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3-D QUANTUM HEISENBERG FERROMAGNET WITH RANDOM ANISOTROPY*

by

R.M. Zorzenon dos Santos[2], A.M. Mariz[1,3]
R.R. dos Santos[2] and C. Tsallis[1]

[1]Centro Brasileiro de Pesquisas Físicas - CBPF/CNPq
Rua Dr. Xavier Sigaud, 150
22290 - Rio de Janeiro, RJ - Brasil

[2]Departamento de Física
Pontifícia Universidade Católica
C.P. 38071, Rio de Janeiro, RJ - Brasil

[3]Departamento de Física
Universidade Federal do Rio Grande do Norte
59000 - Natal, RN - Brasil

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ABSTRACT

We study the critical properties of the 3-D quantum Heisenberg ferromagnet with random anisotropies; that is, the coupling between any pair of nearest-neighbouring spins can be either isotropic (Heisenberg) or anisotropic (Ising-or XY-like) at random, Within a Migdal-Kadanoff approximation we obtain the full critical frontier and correlation length critical exponents. We found that the isotropic Heisenberg model is unstable (in the context of universality classes) in the presence of a small concentration of couplings with lower symmetry.

Key-words: Heisenberg ferromagnet; Random anisotropy; Criticality; Quantum system.

Antiferromagnetic systems with random anisotropies have attracted a great number of experimental (Katsumata 1983, and references therein) and theoretical (Aharony 1983, and references therein) investigations over recent years. In these systems the coupling between any pair of neighbouring spins can have O(n) symmetry with n being either n_1 or n_2 at random. For instance, $Fe_{(1-p)}Co_pBr_2$ behaves essentially as an Ising antiferromagnet when p=0, whereas for p=1 it behaves as an XY antiferromagnet (Katsumata et al 1984). On the other hand, Komoda and Pekalski 1981 considered a ferromagnetic system in which the magnetic interactions were either Ising - or Heisenberg - like and obtained the phase diagram (T_c as a function of p_s, the site concentration) within an effective Hamiltonian method. Furthermore, Pekalski (1977, 1984) and Mariz and Tsallis (1984) investigated a generalized model in two-dimensions by series expansions and by Real-Space Renormalization Group (RSRG) methods, respectively.

The purpose of this letter is to study the critical properties of a Heisenberg ferromagnet with random anisotropies in three dimensions, through a Migdal-Kadanoff (MK) approximation (Migdal 1976, Kadanoff 1976). We consider the following dimensionless Hamiltonian.

$$\mathcal{H} = \sum_{<i,j>} K_{ij}\left[(1+\Delta_{ij})\sigma_i^z\sigma_j^z + (1-\Delta_{ij})(\sigma_i^x\sigma_j^x + \sigma_i^y\sigma_j^y)\right] \qquad (1)$$

where $K_{ij}=J_{ij}/k_BT$(J_{ij} is the exchange coupling) is the same for all bonds, the σ's are Pauli spin operators, and the sum runs over pairs of nearest neighbouring spins on a three dimensional simple cubic lattice. The anisotropy parameter Δ_{ij} is a random variable and the following distribution is associated with each bond:

$$P(K_{ij},\Delta_{ij}) = \left[p\delta(\Delta_{ij}-\Delta) + (1-p)\delta(\Delta_{ij})\right]\delta(K_{ij}-K) \quad (2)$$

with $\Delta\epsilon[-1,1]$ and $K>0$; there is no correlation between anisotropy in different bonds.

Within the MK approximation, adapted to quantum systems (Suzuki and Takano 1979; Barma et al 1979; Stinchcombe 1979,1981; Takano and Suzuki 1981, Castellani et al 1982, Tsallis et al 1984) a Renormalization Group transformation is obtained by first decimating (b-1) spins along each of the d cartesian directions and then combining them in "parallel". Thus, for a linear scaling factor b=2, a 3-site chain is decimated into a 2-site chain by performing a partial trace on the internal site, in such a way that the partition function is preserved, that is,

$$e^{\mathcal{H}^{S}_{12}} = \operatorname*{Tr}_{3} e^{\mathcal{H}_{123}} \quad (3)$$

