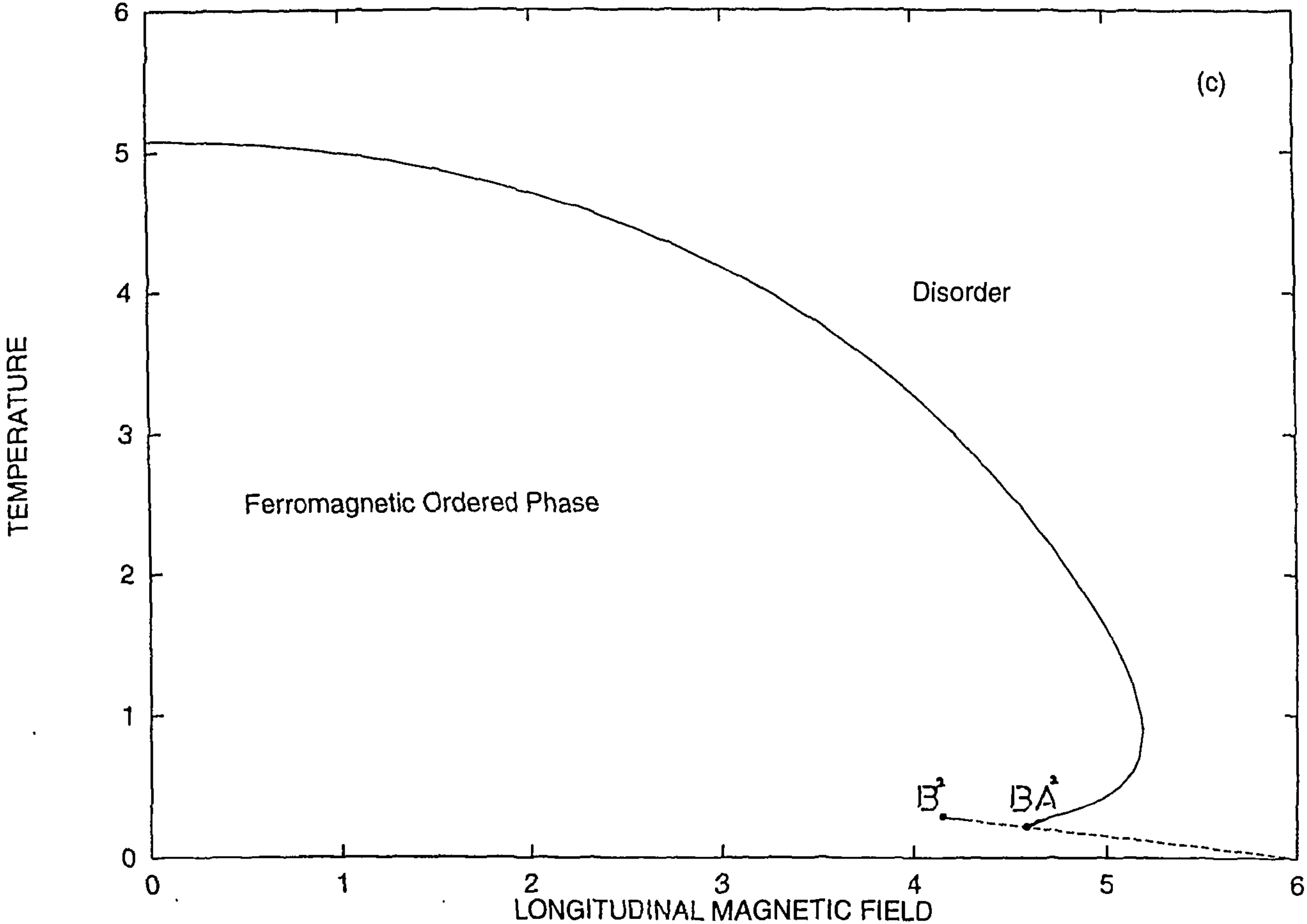
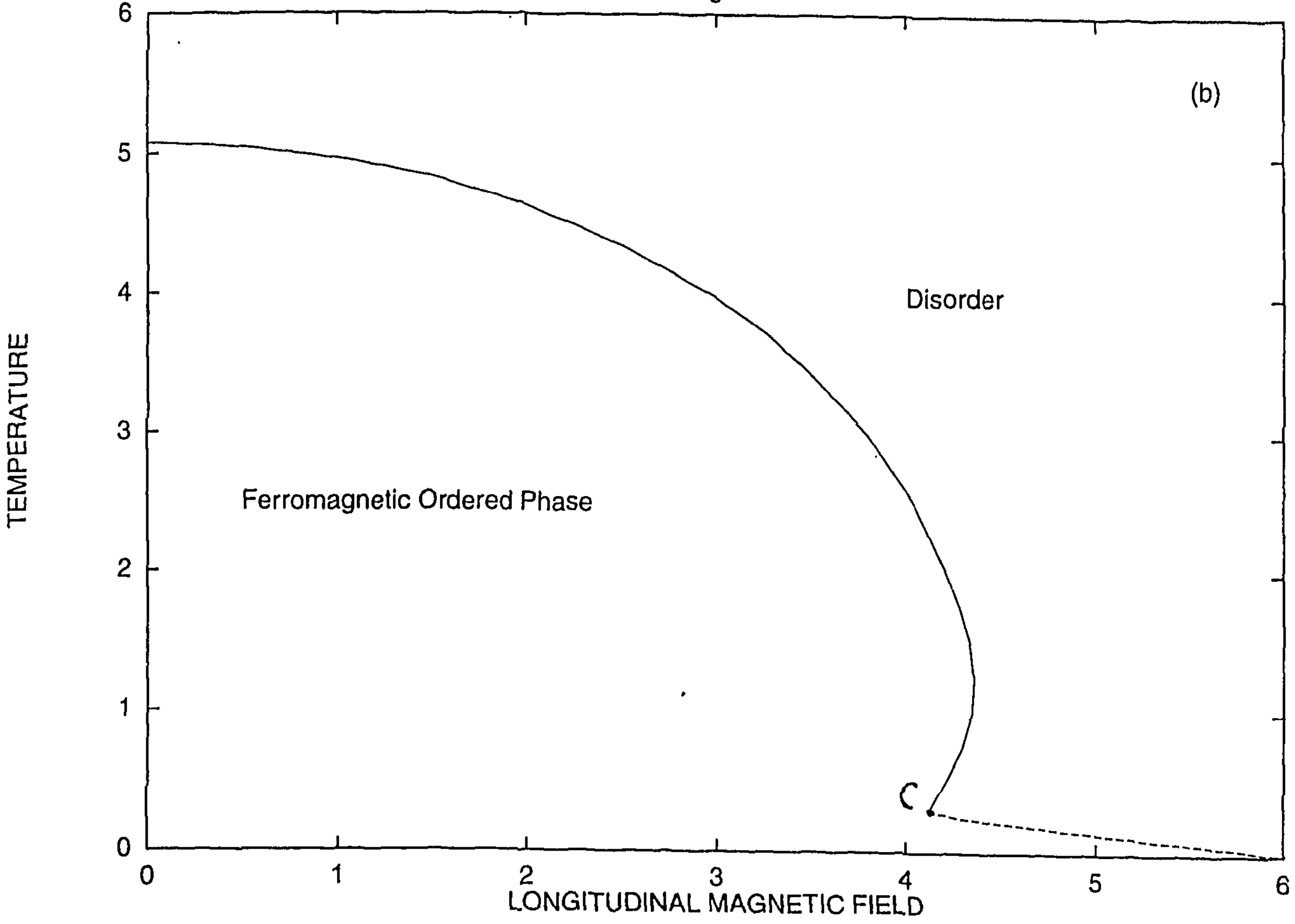
