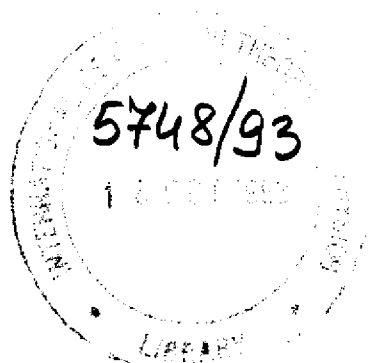


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**INTERNATIONAL CENTRE FOR
THEORETICAL PHYSICS**

**MAGNETIC PROPERTIES
OF A QUANTUM TRANSVERSE
SPIN-1 BLUME-EMERY-GRIFFITHS MODEL**

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**INTERNATIONAL
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ABSTRACT

Using an expansion technique for cluster identities of spin-1 localized spin systems, we study the magnetic properties of a quantum transverse spin-1 Blume-Emery-Griffiths model. The longitudinal and transverse magnetizations and the quadrupolar moments are calculated. General formula applicable to structures with arbitrary coordination number are given.

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1. Introduction

Over several years, some attention have been directed to spin systems which are widespread in very different fields of physics, e.g., in the theory of magnetism, superconductivity, nuclear physics, etc. In particular, because of the fundamental interest in the multi-critical phenomena of physical systems, spin-1 model with single-ion anisotropy[1,2] have been already investigated in some detail using a number of methods, namely the mean field approximation[1,2], effective field approximation [3,4], high-temperature series expansion[5], constant coupling approximation[6], Monte-Carlo technique[7], finite cluster approximation with an expansion technique[8] and so on. All these methods suggest the existence of a tricritical point at which the system changes from second order transition to the first one.

The spin-1 Ising model with nearest-neighbor interactions, both bilinear and biquadratic, and with a crystal-field interaction was introduced by Blume, Emery and Griffiths (BEG)[9] to describe phase separation and superfluid ordering in He³-He⁴ mixtures. With vanishing biquadratic interactions the model is known as the Blume-Capel model [10-11]. The BEG model was subsequently reinterpreted to describe phase transitions in simple[12] and multi-component fluids[13,14]. This model has been extensively studied by different techniques. It has been analyzed using mean field theory[9,12-16], an effective field theory based on the differential operator technique[17,18], real space renormalization group methods[19,21], high- and low-temperature series expansion[22], and Monte-Carlo simulations [16,23-26]. The Ising model in the presence of a transverse field serves for the study of cooperative phenomena and phase transitions in many physical systems[27-29]. The transverse-field or crystal field effects of spin-1 Ising model has been studied by a number of authors[1-31].

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This model including both transverse and crystal-field has been studied by Yang et al[32] within mean field approximation, and by Benyoussef et al[8,33] within an expansion technique for cluster identities of spin-1 localized spin systems[8,33]. But nobody, up to now, has studied the case of the transverse spin-1 BEG model.

The purpose of this paper is to study the magnetic properties of a spin-1 Blume-Emery-Griffiths model in a transverse magnetic field using the Finite cluster approximation [34,35] with an expansion technique for cluster identities of spin -1 localized spin systems established by Ez-Zahraouy et al.[36]. The dependence of longitudinal and transverse magnetizations on the temperature for several values of crystal-field interactions, biquadratic exchange interactions and transverse field, are calculated for coordination number $N=6$. General formula of the magnetizations and quadrupolar moments for an arbitrary coordination number, are given.

The present paper is organized as follows. In section 2 we give the model and the method. The results and discussion are given in section 3.

2. Model and method

The spin-1 BEG model in a transverse magnetic field is described by the following Hamiltonian

$$H = -J \sum_{\langle ij \rangle} S_{ix} S_{jx} - D \sum_{\langle ij \rangle} (S_{iz})^2 (S_{jz})^2 - \Delta \sum_i (S_{iz})^2 - \Omega \sum_i S_{ix} \quad (1)$$

where S_{ix} and S_{iz} are the component of a spin-1 operator at site i , namely

$$S_{ix} = \frac{1}{\sqrt{2}} \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}, \quad S_{iz} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix}, \quad (S_{iz})^2 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

where J and D represent the bilinear and biquadratic nearest-neighbor exchange

couplings between sites i and j respectively, D , Ω are respectively the crystal and transverse fields. The first and second summations run over all neighboring pairs of spins.