where

$$\mathcal{H}_{12}^{(s)} = K_0^{(s)} + K^{(s)}\left[(1+\Delta^{(s)})\sigma_1^z\sigma_2^z + (1-\Delta^{(s)})(\sigma_1^x\sigma_2^x + \sigma_1^y\sigma_2^y)\right] \quad (4)$$

where $K_0^{(s)}$ is an additive constant which makes possible Eq. (3); the label s means "series combination" and

$$\mathcal{H}_{123} = K\left[(1+\Delta_1)\sigma_1^z\sigma_3^z + (1+\Delta_2)\sigma_3^z\sigma_2^z + (1-\Delta_1)(\sigma_1^x\sigma_3^x + \sigma_1^y\sigma_3^y) + (1-\Delta_2)(\sigma_3^x\sigma_2^x + \sigma_3^y\sigma_2^y)\right] \quad (5)$$

where Δ_1 and Δ_2 are distributed according to Eq(2); the fact that $K_{ij} \equiv K$ has been used explicitly.

The evaluation of the trace in Eq(3) is carried out through a procedure previously developed (Caride et al 1983, Mariz et al 1984a):

The density matrices are expanded as

$$e^{\mathcal{H}_{12}^{(s)}} = a^{(s)} + b_{12}^{(s)}(\sigma_1^x\sigma_2^x + \sigma_1^y\sigma_2^y) + c_{12}^{(s)}\sigma_1^z\sigma_2^z \quad (6)$$

and

$$e^{\mathcal{H}_{123}} = a + \sum_{i<j}\{b_{ij}(\sigma_i^x\sigma_j^x + \sigma_i^y\sigma_j^y) + c_{ij}\sigma_i^z\sigma_j^z\} \quad (7)$$

where the sum runs over all sites of the 3-site chain.

The parameters $K_0^{(s)}$, $K^{(s)}$ and $\Delta^{(s)}$ can be determined analitically (Caride et al 1983; Mariz et al 1984a) as functions of $a^{(s)}, b_{12}^{(s)}$ and $c_{12}^{(s)}$. The trace of Eq.(7) yields $a^{(s)}=2a, b_{12}^{(s)}=2b_{12}, c_{12}^{(s)}=2c_{12}$ the remaining terms vanish since they involve a term in σ_3^α. The coefficients a, b_{12} and c_{12}

are determined numerically as functions of K, Δ_1 and Δ_2, and finally we obtain the recursion relations $K_0^{(s)}(K,\Delta_1,\Delta_2)$, $K^{(s)}(K,\Delta_1,\Delta_2)$ and $\Delta^{(s)}(K,\Delta_1,\Delta_2)$. At this point one should note that the procedure outlined above to take the partial trace has been used in the study of the non-random anisotropic Heisenberg model in 3-D through an appropriate two-terminal graph (Mariz et al 1984b). Nevertheless, the process of configurational averaging makes this method inapplicable to that graph for the present problem in view of very long computational times involved.

Neglecting commutation aspects in the bond-moving step of the approximation we get (see Mariz et al 1984a) for a "parallel" combination of four branches (each of them constituted by two bonds in series)

$$\tilde{K}\left[\{K_{ij}^{(\ell)}\},\{\Delta_{ij}^{(\ell)}\}\right] = K_1^{(s)} + K_2^{(s)} + K_3^{(s)} + K_4^{(s)} \tag{8}$$

$$\tilde{\Delta}\left[\{K_{ij}^{(\ell)}\},\{\Delta_{ij}^{(\ell)}\}\right] = \underset{\tilde{K}}{K_1^{(s)}\Delta_1^{(s)}} + K_2^{(s)}\Delta_2^{(s)} + K_3^{(s)}\Delta_3^{(s)} + K_4^{(s)}\Delta_4^{(s)} \tag{9}$$

where $\left(K_r^{(s)},\Delta_r^{(s)}\right)$ denotes the series result associated with the r-th parallel branch of the graph (r=1,...,4), which contains, as a whole, eight bonds identified by ℓ=1,...,8.