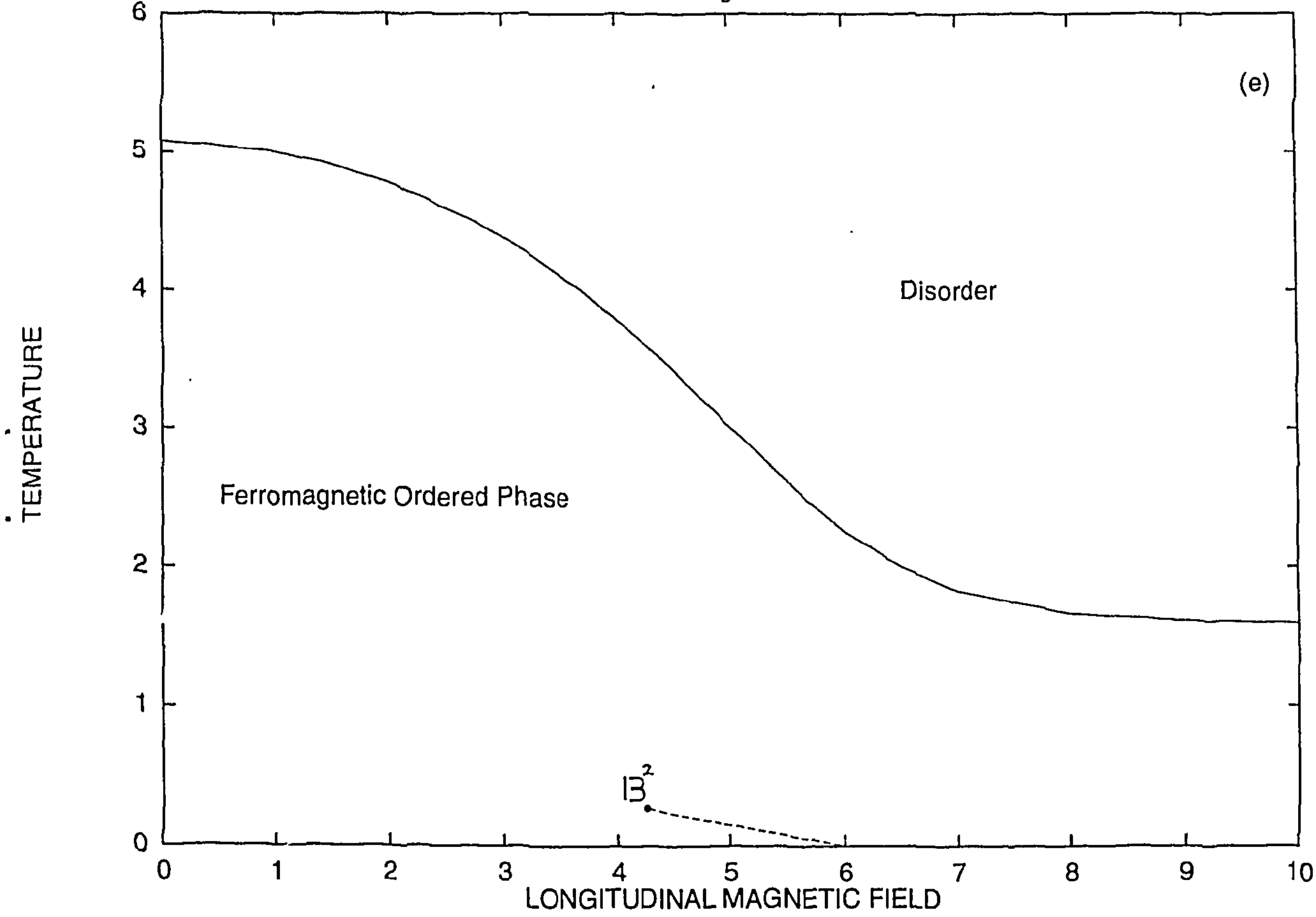

