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Abstract

The effects of amorphized film and diluted surface on phase diagrams and magnetic properties of a spin-1/2 Ising film are investigated within a finite cluster approximation. Depending on the value of the concentration p of the dilution couplings at the surface, it is found that there exists a critical value p_c, when increasing the thickness of the film the critical temperature T_c decreases for p greater than p_c, while it increases for p less than p_c. Moreover, the critical concentration depends on the amorphization δ. Indeed, p_c increases with increasing δ. Besides, the phase diagram represented in (T_c, α), where α represents the strength of the strong coupling at the surface, shows that there exists a critical value of the amorphization $\delta_c = \delta_c(p)$ for $p \neq 1$, for $\delta \leq \delta_c(p)$ a long range order occurs for any value of α at low temperature, while for $\delta > \delta_c(p)$ an order-disorder transition occurs at T=0 and $\alpha = \alpha_c(\delta)$. Magnetization is calculated as a function of the amorphization δ, the concentration p and the strength α of the strong coupling.

I- Introduction

Recently, the determination of the magnetic properties of ferromagnetic thin films, sandwiches and superlattices with a finite thickness d has become a very active field [1-3]. In particular, disordered systems have become the subject of experimental and theoretical interest as a topic in solid state physics owing to the fact that it is possible to find new phenomena in such systems which are unknown in the crystalline case. In fact, experiments of the Mössbauer effect and the magnetization of amorphous ferromagnets indicate that, at least in some materials, there are large fluctuations in the exchange interaction. That fluctuations may be the underlying cause for amorphous magnets which has been proposed by Gubanov [4], Kaneyoshi [5] and Handrich [6]. Furthermore, the magnetic properties of the diluted amorphous systems containing non magnetic impurities are of great interest, since the dilution may cause an additional structural fluctuation in the systems. Theoretically, many works on disordered systems have been published. In particular, surface amorphization has been investigated with the use of bimodal distribution [7] and Gaussian distribution [8] of the exchange integral. The effect of the structural disorder on phase diagram and magnetic properties of spin-1/2 Ising film [9] have also been considered. Furthermore, the disorder was introduced by the quenched randomness of some parameters. For instance, in Refs. 10 and 11 the disorder was represented by the fluctuating magnetic field. In Refs. 12-14 various systems spin 1 with random crystal fields were investigated. In other papers, the properties of disordered magnetic systems have been investigated intensively using bond and site diluted models

[15-20]. In connection with the theory of gelation [21], the diluted system which has both site spin and bond vacancy in the Ising model [22], and the site-bond disorder problem have been studied.

In this paper we study the effect of both type of disorder, namely, diluted surface (layer z=1) and amorphized film ($z \geq 2$), on phase diagrams and magnetic properties of a spin-1/2 ferromagnetic Ising film, by using a single site approximation [23,24]. For the layers z such as $z \geq 2$ the structural disorder is introduced as disorder of the magnetic exchange coupling. Besides, there is a disordered bonds at the surface such as the concentration p is the probability to have a strong coupling $J_{s_1} = (1+\alpha)J_s$ and with 1-p to have a relatively weak coupling $J_{s_2} = (1-\alpha)J_s$. It is found that there exists a critical value p_c of the concentration p, when increasing the thickness of the film the critical temperature T_c decreases for p greater than p_c while it increases for p less than p_c. Moreover, the critical concentration depends on the amorphization of the film δ. Indeed, p_c increases with increasing δ. Besides, the phase diagram represented in (T_c,α) shows that there exists a critical value δ_c of the amorphization δ ($\delta_c = \delta_c(p)$ for $p \neq 1$), for $\delta \leq \delta_c(p)$ a long range order occurs for any value of α, while for $\delta > \delta_c(p)$ an order-disorder transition occurs at T=0 and for $\alpha = \alpha_c(\delta)$.

The paper is organised as follows. In section II, we define the model. The method is explained in Section III. Results and discussions are given in section IV, while section V is reserved for summary and conclusion.

II- Model

We consider a spin-1/2 Ising model of a system of L-coupled squares of a simple cubic lattice. If we consider only nearest-neighbour interactions, the system is governed by the Hamiltonian

$$H = -\sum_{z=1}^{L} \sum_{\langle ij \rangle} J_{ij} \left(S_{i,z} S_{j,z} + S_{i,z} S_{j,z+1} + S_{i,z} S_{j,z-1} \right) \qquad (1)$$

where $S_{i,z} = \pm 1$ is the spin variable of a site i of the layer z, L is the number of layers and J_{ij} are the exchange interactions between nearest neighbour sites which are equal to $\overline{J_S}$ when the sites are at the surface, J_1 when a site is being at surface and its neighbour in the film and $\bar{J}$ when the two sites are in the film (i.e. $z \geq 2$).

We assume that the surface exchange interactions $\overline{J_S}$ fluctuate and are described by a discrete distribution function.

$$P(\overline{J_S}) = p\delta(\overline{J_S} - J_{S_1}) + (1-p)\delta(\overline{J_S} - J_{S_2}) \qquad (2)$$

with

$J_{S_1} = (1+\alpha)J_S$ and $J_{S_2} = (1-\alpha)J_S$.

where p represents the concentration of strong coupling J_{S_1} and the parameter α represents the strength of the exchange interaction J_{S_1} since it allows to increase (decrease) the value of J_{S_1} (J_{S_2}) or to decrease it.

We assume also that the couplings $\bar{J}$ are random exchange interactions between nearest neighbour sites and are distributed by a bimodal distribution namely,

$$P(\bar{J}) = \frac{1}{2}\left(\delta(\bar{J} - J - J\delta) + \delta(\bar{J} - J + J\delta)\right) \tag{3}$$

where $\delta = \frac{\Delta J}{J}$ is a measure of the fluctuation in the exchange coupling $\bar{J}$ and is called amorphization. This distribution has been extensively used by experimentalists to fit their data, especially for Fe-based amorphous alloys [25-26].

III- Method

The method used is the finite cluster method with single site approximation [23,24] which is more appropriate than the mean-field theory in the case of disordered systems. This method, which still neglects correlation between different spins, but takes into account the correlations relation such as $\left\langle (S(x,z))^2 \right\rangle = 1$ exactly, where $\langle \bullet \rangle$ indicates the thermal average. Such a method, is based on a cluster with a selected site labelled 0 and the neighbouring sites with which it directly interacts. Hence, the Hamiltonian containing the central site 0 is given by:

$$H_{0,z} = -\left(J_{0,z-1} S_{0,z-1} + J_{0,z+1} S_{0,z+1} + \sum_{j=1}^{N-2} J_{0,j} S_{j,z} \right) S_{0,z} \tag{4}$$

$J_{0,j}$ is the exchange coupling between the spin at site 0 and the spin at site j. N is the coordination number. N=6 is the simple cubic lattice case.