Starting from a binary distribution (for each of these bonds, see Eq.(2)), the transformed distribution

$$\tilde{P}\left(K_{ij},\Delta_{ij}\right) = \int \prod_{\ell=1}^{8} \left[dK_{ij}^{(\ell)} d\Delta_{ij}^{(\ell)}\, P\left(K_{ij}^{(\ell)},\Delta_{ij}^{(\ell)}\right)\right] \delta\left(K_{ij}-\tilde{K}\right)\delta\left(\Delta_{ij}-\tilde{\Delta}\right) \tag{10}$$

will no longer be of binary form. Since, under iteration these

distributions will evolve to more complicated forms, one has to resort to further approximations. One of the simplest approximations, which retains the essential physical features of the problem, consists in forcing the transformed distribution back into binary form, i.e,

$$P'(K_{ij},\Delta_{ij}) = \left[p'\delta(\Delta_{ij}-\Delta') + (1-p')\delta(\Delta_{ij})\right]\delta(K_{ij}-K') \qquad (11)$$

To obtain the three RG equations (p',K',Δ'), we choose to match the averages of K, Δ and (Δ^2) over the (forced) binary and over the (actual) transformed distributions, that is,

$$\langle K_{ij}\rangle_{P'} = \langle K_{ij}\rangle_{\tilde{P}} \equiv g_1(p,K,\Delta) \qquad (12)$$

$$\langle \Delta_{ij}\rangle_{P'} = \langle \Delta_{ij}\rangle_{\tilde{P}} \equiv g_2(p,K,\Delta) \qquad (13)$$

$$\langle \Delta^2_{ij}\rangle_{P'} = \langle \Delta^2_{ij}\rangle_{\tilde{P}} \equiv g_3(p,K,\Delta) \qquad (14)$$

where <.....> denotes configurational averages with the subscripts referred to both distributions. While Eqs. (12) and (13) are the most natural choices, Eq. (14) has been proposed in order to decouple the random variables p and Δ.

The left-hand-side of Eqs. (12)-(14) are easily worked out to obtain

$$K' = g_1 \qquad (15)$$

$$\Delta' = g_3/g_2 \qquad (16)$$

$$p' = g_2/\Delta' \qquad (17)$$

It is worth noting that when $p'=0$ or $\Delta'=0$ we recover the isotropic Heisenberg critical temperature, in spite of the apparent indeterminacy of Eq.(17).

Solving the recursion relations for critical fixed points (K^*,Δ^*,p^*) and eigenvalues (λ_i), we obtain Table 1 where the critical exponents, have been calculated through

$$\nu_i = \frac{\ell n\ b}{\ell n\ \lambda_i} \qquad (i=T,\Delta)$$

where λ_i are relevant eigenvalues $(\lambda_i>1)$; T and Δ respectively correspond to the thermal and anisotropy correlation length critical exponents.

One only has relevant fixed points in the plane $p=1$, as shown in Table 1 and Fig. 1. For comparison, we also quote the results obtained from series expansion (Domb (1974), Rushbrooke et al (1974), Pfeuty et al (1974), Betts (1974)). Our $p=1$ results are the same as those previously obtained by Takano and Suzuki (1981), as expected. The pure XY fixed point has a residual Ising interaction $(\Delta^* \neq -1)$ and the low temperature XY region $(\Delta<0, p=1)$ is driven towards the zero temperature Heisenberg fixed point under iteration of the RG; this spurious behavior can be attributed to different ground state properties of the 3-site chain and the renormalized 2-site chain, as pointed out by Castellani et al (1982).

In Fig.1 we show the critical surface (full lines) which is the boundary between the ferromagnetic and paramagnetic phases. One expects that this critical surface is properly described within the present approach, since the spurious behaviour for $\Delta<0$ only dominates the low-temperature region. In fact, points in the random region ($p\neq1$) of the critical surface are attracted (under RG iterations) to the pure XY (Ising) fixed point if $\Delta<0$ ($\Delta>0$). Thus, three Universality classes are present, as expected: (i) the ABC and BH critical lines have Heisenberg model exponents; (ii) the whole surface with $\Delta<0$, $p>0$ belongs to the XY Universality class; (iii) the whole surface with $\Delta>0$, $p>0$ belongs to the Ising Universality class. This means that a small amount of bonds with lower symmetry embedded in a majority of Heisenberg-like bonds is enough to change the O(3) symmetry.