(c)
Disorder
Ferromagnetic Ordered Phase
B
BA
TEMPERATURE
LONGITUDINAL MAGNETIC FIELD
0
1
2
3
4
5
6

Fig.1



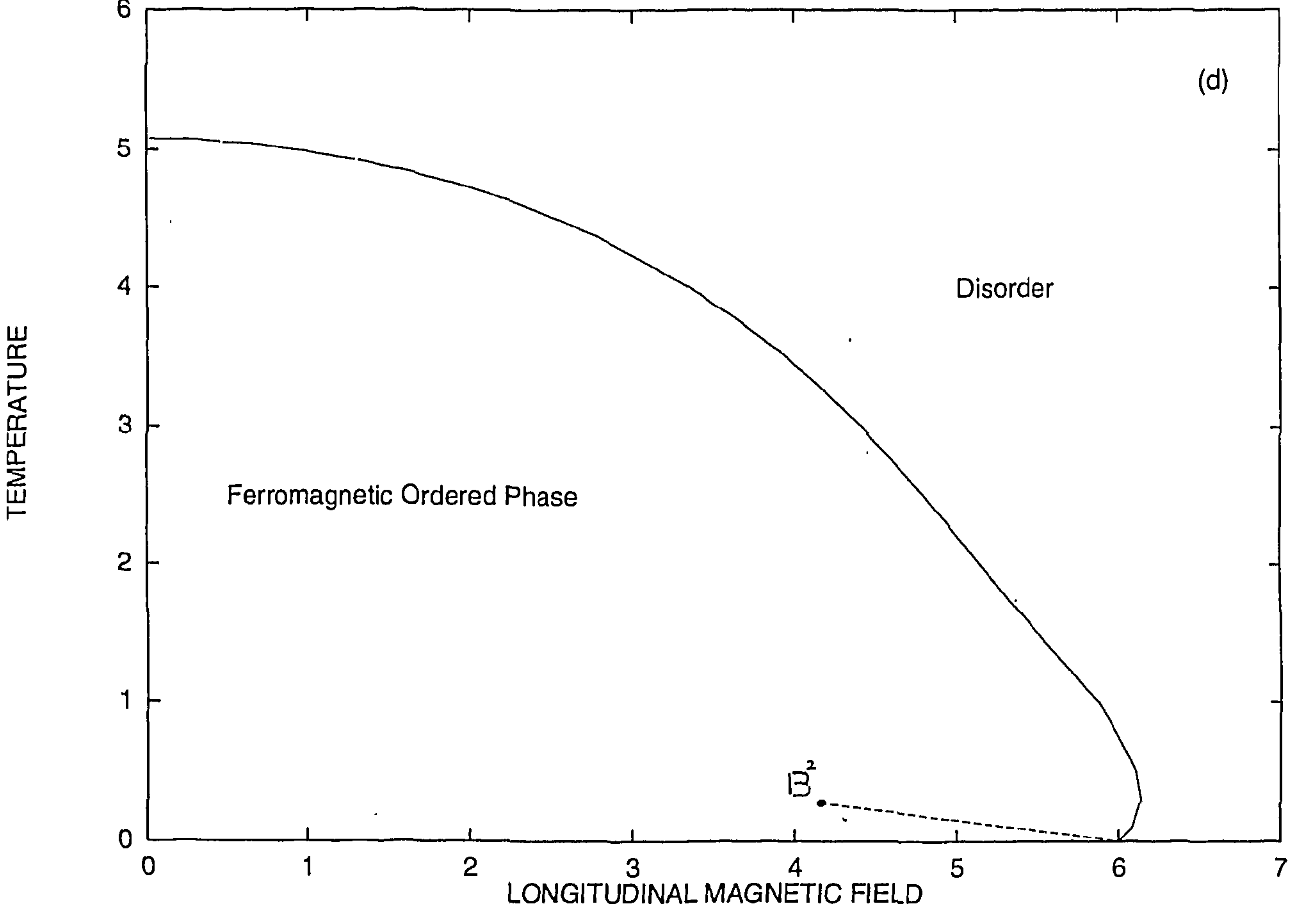
(b)
Disorder
Ferromagnetic Ordered Phase
C
TEMPERATURE
LONGITUDINAL MAGNETIC FIELD
0
1
2
3
4
5
6