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

$$\left\langle \left\langle S_{0,z} \right\rangle_c \right\rangle = \left\langle \frac{Tr_0 \, S_{0,z} \exp(-\beta H_{0,z})}{Tr_0 \exp(-\beta H_{0,z})} \right\rangle, \tag{5}$$

where $\left\langle S_{0,z} \right\rangle_c$ denotes the average value of the spin 0 of the layer z for a given configuration c of the nearest-neighbouring spins. $\underset{0}{Tr}$ means the trace performed over $S_{0,z}$ only. $\beta = 1/K_B T$, T is the absolute temperature and K_B is the Boltzmann constant.

By calculating the inner trace in eq. (5), $\left\langle S_{0,z} \right\rangle_c$ is given by :

$$\left\langle S_{0,z} \right\rangle_c = \tanh\left[\frac{1}{K_B T} \left(J_{0,z-1} S_{0,z-1} + J_{0,z+1} S_{0,z+1} + \sum_{j=1}^{N-2} J_{0,j} S_{j,z} \right) \right] \tag{6}$$

The magnetization m_z of the layer z is given by performing the average $\langle \bullet \rangle_D$ over the disorder of the exchange coupling at the surface, and the average $\langle \bullet \rangle$ over the spin configurations, namely

$$m_z = \left\langle \left\langle \left\langle S_{0,z} \right\rangle_c \right\rangle \right\rangle_D \tag{7}$$

with

$$\left\langle \left\langle S_{0,z} \right\rangle_c \right\rangle_D = \int \left\langle S_{0,z} \right\rangle_c \prod_{j=1}^{N-2} P\left(J_{0,j}\right) dJ_{0,j} P\left(J_{0,z-1}\right) P\left(J_{0,z+1}\right) dJ_{o,z-1} dJ_{0,z+1} \quad (8)$$

To develop this expression we use the expansion technique for cluster identities of a spin-1/2 Ising system [27,28].

The magnetisation of the layer z is given by:

at the surface,

$$m_s = \frac{1}{2^{N-2}} \sum_{k_3=0}^{N-2} C_{k_3}^{N-2} \sum_{p_3=0}^{N-2} \sum_{p_2=0}^{1} U_{p_2 p_3 k_3} (m_S)^{p_3} (m_1)^{p_2} C_{p_3}^{N-2} \quad (9)$$

for z=1,

$$m_1 = \frac{1}{2^N} \sum_{k_1=0}^{1} \sum_{k_2=0}^{1} \sum_{k_3=0}^{N-2} C_{k_3}^{N-2} \sum_{p_2=0}^{1} \sum_{p_1=0}^{1} \sum_{p_3=0}^{N-2} A_{p_1 p_2 p_3, k_1, k_2, k_3} (m_s)^{p_1} (m_1)^{p_3} (m_2)^{p_2} C_{p_3}^{N-2} \quad (10)$$

for z=L,

$$m_L = \frac{1}{2^{N-1}} \sum_{k_2=0}^{1} \sum_{k_3=0}^{N-2} C_{k_3}^{N-2} \sum_{p_2=0}^{1} \sum_{p_3=0}^{N-2} B_{p_2 p_3 k_2 k_3} (m_L)^{p_3} (m_{L-1})^{p_2} C_{p_3}^{N-2} \quad (11)$$

and for z=2, $\cdots$,L-1

$$m_z = \frac{1}{2^N} \sum_{k_1=0}^{1} \sum_{k_2=0}^{1} \sum_{k_3=0}^{N-2} C_{k_3}^{N-2} \sum_{p_2=0}^{1} \sum_{p_1=0}^{1} \sum_{p_3=0}^{N-2} V_{p_1 p_2 p_3, k_1, k_2, k_3} (m_{z-1})^{p_1} (m_z)^{p_3} (m_{z+1})^{p_2} C_{p_3}^{N-2} \tag{12}$$

with

$$U_{p_2 p_3 k_3} = \frac{1}{2^{N-1} C_{p_3}^{N-2}} \sum_{i_2=0}^{1} \sum_{i_3=0}^{k_3} \sum_{j_3=0}^{N-2-k_3} \sum_{\mu_2=0}^{i_2} \sum_{\mu_3=0}^{i_3} \sum_{\nu_3=0}^{j_3} (-1)^{\mu_2+\mu_3+\nu_3}$$
$$\times C_{\mu_2}^{i_2} C_{p_2-\mu_2}^{1-i_2} C_{i_3}^{k_3} C_{j_3}^{N-2-k_3} C_{\mu_3}^{i_3} C_{\nu_3}^{j_3} C_{p_3-\mu_3-\nu_3}^{N-2-i_3-j_3} \tag{13}$$
$$\times \tanh[\beta(J_{S_1}(k_3 - 2i_3) + J_{S_2}(N-2-k_3-2j_3) + J_1(1-2i_2))]$$

$$A_{p_1 p_2 p_3 k_1 k_2 k_3} = \frac{1}{2^N C_{p_3}^{N-2}} \sum_{i_1=0}^{k} \sum_{i_2=0}^{k} \sum_{i_3=0}^{k_3} C_{i_3}^{k_3} \sum_{j_1=0}^{1-k} \sum_{j_2=0}^{1-k} \sum_{j_3=0}^{N-2-k_3} \sum_{\mu_1=0}^{i} \sum_{\mu_2=0}^{i} \sum_{\mu_3=0}^{i}$$
$$\sum_{\upsilon_1=0}^{j} \sum_{\upsilon_2=0}^{j} \sum_{\upsilon_3=0}^{j} (-1)^{\mu+\upsilon} C_{j_3}^{N-2-k_3} C_{\mu_3}^{i_3} C_{\upsilon_3}^{j_3} C_{p_1-\mu_1-\upsilon_1}^{1-i_1-j_1} C_{p_2-\mu_2-\upsilon_2}^{1-i_2-j_2} C_{p_3-\mu_3-\upsilon_3}^{N-2-i_3-j_3}$$
$$\tanh[\beta(J(1-\delta)(k_3 - 2i_3) + J(1+\delta)(N-2-k_3-2j_3) + J(1-\delta)(k_2 - 2i_2) +$$
$$J(1+\delta)(1-k_2-2j_2) + J_1(1-\delta_1)(k_1 - 2i_1) + J_1(1+\delta_1)(1-k_1-2j_1))] \tag{14}$$