In Fig.2 we show the critical temperature as a function of the anisotropy parameter Δ for several concentrations (p) of anisotropic bonds. We see that for small p there is only a small change in the critical temperature as Δ varies from 0 to ±1, although there is a change in Universality classes as mentioned above. A similar behaviour is present in the plots of the critical temperature as a function of p for several values of Δ (Figs. 3 and 4). One should note that the curves $T_c(p)$ obtained by Komoda and Pekalski (1981) have

inflection points which are absent in ours (see Fig.3). This difference probably comes about because their Hamiltonian allows for three different couplings as the site concentration p_s varies from 0 to 1: Ising (with probability p_s^2), anisotropic Heisenberg (with probability $2p_s(1-p_s)$) and isotropic Heisenberg (with probability $(1-p_s)^2$). In our formulation, Ising and anisotropic Heisenberg couplings are treated on equal footing.

We are currently investigating a more complex model, where a ternary (instead of binary) distribution is introduced for the couplings: p_1 is the bond concentration of Ising or XY interactions ($\Delta_{ij}=\pm 1$), p_2 is that of anisotropic Heisenberg interactions ($\Delta_{ij}=\Delta\epsilon[-1,1]$) and finally p_3 is that of isotropic Heisenberg interactions ($\Delta_{ij}=0$) ($p_1+p_2+p_3=1$). The treatment of such a model within the present formalism (which recovers, for $p_1=0$, that treated here) would allow for interesting comparisons with the case focused by Komoda and Pękalski (1981) (which corresponds to $p_1=p_s^2$, $p_2=2p_s(1-p_s)$ and $p_3=(1-p_s)^2$).

As a final remark, it would be interesting to extend our analysis to the antiferromagnetic case, in order to study the intermediate phases present in some antiferromagnets with random anisotropies (Katsumata (1983)) which come about as a result of competing interactions together with random field effects (Aharony 1983).

To summarize, we studied the finite temperature critical behaviour of the three-dimensional quantum Heisenberg ferromagnet with random anisotropy . We found, in accordance with intuitive expectation, that the isotropic Heisenberg critical behaviour is unstable when a small concentration of couplings with lower symmetry are present.

TABLE AND FIGURE CAPTIONS

Table 1 - Critical fixed points and correlation length critical exponents obtained from Migdal-Kadanoff RG; For comparison series results are also shown. Numbers in square brackets for the XY model represent the intersection of the critical curve with the line $\Delta=-1$.

Figure 1 - The full critical surface (in the $p, \Delta, k_BT/J$ space) of the 3-D quantum Heisenberg model with random anisotropy. The non-trivial Ising (I), Isotropic Heisenberg (H) and XY fixed points are shown.

Figure 2 - The critical temperature (k_BT_C/J) as function of the anisotropy parameter Δ for several concentrations of anisotropic bonds (p).

Figure 3 - The critical temperature (k_BT_C/J) as function of the concentration p for several values of $\Delta>0$.

Figure 4 - The same as Fig.3, but with $\Delta<0$.

TABLE 1

MODEL	CRITICAL FIXED POINTS AND EXPONENTS	MK+	SERIES
Ising	$\left(\Delta^*, \frac{k_B T_C^*}{J}\right)$	(1,7.66)	(1,9.09) (1)
	ν_T	1.06	0.63 (1)
Isotropic Heisenberg	$\left(\Delta^*, \frac{k_B T_C^*}{J}\right)$	(0,2.91)	(0,3.33) (2)
	ν_T	1.39	0.72 (2)
	$\phi = \frac{\nu_T}{\nu_\Delta}$	1.56	1.25 (3)
XY	$(\Delta^*, k_B T_C^*/J)$	(-0.88,6.80) [-1,7.26]	(-1,8.00) (4)
	ν_T	1.16	0.67 (4)

+ All values reproduce those associated with the pure model (p=1), firstly obtained by Takano and Suzuki (1981).