Fig.1



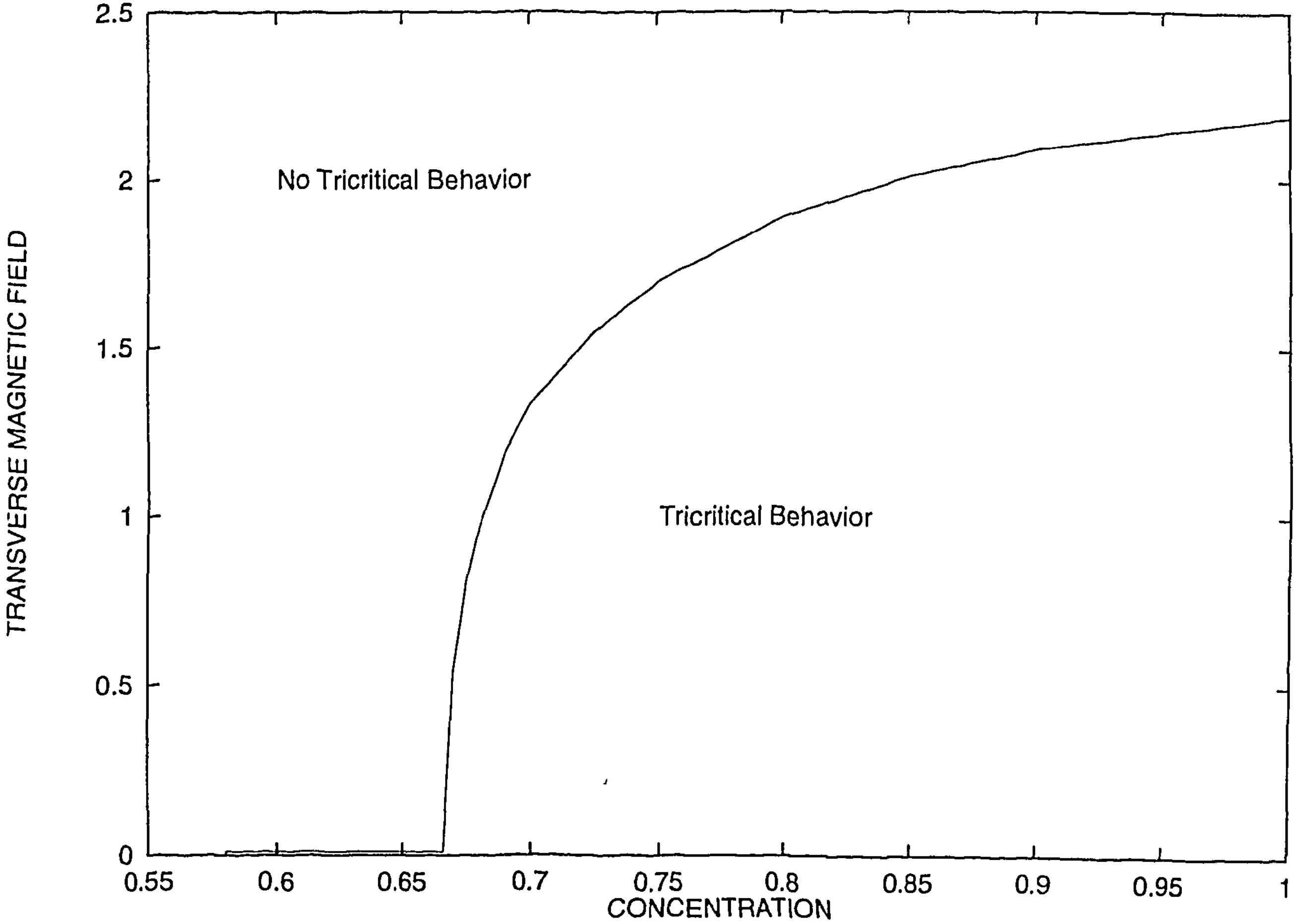
(e)
Disorder
Ferromagnetic Ordered Phase
TEMPERATURE
6
5
4
3
2
1
0
0
1
2
3
4
5
6
7
8
9
10
LONGITUDINAL MAGNETIC FIELD

Fig.1



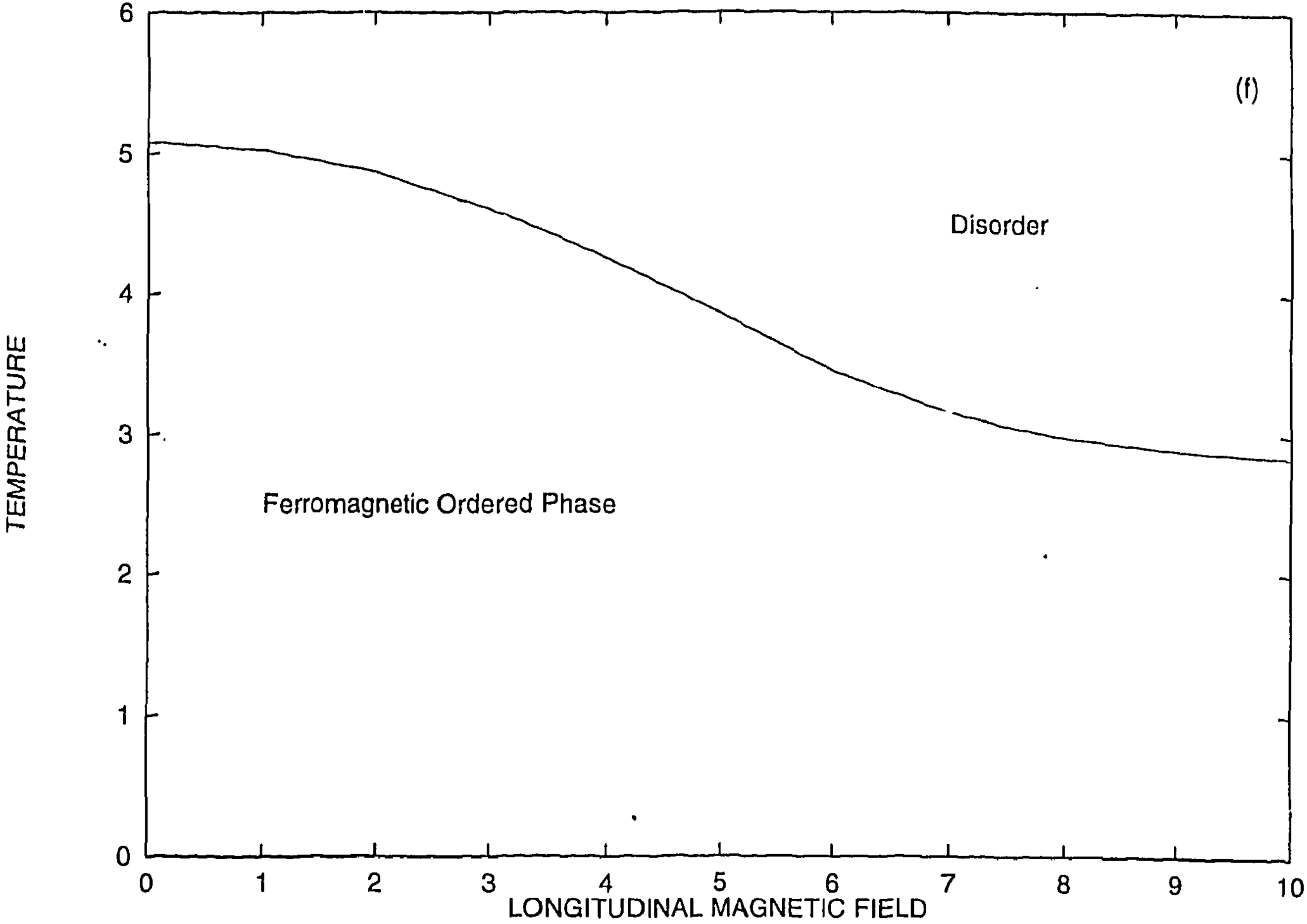
(d)
Disorder
Ferromagnetic Ordered Phase
TEMPERATURE
LONGITUDINAL MAGNETIC FIELD
0
1
2
3
4
5
6
7

