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ABSTRACT

The three dimensional spin-1 Ising model with crystal field interactions exhibit tricritical behavior. Using an expansion technique for cluster identities of spin-1 localized spin systems, we study the influence of transverse magnetic field on this behavior. Temperature-crystal-field phase diagrams is investigated for different values of transverse field. The longitudinal and transverse magnetizations, the quadrupolar moments are calculated. General formulae, applicable to structures with arbitrary coordination number N, are given.

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1.Introduction

Spin systems are widespread in very different fields of physics ,e.g., in the theory of magnetism, superconductivity, nuclear physics, etc. Special methods of theoretical physics are needed to describe the systems since commutation relations for spin components differ from the corresponding relations in both Bose and Fermi systems.The study of phase transitions in the Ising and the Heisenberg models has been the subject of much interest [1-7]. Phase diagrams of such models show various types of multicritical phenomena [3,4,7]. The Ising model in the presence of a transverse field serves for the study of cooperative phenomena and phase transitions in many physical systems [8-10]. The diluted three-dimensional spin-1 Ising model with crystal field interactions is studied by Saber[11] within Finite cluster approximation, The spin-1 Ising model with a random crystal field is studied by Benyoussef et al[12], Boccara et al[13] within mean field solution. Our aim is to study the influence of the transverse magnetic field on the phase diagram and magnetic properties of spin-1 Ising model with crystal field interactions. We use the finite cluster approximation [14,15] with an expansion technique for cluster identities of spin-1 localised spin systems established by Ez-Zahraouy et al[16]. Phase diagram for coordination number N=6 is represented in the T-D space for differents values of Ω, where T, Ω and D are respectively temperature, transverse field and longitudinal crystal field. Magnetizations and quadrupolar moments are determined for several values of the crystal field for fixed value of transverse field.

for N=6. In section 2 we give the method and we calculate the state equations. Section 3 is reserved to results and discussion.

2. Finite cluster approximation.

We consider a spin-1 Ising system in a simple cubic lattice described by a Hamiltonian corresponding to paramangnet of the longitudinal-axis type in a transverse magnetic field.

$$H = -\sum_{<ij>} J_{ij} S_{iz} S_{jz} - \Omega \sum_{i} S_{ix} + D \sum_{i} S_{iz}^2 \qquad (1)$$

Where S_{ix} and S_{iz} are respectively the x-component and the z-component of spin-1 operator at site i, Ω represents the transverse field and J_{ij} is the exchange interaction between spins at site i and j, in this paper J_{ij} is constant and equal J. <ij> runs over all nearest - neighbour pairs of spins , and D is the crystal field.

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, then the Hamiltonian containing 0, namely

$$H_0 = AS_{0z} + BS_{0x} + DS_{0z}^2 \qquad (2)$$

where

$$A = -J\theta \quad ; \quad B = -\Omega \qquad (3)$$

with $\theta = \sum_{j=1}^{N} S_{jz}$

This single-site Hamiltonian can readily be diagonalised and its eigenvalues and eigenvectors found. The three eigenvectors corresponding to the eigenvalues

$$\lambda_k = 2(D + \sqrt[3]{\rho}\ cos(\phi_k))/3 \qquad (4)$$

with $$\phi_k = \frac{1}{3} Arc\cos(-27q/2\rho) + 2(k-1)\Pi/3 \qquad (5)$$

and $$\rho = \frac{3\sqrt{3}}{2}\sqrt{27q^2 + \sqrt{|4p^3 + 27q^2|}} \qquad (6)$$

$$p = -(A^2 + B^2) - D^2/3 \quad ; \quad q = -D(2A^2 + 2/9D^2 + B^2)/3 \qquad (7)$$

are

$$|\Psi\rangle_k = \alpha_k|+\rangle + \beta_k|-\rangle + \gamma_k|0\rangle \qquad (8)$$

with

$$\alpha_k = \frac{|B(\lambda_k - D + A)|}{\sqrt{2}\sqrt{B^2((\lambda_k - D)^2 + A^2) + ((\lambda_k - D)^2 - A^2)^2}} \qquad (9)$$

$$\beta_k = \frac{\lambda_k - D - A}{\lambda_k - D + A}\alpha_k \quad ; \quad \gamma_k = \frac{\sqrt{2}}{B}(\lambda_k - D - A)\alpha_k \qquad (10)$$