(1) Domb (1974)
(2) Rushbrooke et al (1974)
(3) Pfeuty et al (1974)
(4) Betts (1974)

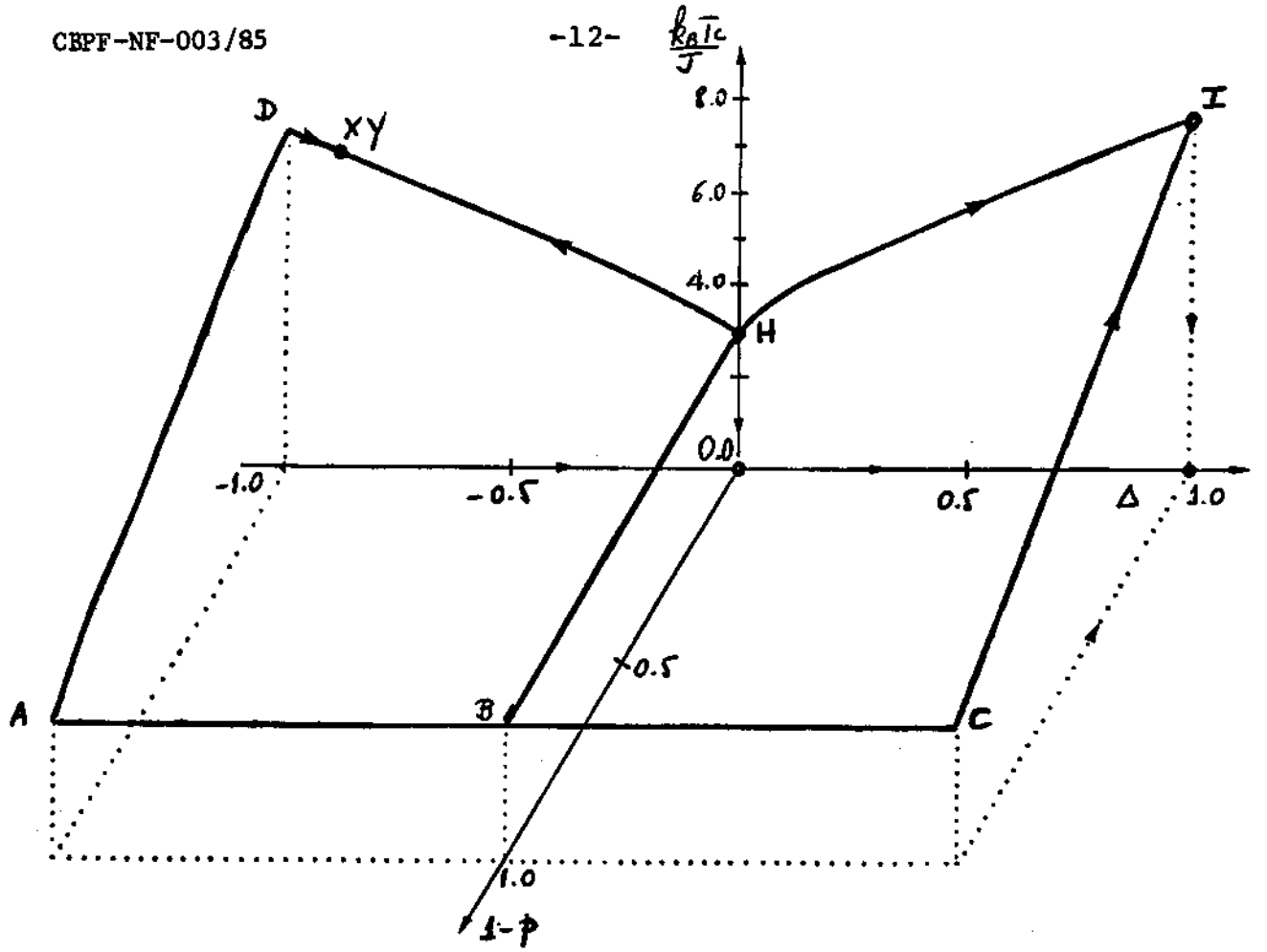