$$B_{p_2 p_3 k_2 k_3} = \frac{1}{2^{N-1} C_{p_3}^{N-2}} \sum_{i_2=0}^{k_2} \sum_{i_3=0}^{k_3} \sum_{j_2=0}^{1-k_2} \sum_{j_3=0}^{N-2-k_3} \sum_{\mu_2=0}^{i_2} \sum_{\mu_3=0}^{i_3} C_{i_3}^{k_3}$$

$$\sum_{\upsilon_2=0}^{j_2} \sum_{\upsilon_3=0}^{j_3} (-1)^{\mu_3+\mu_2+\upsilon_3+\upsilon_2} C_{j_3}^{N-2-k_3} C_{\mu_3}^{i_3} C_{\upsilon_3}^{j_3} C_{p_2-\mu_2-\upsilon_2}^{1-i_2-j_2}$$

$$C_{p_3-\mu_3-\upsilon_3}^{N-2-i_3-j_3} \tanh[\beta J((1-\delta)(k_2+k_3-2(i_2+i_3)) +$$

$$(1+\delta)(N-1-(k_2+k_3)-2(j_2+j_3)))]$$

(15)

and

$$V_{p_1 p_2 p_3 k_1 k_2 k_3} = \frac{1}{2^N C_{p_3}^{N-2}} \sum_{i_1=0}^{k_1} \sum_{i_2=0}^{k_2} \sum_{i_3=0}^{k_3} C_{i_3}^{k_3} \sum_{j_1=0}^{1-k_1} \sum_{j_2=0}^{1-k_2} \sum_{j_3=0}^{N-2-k_3} \sum_{\mu_1=0}^{i_1} \sum_{\mu_2=0}^{i_2} \sum_{\mu_3=0}^{i_3}$$

$$\sum_{\upsilon_1=0}^{j_1} \sum_{\upsilon_2=0}^{j_2} \sum_{\upsilon_3=0}^{j_3} (-1)^{\mu+\upsilon} C_{j_3}^{N-2-k_3} C_{\mu_3}^{i_3} C_{\upsilon_3}^{j_3} C_{p_1-\mu_1-\upsilon_1}^{1-i_1-j_1} C_{p_2-\mu_2-\upsilon_2}^{1-i_2-j_2} C_{p_3-\mu_3-\upsilon_3}^{N-2-i_3-j_3}$$

$$\tanh[\beta(J(1-\delta)(k_3-2i_3)+J(1+\delta)(N-2-k_3-2j_3)+J(1-\delta)(k_2-2i_2)+$$

$$J(1+\delta)(1-k_2-2j_2)+J_1(1-\delta_1)(k_1-2i_1)+J_1(1+\delta_1)(1-k_1-2j_1))]$$

(16)

IV- Results and discussion

Equations (9)-(16), are solved numerically. However, the transition temperature T_c as a function of the thickness L of the film is plotted in Fig. 1. As is seen, T_c may increase or

decrease with L according to the values of the concentration p. For p greater than p_c=0.5, the transition temperature decreases with L and asymptotically tends to the bulk transition. However, for p less than p_c, the critical temperature increases with the thickness L. In fact, for a large value of p, there is a dominance of a large coupling J_{S_1} at the surface which give a large value of the transition temperature to the system. Furthermore, when the amorphization δ in the film increases, the critical concentration p_c also increases and then for any value of the probability p less than p_c, the transition temperature increases with the thickness L. This is due to the fact that the amorphization reduces the value of the transition temperature. Fig. 2 shows the dependence of the transition temperature T_c on the strength of the strong coupling J_{S_1} for three values of the concentration p, namely p=0 (Fig. 2a), p=0.4 (Fig. 2b) and p=1 (Fig. 2c). It is clear, from Fig. 2a and 2b that there exists a critical value δ_c of the amorphization δ for which the critical transition reduces to zero. However by increasing the concentration p, the system needs a large value of the amorphization δ in order to reduce its critical temperature to zero. Consequently, $\delta_{c(p)}$ increases with increasing p until to disappear in the special case of p=1 where, contrary to the case p<1, the critical temperature increases with increasing the parameter α. In order to understand further, in Fig. 3 the critical temperature $K_B T_c/J$ is plotted as a function of the amorphization δ for α=0.4 and for several values of the concentration p. The order-disorder transition temperature decreases when δ increases. This variation is more pronounced for a relatively small value of the concentration p. For the same value of the strength of J_{S_1} as in Fig. 3, Fig. 4

gives the dependence of the transition temperature as a function of the concentration p for a pure case and for several values of the amorphization δ. It is clear that the transition temperature increases with increasing the concentration p which favours a strong coupling at the surface and imposes a large value of the transition temperature to the system.

The corresponding magnetizations of the previous phase diagram (Fig. 2) are presented as functions of the amorphization δ (Fig. 5). As is seen, the total magnetization of the system decreases with increasing the amorphization δ and that for a relatively small value of p, the transition temperature reduces to zero at $\delta = \delta_c$. Typical magnetization profiles are depicted in Fig. 6 for a film of thickness L=20 and for several values of the concentration p. It is clear that for $p \neq 1$ the transition temperature of the system increases from its surface value to the bulk one. However, for the special case p=1, the magnetization decreases when we move from the surface to the bulk. However, for any value of the concentration p and far from the diluted surface, the magnetization keeps a fixed value and decreases when we approach the second pure surface (z=L). Fig. 7 gives the profile of the magnetizations for $p = p_c = 0.5$ and for several values of the amorphization δ. It is clear that the magnetization increases from its surfaces values to the bulk one and decreases with increasing the amorphization δ. However, it is noted that for p=1, the magnetization of the diluted surface is never equal to zero and this for any value of the amorphization δ.

V- Conclusion

We have studied the effects of diluted surface and amorphized film on the phase diagrams and magnetic properties of a spin-1/2 Ising film by using a single cluster approximation. Many relevant results are obtained. Indeed, on one hand, depending on the value of the concentration p at the surface, there exists a critical value p_c, when increasing the thickness of the film the critical temperature T_c decreases for p greater than p_c while it increases for p less than p_c. Moreover, the critical concentration depends on the amorphization δ. Indeed, p_c increases with increasing δ. On the other hand, the phase diagram represented in (T_c, α), shows that there exists a critical value of the amorphization $\delta_c = \delta_c(p)$ for $p \neq 1$, for $\delta \leq \delta_c(p)$ a long range order occurs for any value of α while for $\delta > \delta_c(p)$ an order-disorder transition occurs at T=0 and for $\alpha = \alpha_c(\delta)$.