In a representation in which S_{0z} is diagonal. The starting point of single-site cluster approximation is a set of formal identities of the type

$$\left\langle \left\langle S_{0\alpha}^{p} \right\rangle_{c} \right\rangle = \left\langle \frac{\mathrm{trace}_0\left[S_{0\alpha}^{p}\exp(-\beta H_0)\right]}{\mathrm{trace}_0\left[\exp(-\beta H_0)\right]} \right\rangle \tag{11}$$

Where $S_{0\alpha}^{p}$ is the α-component of the spin operator S_0 raised to the power p. $\left\langle S_{0\alpha}^{p} \right\rangle_{c}$ denotes the mean value of $S_{0\alpha}^{p}$ for a given configuration c of all other spins, i.e when all other spins S_i $(i \neq 0)$ have fixed values. $\langle \ldots \rangle$ denotes the average over all spin configurations. trace_0 means the trace performed over S_0 only. $\beta = \frac{1}{K_B T}$, T the absolute temperature and K_B is the Boltzmann constant. The equations (11) are not exact for an Ising system in a transverse field, they have nevertheless, been accepted as a reasonable starting point in many studies of that system[17]. Let $< S_{0\alpha} >_C$ and $< S_{0\alpha}^2 >_C$ denotes respectively the mean value of $S_{0\alpha}$ and $S_{0\alpha}^2$ for a fixed configuration c for all other spins.

To calculate, $< S_{0z} >_C$ and $< S_{0\alpha}^2 >_C$, one has to effect the inner traces in eqs.(11) over the states of the spin 0 and this is the most easily performed using the eigenstates of eqs.(8) as the basic states. In this way, it follows on setting p=1 and 2 in turn in eqs.(11) that

$$\left\langle S_{0z} \right\rangle_C = \frac{\sum_{k=1}^{3} (\alpha_k^2 - \beta_k^2) \exp(-\beta\lambda_k)}{\sum_{k=1}^{3} \exp(-\beta\lambda_k)} \tag{12}$$

$$\left\langle S_{0x} \right\rangle_C = \sqrt{2}\, \frac{\sum_{k=1}^{3} (\alpha_k + \beta_k)\gamma_k \exp(-\beta\lambda_k)}{\sum_{k=1}^{3} \exp(-\beta\lambda_k)} \tag{13}$$

$$\left\langle S_{0z}^2 \right\rangle_C = \frac{\sum_{k=1}^{3} (\alpha_k^2 + \beta_k^2) \exp(-\beta\lambda_k)}{\sum_{k=1}^{3} \exp(-\beta\lambda_k)} \tag{14}$$

$$\left\langle S_{0x}^2 \right\rangle_C = \frac{\sum_{k=1}^{3} ((\alpha_k + \beta_k)^2 / 2 + \gamma_k^2) \exp(-\beta\lambda_k)}{\sum_{k=1}^{3} \exp(-\beta\lambda_k)} \tag{15}$$

The magnetizations m_α $(\alpha=z,x)$ and the quadrupolar moments q_α $(\alpha=z,x)$ are given by :

$$m_\alpha = \left\langle f_\alpha(\theta) \right\rangle \quad ; \quad q_\alpha = \left\langle g_\alpha(\theta) \right\rangle$$

with

$$f_\alpha(\theta) = \left\langle S_{0\alpha} \right\rangle_C \tag{16}$$

$$g_\alpha(\theta) = \left\langle S_{0\alpha}^2 \right\rangle_C \qquad (17)$$

Where $\langle \ldots \rangle$ denotes the average over all configurations of the spins $S_{jz}(j \neq 0)$. To calculate $\langle f_\alpha(\theta) \rangle$ and $\langle g_\alpha(\theta) \rangle$ we have used the expansion technique for spin-1 Ising systems as follows[14]:

Suppose one considers the general product $\prod_{i=1}^{N}(\sum_{p_i=0}^{2} S_{iz}^{p_i})$ that contains 3^N terms. From these terms one may collect together all those terms containing p factors of S_{iz}^2 and q factors of S_{iz}. Such a group is to be denoted by $\{S_z^2, S_z\}_{N,p,q}$. For example, if N=4, p=1 and q=2, then

$$\begin{aligned}\{S_z^2, S_z\}_{4,1,2} = {} & S_{1z}^2(S_{2z}S_{3z} + S_{2z}S_{4z} + S_{3z}S_{4z}) + S_{2z}^2(S_{1z}S_{3z} + S_{1z}S_{4z} + S_{3z}S_{4z}) \\ & + S_{3z}^2(S_{1z}S_{2z} + S_{1z}S_{4z} + S_{2z}S_{4z}) + S_{4z}^2(S_{1z}S_{2z} + S_{1z}S_{3z} + S_{2z}S_{3z})\end{aligned} \qquad (18)$$

Our aim is to expand the functions of eqs.(16) and (17) in terms of these $\{S_z^2, S_z\}_{N,p,q}$. Thus, if one writes

$$f_\alpha(\sum_{i=1}^{N} S_{iz}) = \sum_{q=0}^{N}\sum_{p=0}^{N-q} A_{pq}^{(\alpha)}(N)\{S_z^2, S_z\}_{N,p,q} \qquad (19)$$

$$g_\alpha(\sum_{i=1}^{N} S_{iz}) = \sum_{q=0}^{N}\sum_{p=0}^{N-q} B_{pq}^{(\alpha)}(N)\{S_z^2, S_z\}_{N,p,q}, \qquad (20)$$

the problem is to find the coefficients $A_{pq}^{(\alpha)}(N)$ and $B_{pq}^{(\alpha)}(N)$. To achieve this it is advantageous to transform the spin-1 system to a spin-$\frac{1}{2}$ representation containing the Pauli operators $\sigma_{iz} = \pm 1$. This may be accomplished by setting $S_{iz} = \tau_{iz}\sigma_{iz}$ with τ_{iz}=0,1. In this representation, eqs(19) and (20) become

$$f_\alpha(\sum_{i=1}^{N} \tau_{iz}\sigma_{iz}) = \sum_{q=0}^{N}\sum_{p=0}^{N-q} A_{pq}^{(\alpha)}(N)\{\tau_z, \tau_z\sigma_z\}_{N,p,q} \qquad (21)$$

$$g_\alpha(\sum_{i=1}^{N} \tau_{iz}\sigma_{iz}) = \sum_{q=0}^{N}\sum_{p=0}^{N-q} B_{pq}^{(\alpha)}(N)\{\tau_z, \tau_z\sigma_z\}_{N,p,q} \qquad (22)$$

and must hold for arbitrary choices of τ_{iz}. Suppose one now chooses the first r out of the N operators τ_{iz} to be unity, and the remainder zero. Then eqs.(21) and (22) give

$$f_\alpha(\sum_{i=1}^{r} \sigma_{iz}) = \sum_{q=0}^{r}\sum_{p=0}^{r-q} A_{pq}^{(\alpha)}(N) C_p^{r-q}\{\sigma_z\}_{r,q} \qquad (23)$$

$$g_\alpha(\sum_{i=1}^{r} \sigma_{iz}) = \sum_{q=0}^{r}\sum_{p=0}^{r-q} B_{pq}^{(\alpha)}(N) C_p^{r-q}\{\sigma_z\}_{r,q} \qquad (24)$$

where $\{\sigma_z\}_{r,q}$ is the sum of all possible products of q spin operators, σ_{iz}, out of a maximum of r, and the C_n^m are the binomial coefficients $m!/n!(m-n)!$. That is,