Fig.2



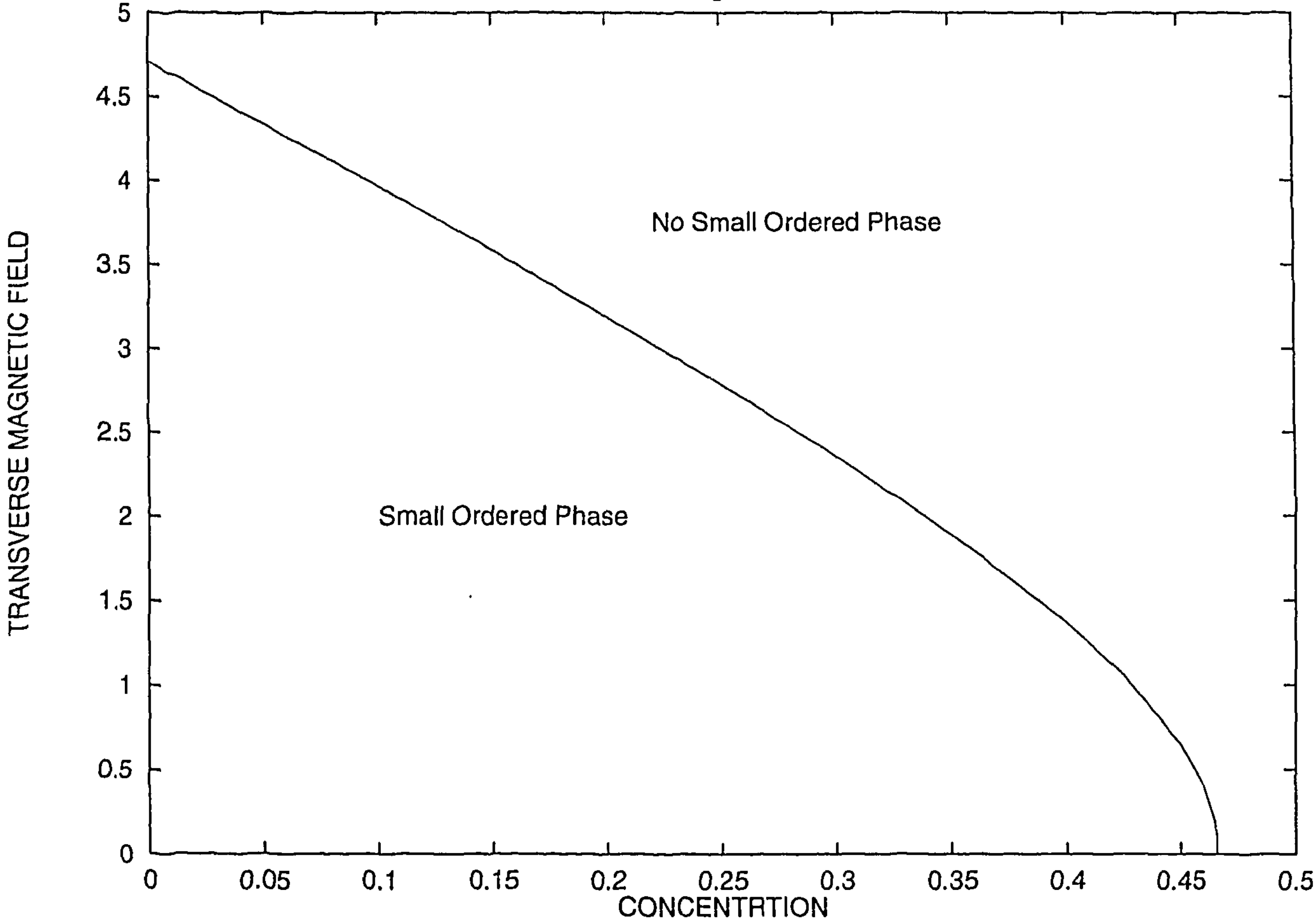
2.5
2
1.5
1
0.5
0
TRANSVERSE MAGNETIC FIELD
No Tricritical Behavior
Tricritical Behavior
0.55
0.6
0.65
0.7
0.75
0.8
0.85
0.9
0.95
1
CONCENTRATION