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Figure captions

Fig. 1: The dependence of the critical temperature T_c on the film thickness L for $\delta = 0$ and $\alpha = 0.4$.

Fig. 2: The dependence of the critical temperature T_c on the parameter α for p=0 (a), p=0.4 (b) and p=1 (c).

Fig. 3: The dependence of the critical temperature T_c on the amorphization δ for $\alpha = 0.4$.

Fig. 4: The dependence of the critical temperature T_c on the concentration p for $\alpha = 0.4$.

Fig. 5: The total magnetization M_T dependence on the amorphization δ for T=1 and $\alpha = 1$.

Fig. 6: The magnetization profiles M(z) for δ=0, $\alpha = 0.4$. and T=4.5.

Fig. 7: The magnetization profiles M(z) for p=0.5, $\alpha = 0.4$. and T=4.5.

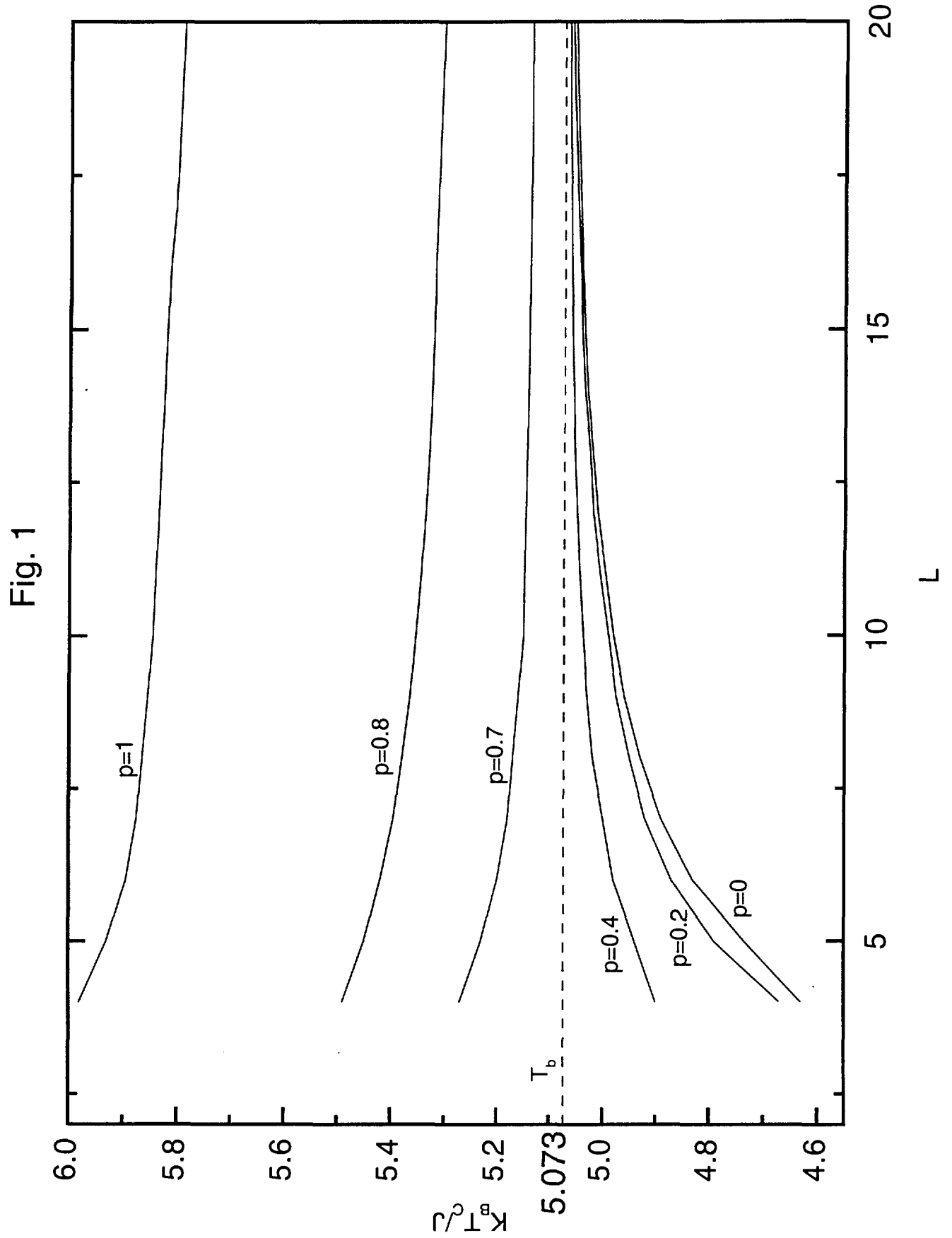
Fig. 1
6.0
5.8
5.6
5.4
5.2
5.073
5.0
4.8
4.6
$K_B T_c / J$
T_b
5
10
15
20
L
p=1
p=0.8
p=0.7
p=0.4
p=0.2
p=0