$$f_\alpha(\sum_{i=1}^{r} \sigma_{iz}) = \sum_{q=0}^{r} b_q^{(\alpha)}(r)\{\sigma_z\}_{r,q} \qquad (25)$$

$$g_\alpha\left(\sum_{i=1}^{r}\sigma_{iz}\right)=\sum_{q=0}^{r}d_q^{(\alpha)}(r)\{\sigma_z\}_{r,q} \tag{26}$$

with

$$b_q^{(\alpha)}(r)=\sum_{p=0}^{r-q}A_{pq}^{(\alpha)}(N)C_p^{r-q} \tag{27}$$

$$d_q^{(\alpha)}(r)=\sum_{p=0}^{r-q}B_{pq}^{(\alpha)}(N)C_p^{r-q}. \tag{28}$$

The spin-1 problem of eqs.(19) and (20) containing N spins has thus been transformed to a spin-1/2 problem containing r spins. The advantage of doing this is that it now enables one to use directly the results already established in ref.[18] for the spin-$\frac{1}{2}$ system. It may also be noted that whereas the coefficients $b_q^{(\alpha)}(r)$ and $d_q^{(\alpha)}(r)$ for the spin-1/2 problem depend on the total number of spins present, the coefficients $A_{pq}^{(\alpha)}(N)$ and $B_{pq}^{(\alpha)}(N)$ are in fact independent of N, as is clear from eqs.(27) and (28). Thus the label N is superfluous and may henceforth be dropped. This could, of course, have been inferred directly from eqs.(19) and (20) by setting one of the S_{iz} spins equal to its zero value throughout. Specialising the results of ref.[18] to a single group of r spins, one has for the current problem

$$b_q^{(\alpha)}(r)=\frac{1}{2^r C_q^r}\sum_{i=0}^{r}C_i^r\varepsilon_i(r,q)\,f_{i\alpha}(r) \tag{29}$$

$$d_q^{(\alpha)}(r)=\frac{1}{2^r C_q^r}\sum_{i=0}^{r}C_i^r\varepsilon_i(r,q)\,g_{i\alpha}(r) \tag{30}$$

where

$$\varepsilon_i(r,q)=\sum_{\mu=0}^{i}(-1)^\mu C_\mu^i C_{q-\mu}^{r-i} \tag{31}$$

and

$$f_{i\alpha}(r)=f_\alpha(r-2i) \tag{32}$$

$$g_{i\alpha}(r)=g_\alpha(r-2i) \tag{33}$$

Once the coefficients $b_q^{(\alpha)}(r)$ and $d_q^{(\alpha)}(r)$ have been calculated, the coefficients $A_{pq}^{(\alpha)}$ and $B_{pq}^{(\alpha)}$ may be found by the following procedure. First, $A_{0q}^{(\alpha)}$ and $B_{0q}^{(\alpha)}$ are got by setting r=q in eqs.(29) and (30). That is

$$A_{0q}^{(\alpha)}=b_q^{(\alpha)}(q)\quad;\quad B_{0q}^{(\alpha)}=d_q^{(\alpha)}(q) \tag{34}$$

Then, the other $A_{pq}^{(\alpha)}$ and $B_{pq}^{(\alpha)}$ may be obtained by expressing eqs.(29) and (30) as a reccurence relation, namely as

$$A_{r,q,q}^{(\alpha)}=b_q^{(\alpha)}(r)-\sum_{p=0}^{r-q-1}A_{pq}^{(\alpha)}C_p^{r-q} \tag{35}$$

$$B_{r-q,q}^{(\alpha)}=d_q^{(\alpha)}(r)-\sum_{p=0}^{r-q-1}B_{pq}^{(\alpha)}C_p^{r-q} \tag{36}$$