Fig.1



(f)
Disorder
Ferromagnetic Ordered Phase
TEMPERATURE
LONGITUDINAL MAGNETIC FIELD
0
1
2
3
4
5
6
7
8
9
10

Fig.4



5
4.5
4
3.5
3
2.5
2
1.5
1
0.5
0
TRANSVERSE MAGNETIC FIELD
No Small Ordered Phase
Small Ordered Phase
0
0.05
0.1
0.15
0.2
0.25
0.3
0.35
0.4
0.45
0.5
CONCENTRTION

Fig.3

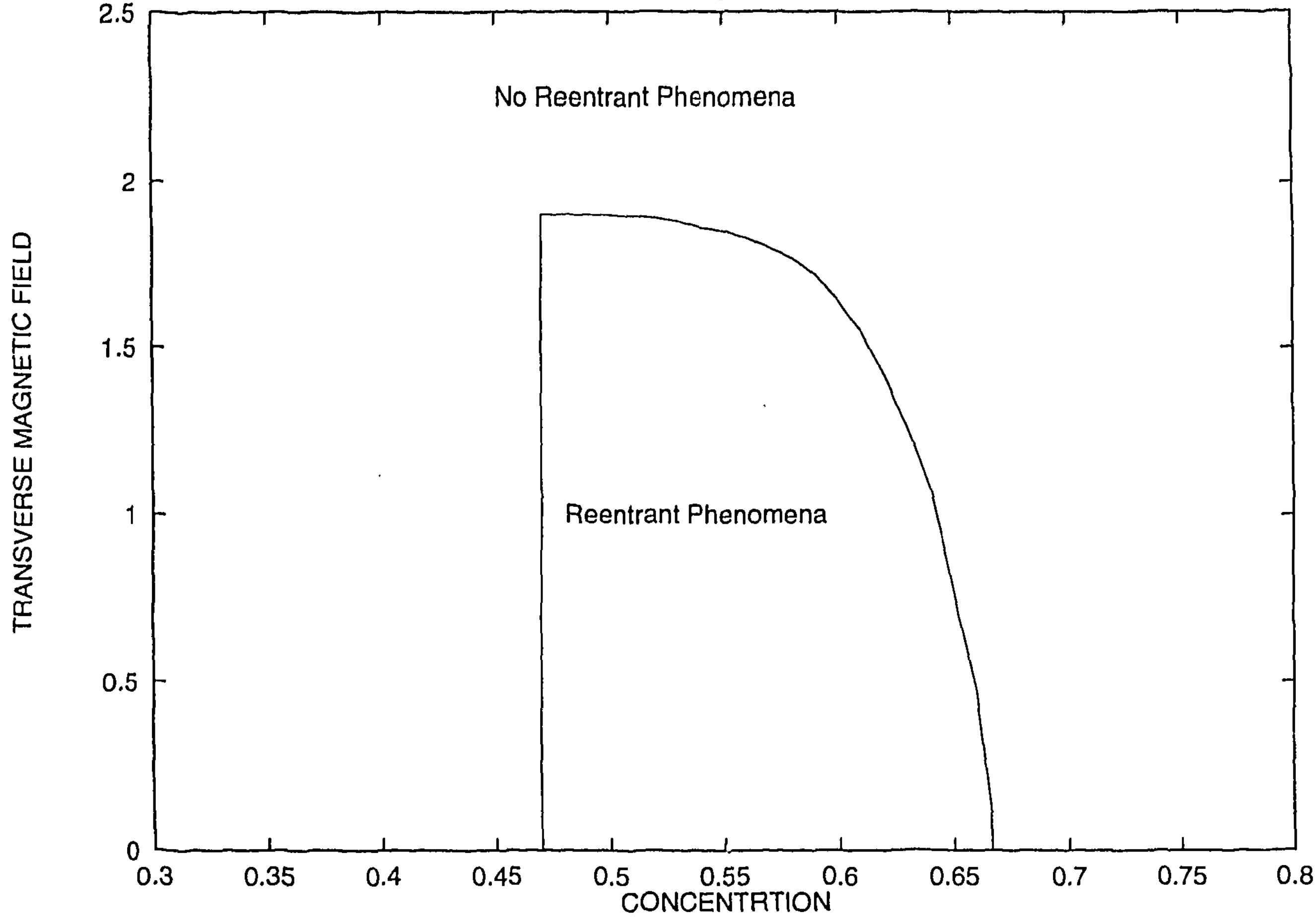

No Reentrant Phenomena
Reentrant Phenomena
TRANSVERSE MAGNETIC FIELD
CONCENTRTION
2.5
2
1.5
1
0.5
0
0.3
0.35
0.4
0.45
0.5
0.55
0.6
0.65
0.7
0.75
0.8