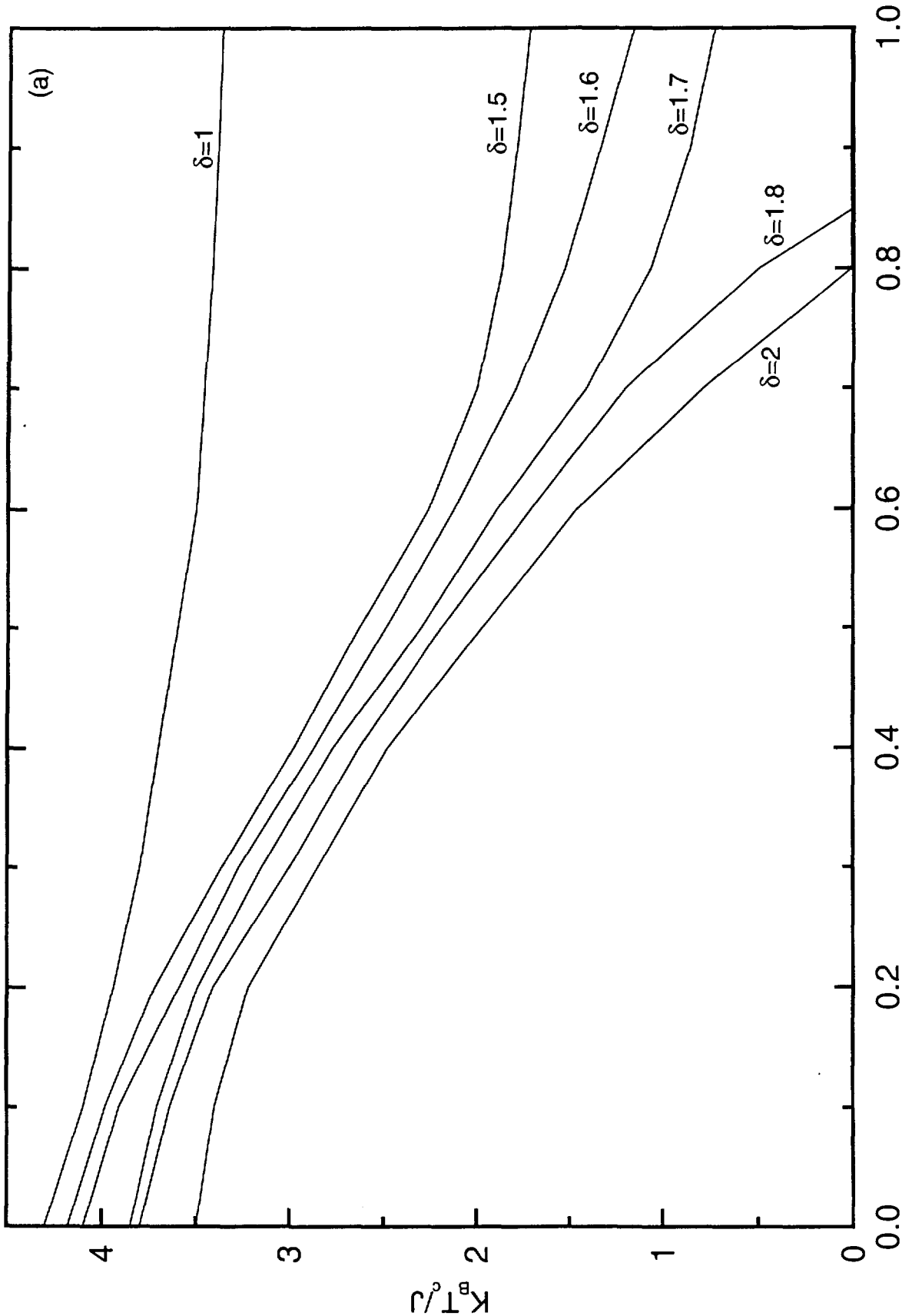

Fig. 2

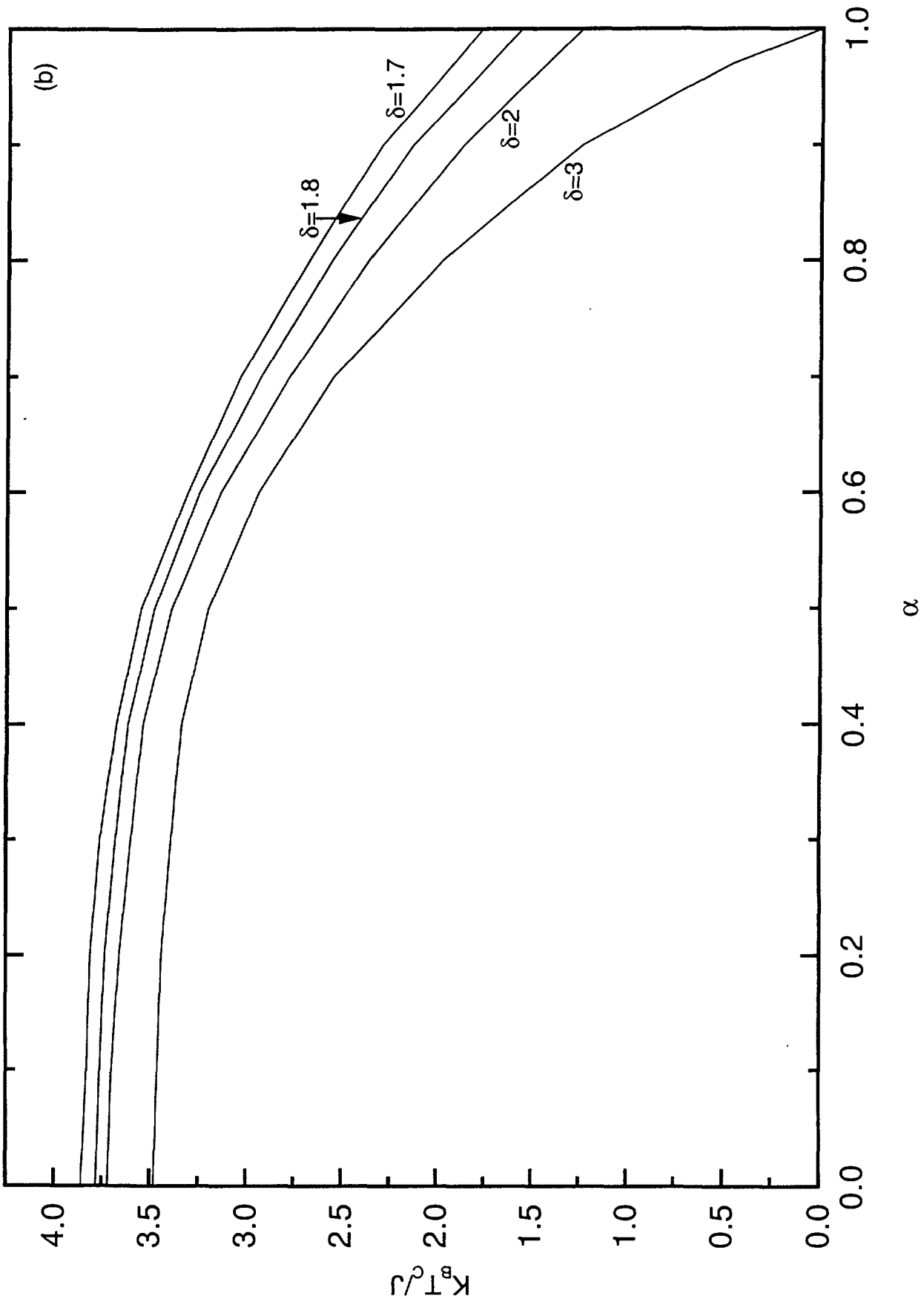

Fig. 2