Then the magnetizations $m_\alpha(\alpha=z,x)$ and the quadrupolar moments $q_\alpha(\alpha=z,x)$ are given for an arbitrary coordination number N, by

$$m_\alpha = \sum_{q=0}^{N}\sum_{p=0}^{N-q} A_{pq}^{(\alpha)} \left\langle \left\{ S_z^2, S_z \right\}_{N,p,q} \right\rangle \tag{37}$$

$$q_\alpha = \sum_{q=0}^{N}\sum_{p=0}^{N-q} B_{pq}^{(\alpha)} \left\langle \left\{ S_z^2, S_z \right\}_{N,p,q} \right\rangle \tag{38}$$

Using the simplest approximation of the Zernike decoupling of the type

$$\left\langle S_\nu S_\mu \ldots S_{k_z} \ldots \right\rangle \equiv \left\langle S_{i_z} \right\rangle \left\langle S_\mu \right\rangle \ldots \left\langle S_{k_z} \right\rangle \ldots \quad \text{for } i \neq j \neq k \neq \ldots,$$

and seeing that the number of elements of the group $\left\{ S_z^2, S_z \right\}_{N,p,q}$ is equal $C_p^N C_q^{N-p}$, the eqs.(37) and (38) become

$$m_\alpha = \sum_{q=0}^{N}\sum_{p=0}^{N-q} A_{pq}^{(\alpha)} m_z^q q_z^p C_p^N C_q^{N-p} \tag{39}$$

$$q_\alpha = \sum_{q=0}^{N}\sum_{p=0}^{N-q} B_{pq}^{(\alpha)} m_z^q q_z^p C_p^N C_q^{N-p} \tag{40}$$

Let put $m = m_z = \langle S_z \rangle$ and $x = q_z = \langle S_z^2 \rangle$, and if we replace x in (39) by its expression taken from (40), we obtain an equation for m of the form

$$m = am + bm^3 + \ldots \tag{41}$$

where

$$a = N\left(A_{01}^{(z)} + \sum_{p=1}^{N-1} A_{p1}^{(z)} C_p^{N-1} x_0^p \right) \tag{42}$$

with x_0 the solution of the following equation

$$x_0 = B_{00}^{(z)} + \sum_{p=1}^{N} B_{p0}^{(z)} C_p^N x_0^p \tag{43}$$

The critical temperature of the second order transition is determined by a=1. In the vicinity of second order transition the magnetization m_z is determined by:

$$m_z^2 = \frac{1-a}{b} \tag{44}$$

At this temperature the transverse magnetization is given by

$$m_x = \sum_{p=0}^{N} A_{p0}^{(x)} C_p^N x_0^p \tag{45}$$

and the quadrupolar moments q_α (α=z,x) are given by

$$q_\alpha = \sum_{p=0}^{N} B_{p0}^{(\alpha)} C_p^N x_0^p \tag{46}$$

The right-hand side of eq.(44) must be positive. If this is not the case the transition is of first order. The point at which a=1 and b=0 is the tricritical point. To obtain the expression for b one has to solve (40) for small m. The solution is of the form

$$x = x_0 + x_1 m^2 \tag{47}$$

Where x_1 is given by :

$$x_1 = \sum_{p=0}^{N-2} B_{p2}^{(z)} C_2^N C_p^{N-2} x_0^p + \sum_{p=1}^{N} p B_{p0}^{(z)} C_p^N x_0^{p-1} x_1 \tag{48}$$

That is

$$x_1 = \frac{\sum_{p=0}^{N-2} B_{p2}^{(z)} C_2^N C_p^{N-2} x_0^p}{1 - \sum_{p=1}^{N} p B_{p0}^{(z)} C_p^N x_0^{p-1}} \tag{48}$$

This yields

$$b = \sum_{p=0}^{N-3} A_{p3}^{(z)} C_3^N C_p^{N-3} x_0^p + N \sum_{p=1}^{N-1} p A_{p1}^{(z)} C_p^{N-1} x^{p-1} x_1 \tag{50}$$

3-Results and discussion.