Fig. 5

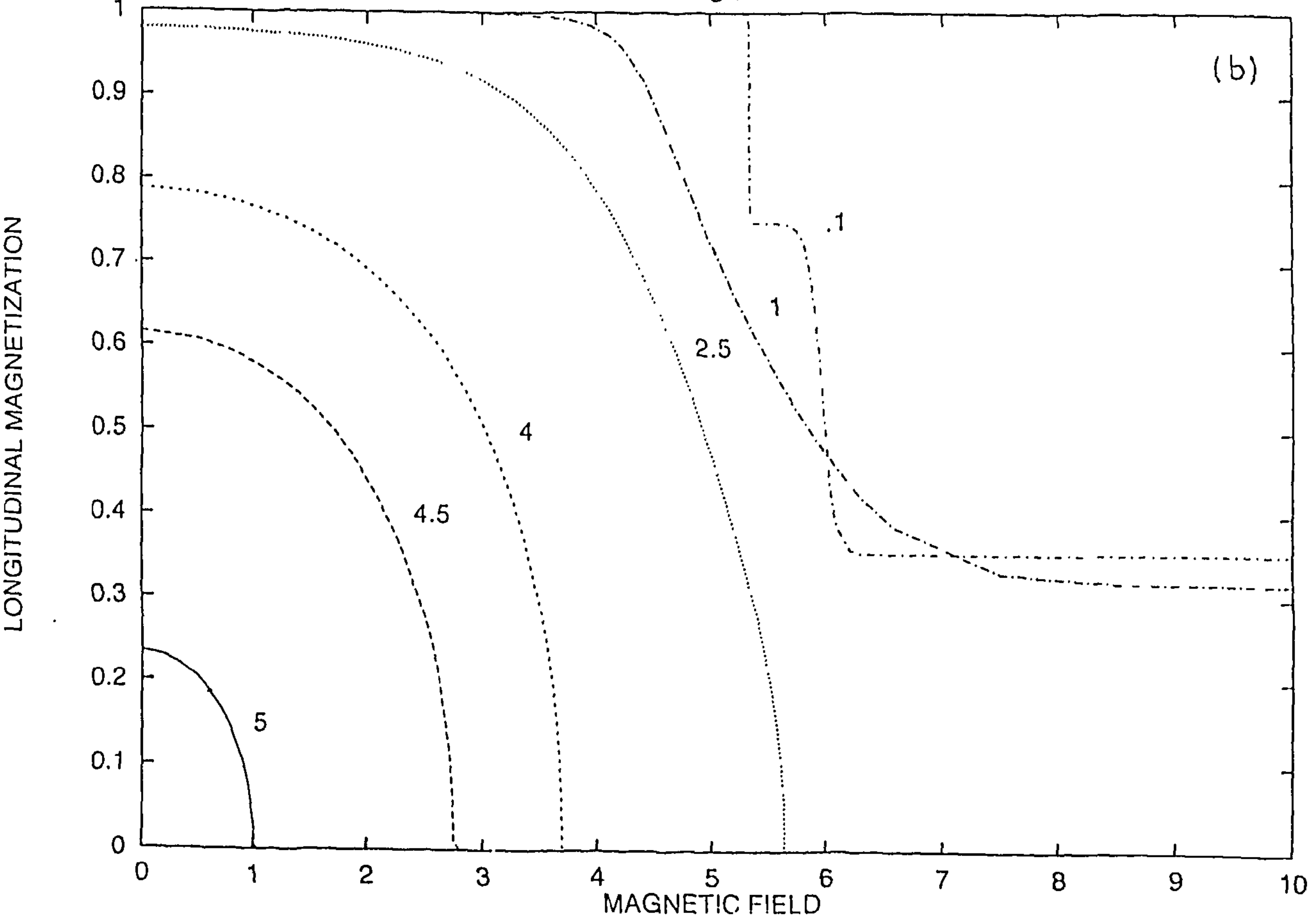

(b)
LONGITUDINAL MAGNETIZATION
MAGNETIC FIELD
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
0
1
2
3
4
5
6
7
8
9
10
5
4.5
4
2.5
1
.1