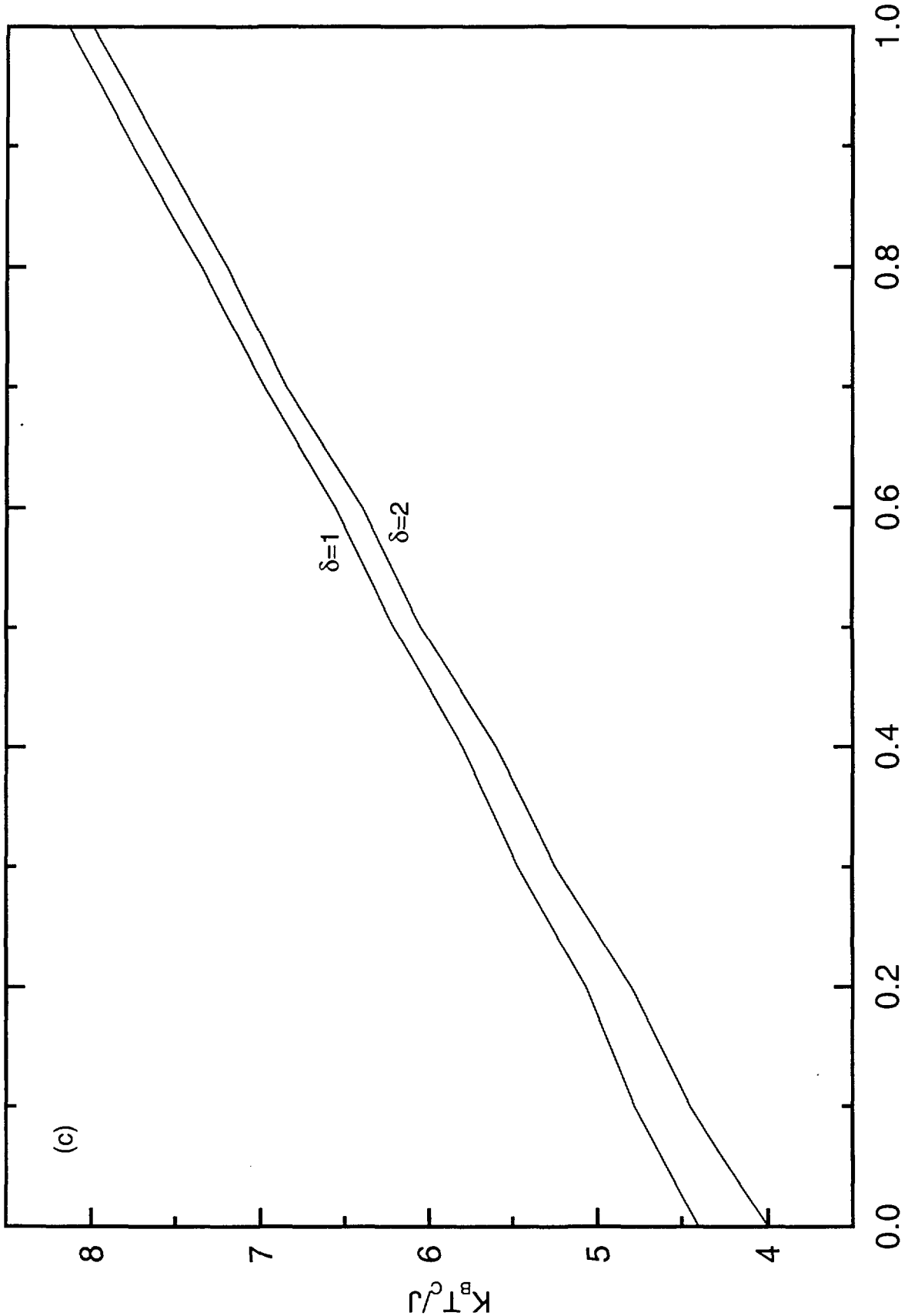
Fig. 2
(c)
δ=1
δ=2
$K_B T_c/J$
α
0.0
0.2
0.4
0.6
0.8
1.0
4
5
6
7
8