In this section we present results of the Hamiltonian (1) on a simple cubic lattice (N=6). The dependence of the magnetizations m_z, and m_x, and the quadrupolar moments q_z and q_x on the temperature for a fixed value of the transverse field Ω is shown in fig2,3,4,5 for several values of the strength of the longitudinal crystal field D. First order transition is characterised by the gap of the longitudinal magnetization m_z at the transition temperature ,showing in fig.2.(D=2.95, 2.85) in agreement with ref.[19]. While the magnetization m_z decreases continuousely in the vicinity of the transition temperature and vanishes at $T=T_c$, this is the second order transition. It is seen that the critical crystal field above which first order transition appears (fig.1.)

decreases when increasing the transverse field. The resulting phase diagram is shown in fig.1. From fig.3 it can be seen that there exists a tricritical line TCL separating the surfaces of second and first order transitions. This line ends on tricritical points in the T-D and D-Ω planes. The temperature dependence of the longitudinal and transverse magnetizations for different value of the longitudinal crystal field is exhibited in fig.2 and fig.3. The transverse magnetization m_x increases with the strength of the longitudinal magnetic field at low temperature and passes through a pic for the first order transition and a cusp for the second order transition temperature of m_z and then falls off rapidly as determined by the relation (45). Figures 2 and 3 also display the extent to which the components of magnetization depend on the lattice coordination number. Finally, in figures 4 and 5, the temperature dependence of the longitudinal (q_z) and the transverse (q_x) quadrupolar moments is displayed for the simple cubic lattice for a typical value of the crystal field. At low temperature, The longitudinal quadrupolar moment decreases, for $T > T_c$, the latter increases when increasing temperature, or decreasing the strength of the crystal field, while the transverse quadrupolar moment increases, when increasing the strength of the longitudinal crystal field. In the vicinity of the second order transition temperature the quadrupolar moments $q_\alpha(\alpha=z,x)$ passes through a cusp as determined by the relation (46). we conclude that the tricritical behaviour due to presence of crystal field interactions desappears for sufficiently large transverse magnetic field Ω.

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Figure Captions

Figure1. Phase diagram in D-T space for N=6. TCL is the tricritical line. Dashed lines correspond to first order transition. The number accompanying each curve denotes the value of Ω/J.

Figure2. The temperature dependence of the longitudinal magnetization when Ω/J =0.5. The number accompanying each curve denotes the value of D/J.

Figure3. The temperature dependence of the transverse magnetization when Ω/J=0.5. The number accompanying each curve denotes the value of D/J.

Figure4. The temperature dependence of the longitudinal quadrupolar moment for the cubic lattice, when Ω/J=0.5 . The number accompanying each curve denotes the value of D/J.

Figure5. The temperature dependence of the transverse quadrupolar moment when Ω/J=0.5. The number accompanying each curve denotes the value of D/J.