Figure 1

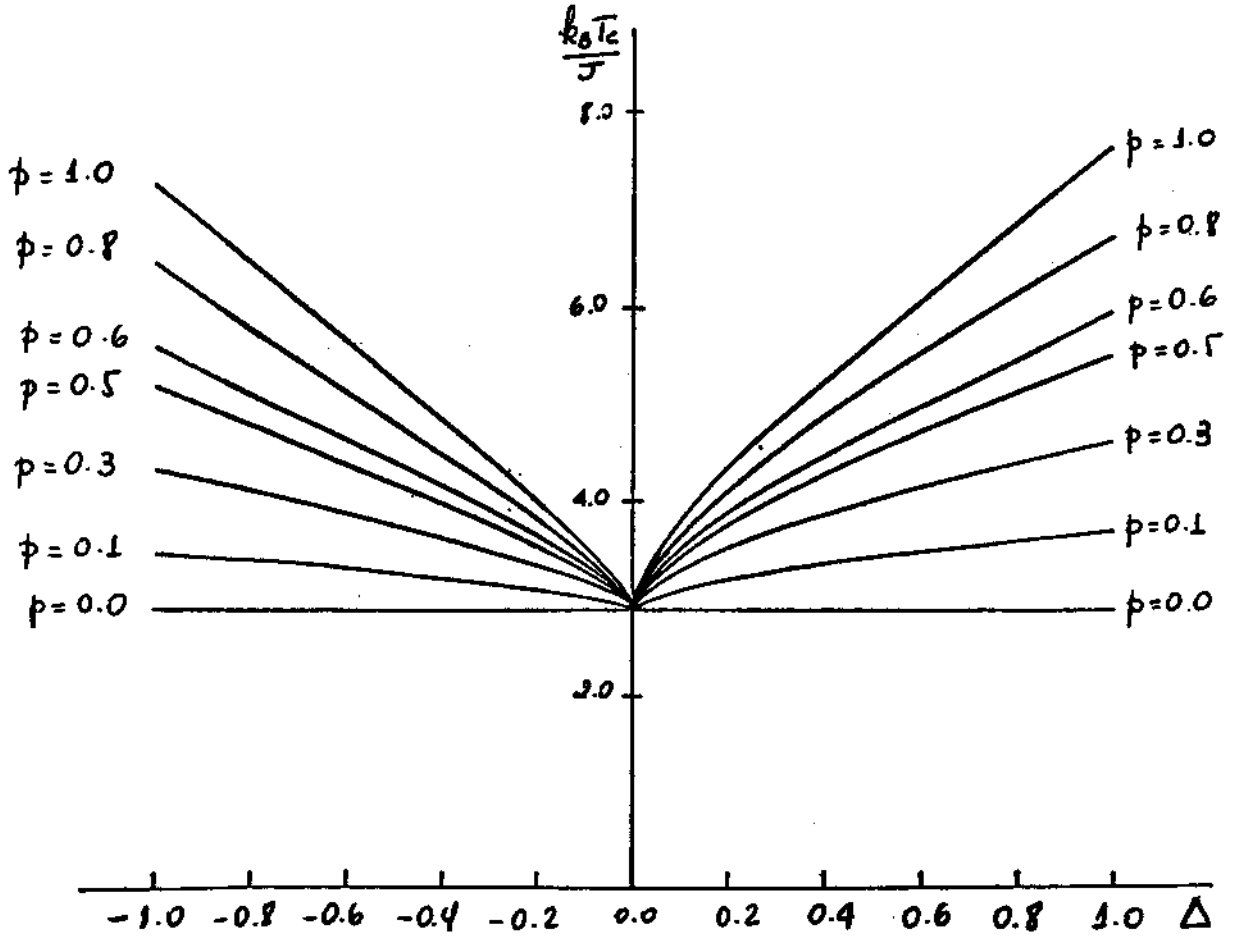

Figure 2

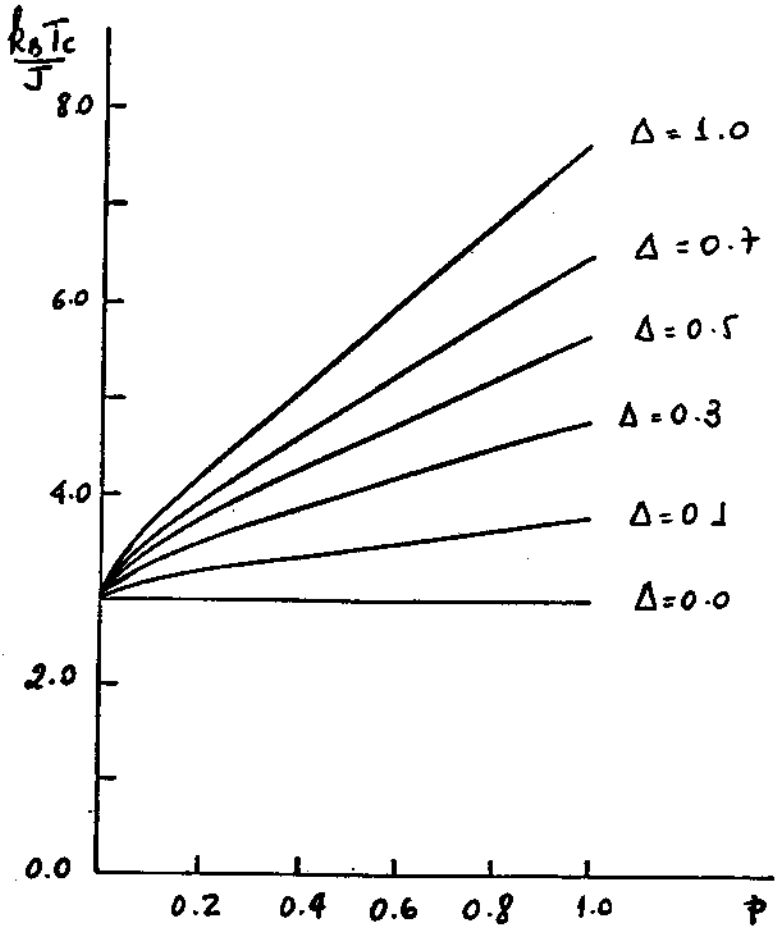