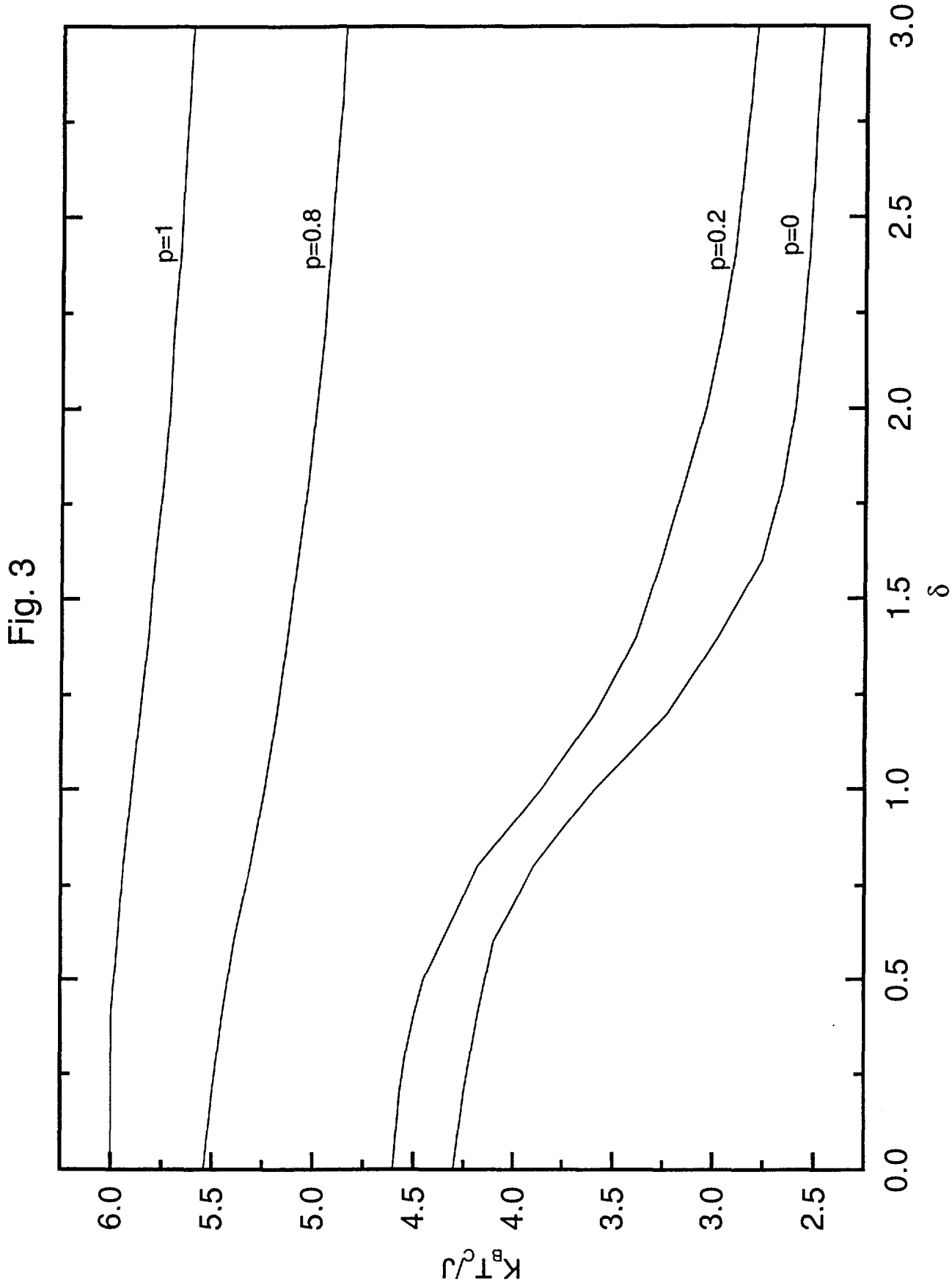

Fig. 3

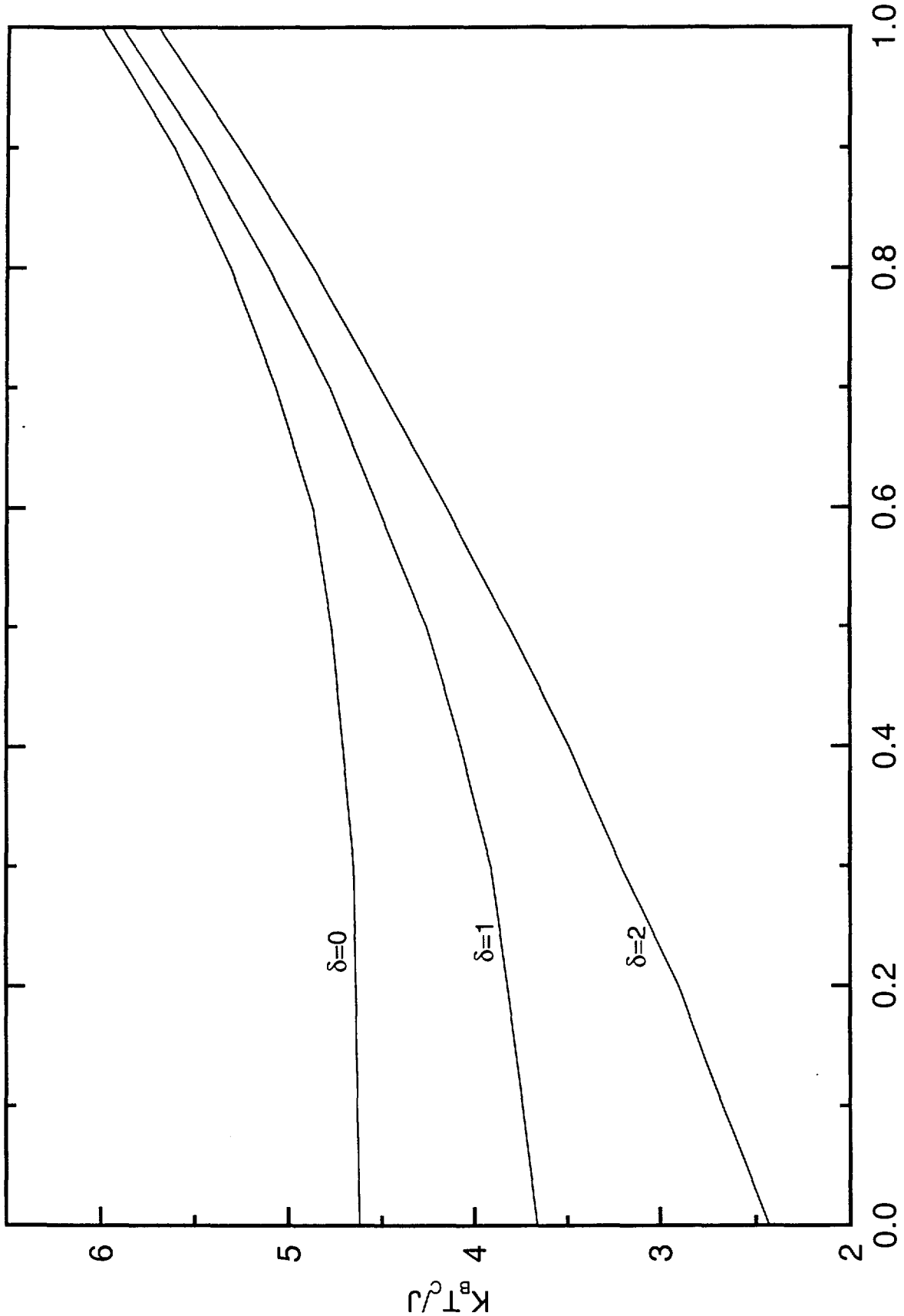
Fig. 4
k_BT_c/J
p
δ=0
δ=1
δ=2
0.0
0.2
0.4
0.6
0.8
1.0
2
3
4
5
6