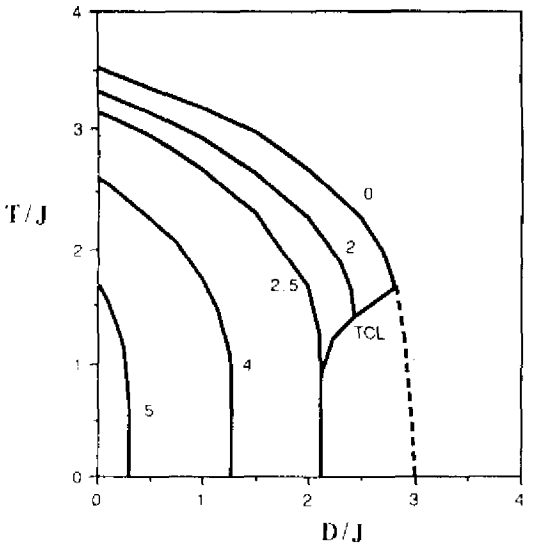

FIG 1

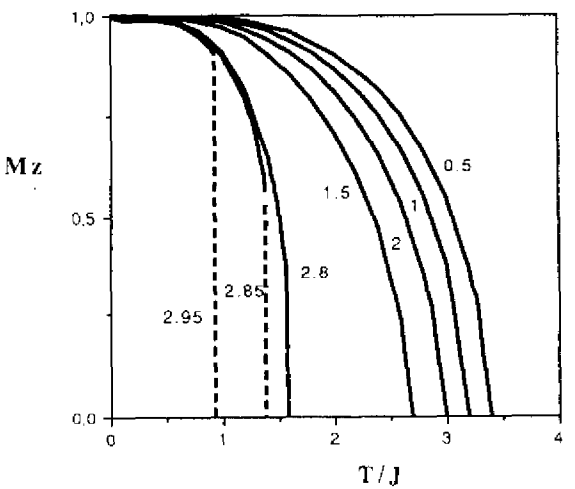

FIG.2

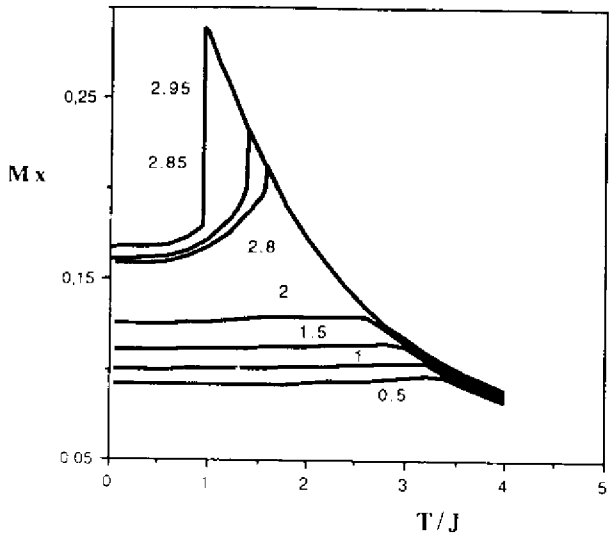

FIG.3

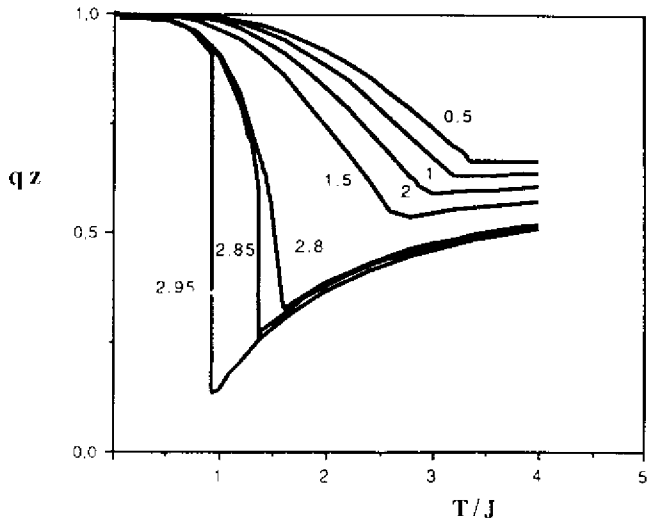

FIG.4

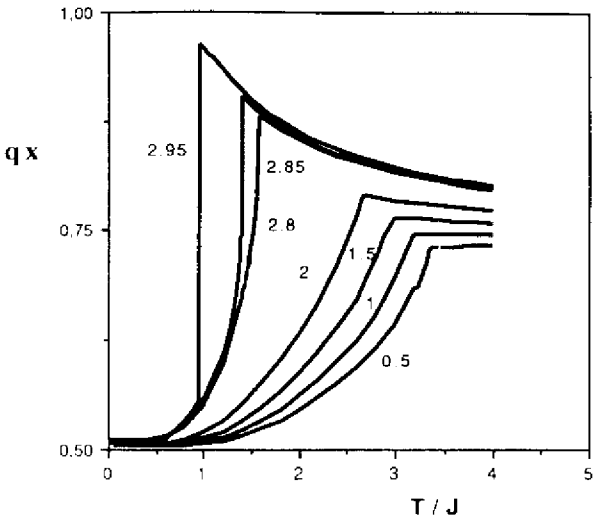

FIG.5