Figure 3

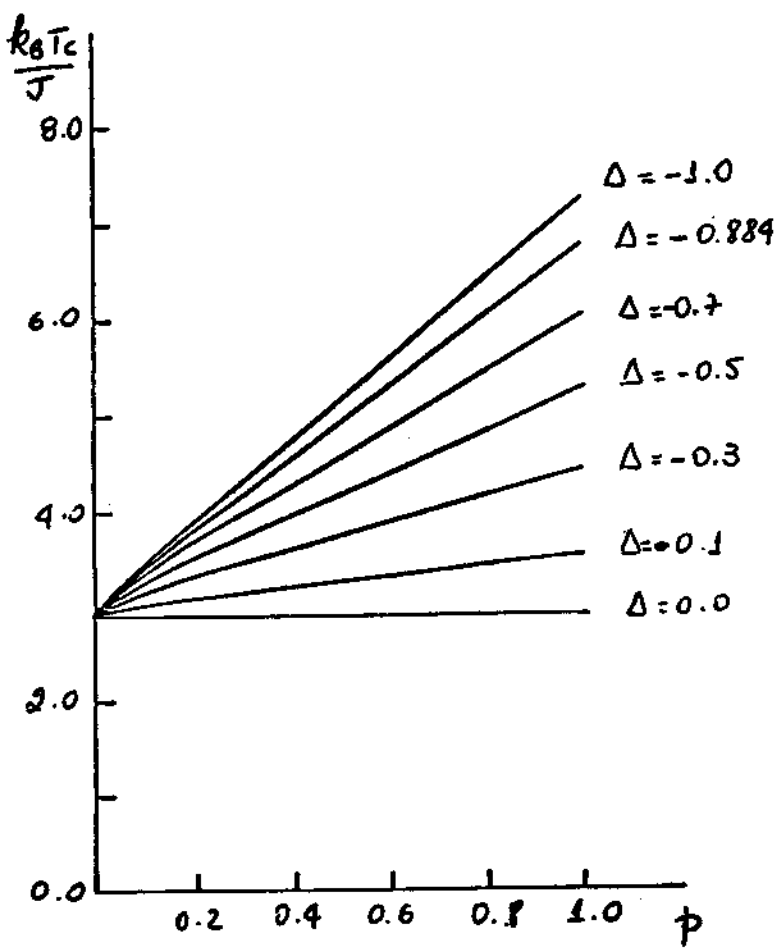

Figure 4

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