Fig. 5

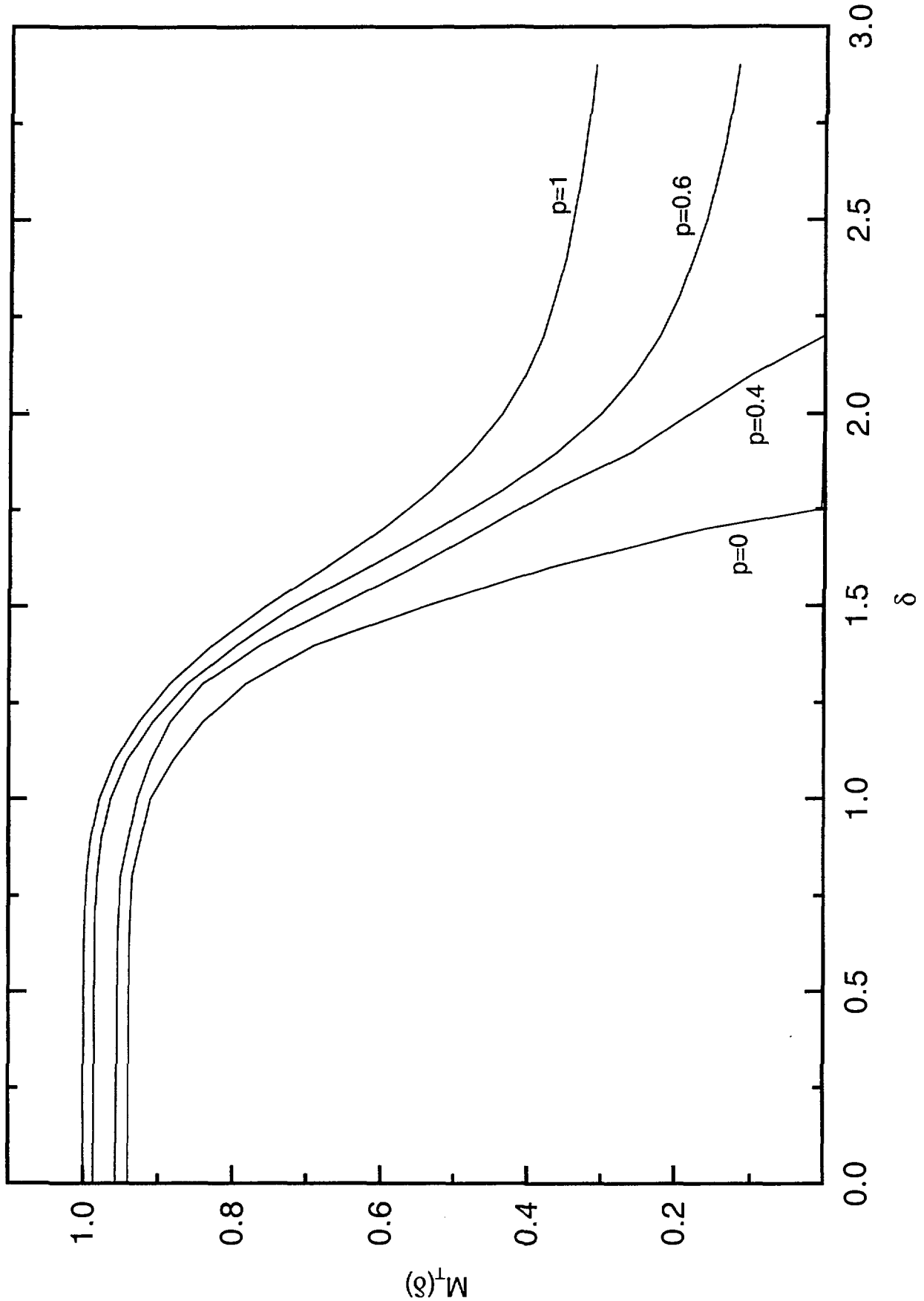

Fig. 6

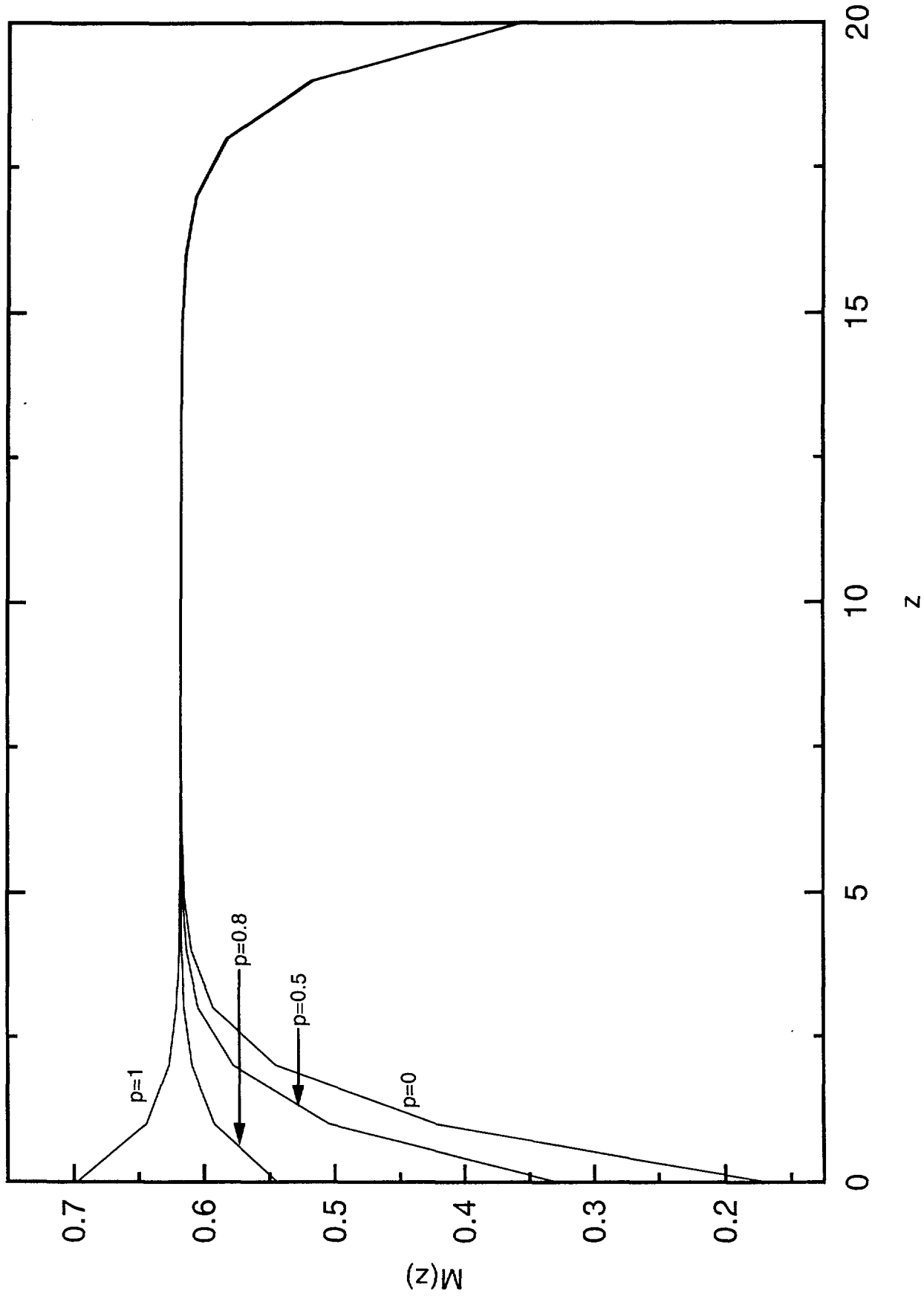

Fig. 7