Fig.5

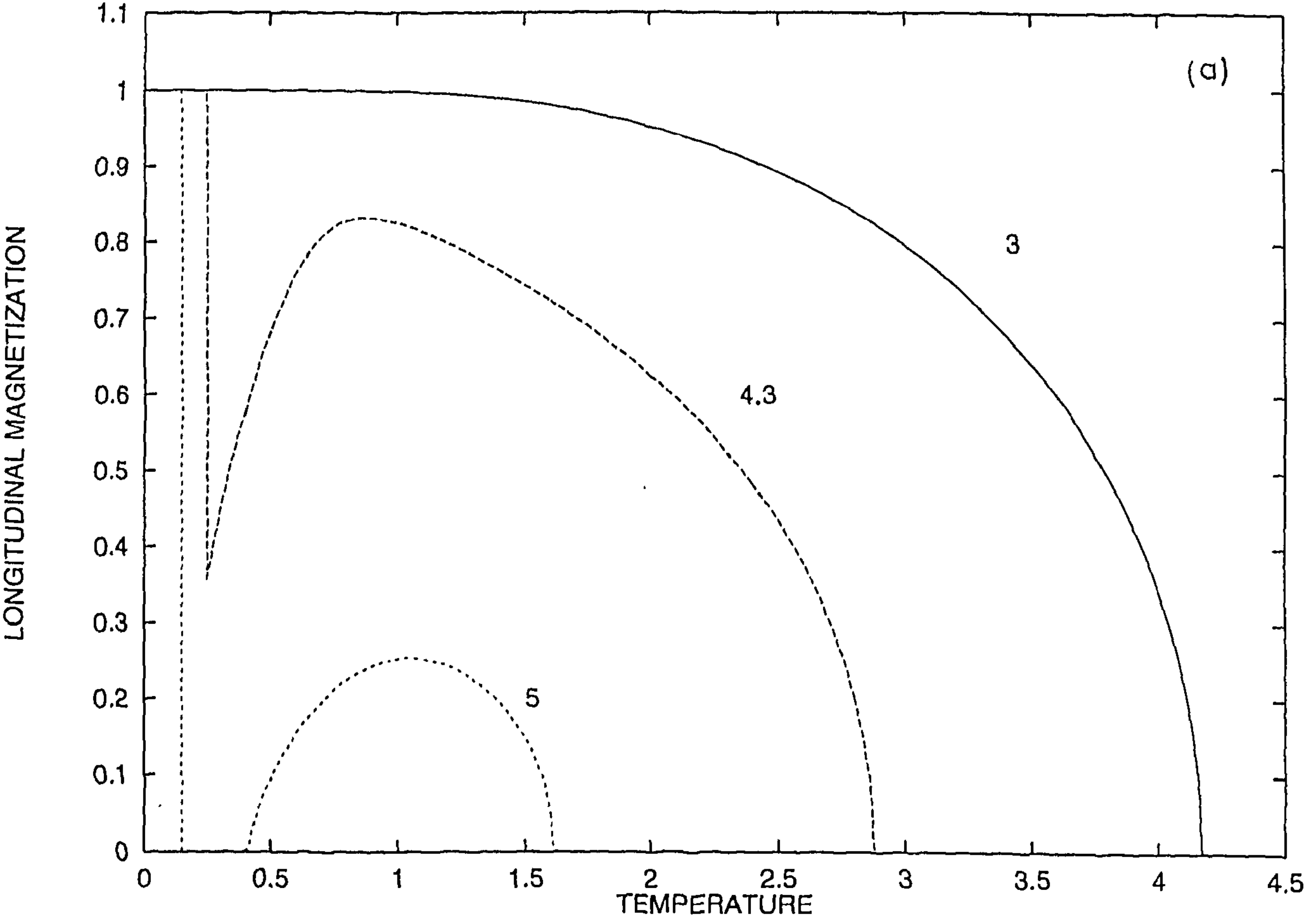
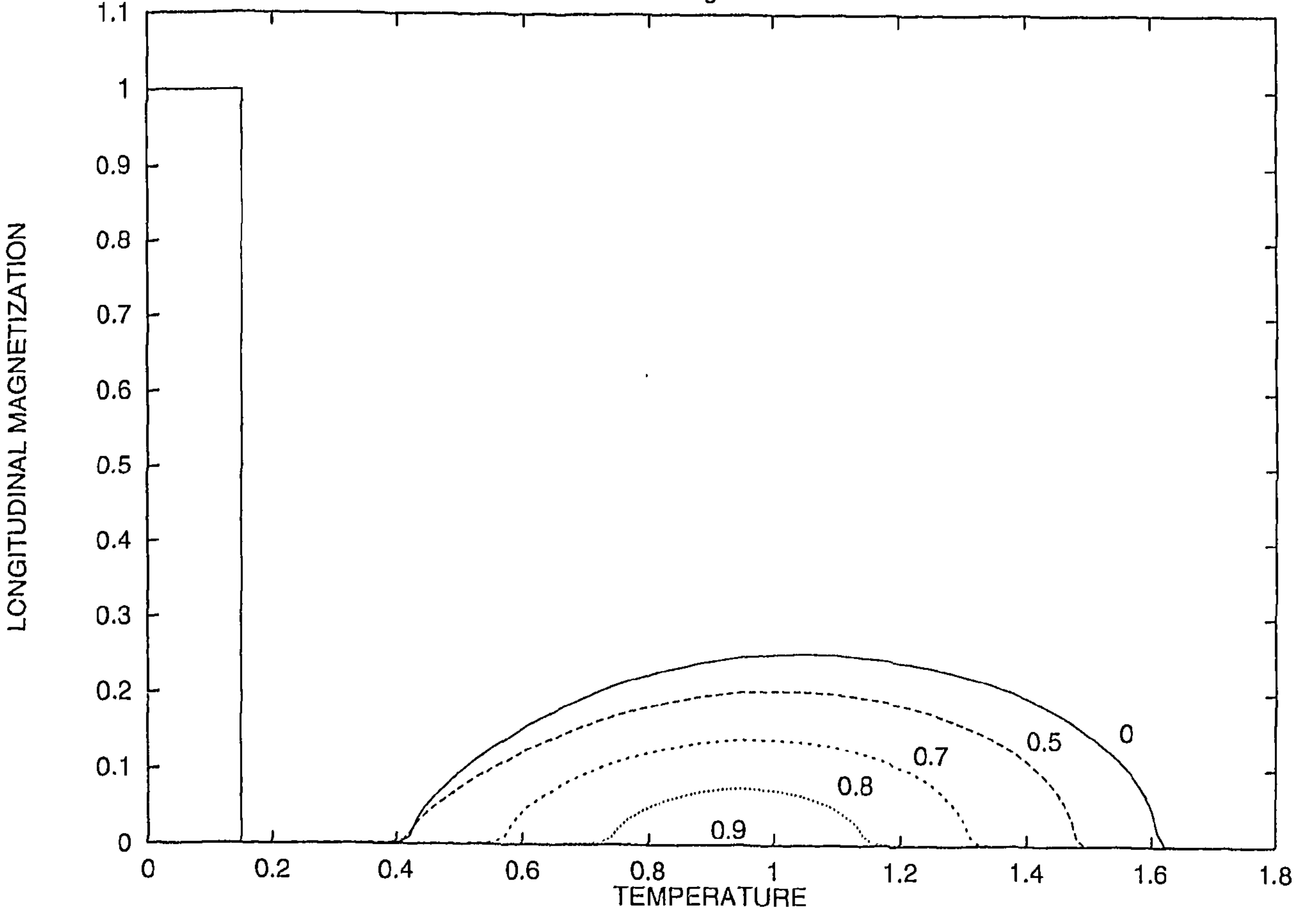

(a)
LONGITUDINAL MAGNETIZATION
TEMPERATURE
3
4.3
5
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
1.1
0.5
1
1.5
2
2.5
3
3.5
4
4.5

Fig. 6


LONGITUDINAL MAGNETIZATION
TEMPERATURE
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
1.1
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
1.8
0.9
0.8
0.7
0.5
0