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

$$H_0 = A S_{0z} + (\Delta + C)(S_{0z})^2 + B S_{0x} \quad (2)$$

where

$$A = -J\theta \quad ; \quad B = -\Omega \quad ; \quad C = -D\zeta \quad (3)$$

with

$$\theta = \sum_{j=1}^N S_{jx} \quad ; \quad \zeta = \sum_{j=1}^N (S_{jz})^2$$

This single-site Hamiltonian can really be diagonalized and its eigenvalues and eigenvectors are easily obtained. The three eigenvectors corresponding to the eigenvalues

$$\lambda_k = 2(\Delta + C + \rho^3 \cos(\phi_k))/3 \quad , \quad \text{for } k=1,2,3 \quad (4)$$

with

$$\phi_k = \frac{1}{3} \text{Arccos}(-27q/2\rho) + 2(k-1)\pi/3 \quad (5)$$

and

$$\rho = \frac{3\sqrt{3}}{2} (27q^2 + 4p^3 + 27q^2)^{1/2} \quad (6)$$

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

are

$$|\Psi_k\rangle = \alpha_k |+\rangle + \beta_k |-\rangle + \gamma_k |0\rangle \quad (8)$$

with

$$\alpha_k = \frac{|B(\lambda_k - \Delta - C + A)|}{\sqrt{2[B^2((\lambda_k - \Delta - C)^2 + A^2) + ((\lambda_k - \Delta - C)^2 - A^2)^2]^{1/2}}} \quad (9)$$

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

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

$$\langle\langle (S_{0\alpha})^p \rangle\rangle_c = \langle \frac{\text{tr}_0 \{ (S_{0\alpha})^p \exp(-\beta H_0) \}}{\text{tr}_0 \{ \exp(-\beta H_0) \}} \rangle \quad (11)$$

where $(S_{0\alpha})^p$ is the α -component of the spin operator S_0 raised to the power p , $\langle (S_{0\alpha})^p \rangle_c$ 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. $\langle \dots \rangle$ denotes the average over all spin configurations. tr_0 means the trace performed over $S_{0\alpha}$ only. $\beta = 1/K_B T$, 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[37].

Let $\langle S_{0\alpha} \rangle_c$ and $\langle (S_{0\alpha})^2 \rangle_c$ 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, $\langle S_{0\alpha} \rangle_c$ and $\langle (S_{0\alpha})^2 \rangle_c$, 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 it turn in eqs.(11) that

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

$$\langle S_{0z} \rangle_c = \sqrt{2} \frac{\sum_{k=1}^3 (\alpha_k + \beta_k) \gamma_k \exp(-\beta \lambda_k)}{\sum_{k=1}^3 \exp(-\beta \lambda_k)} \quad (13)$$

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

$$\langle (S_{0z})^2 \rangle_c = \frac{\sum_{k=1}^3 ((\alpha_k + \beta_k)^2 / 2 + \gamma_k^2) \exp(-\beta \lambda_k)}{\sum_{k=1}^3 \exp(-\beta \lambda_k)} \quad (15)$$

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

by:

$$m_\alpha = \langle f_\alpha(\theta, \zeta) \rangle \quad ; \quad q_\alpha = \langle g_\alpha(\theta, \zeta) \rangle$$

with

$$f_\alpha(\theta, \zeta) = \langle S_{0\alpha} \rangle_c \quad (16)$$

$$g_\alpha(\theta, \zeta) = \langle (S_{0\alpha})^2 \rangle_c \quad (17)$$

where $\langle \dots \rangle$ denotes the average over all configurations of the spins $S_{ij} (j \neq 0)$. To calculate $\langle f_\alpha(\theta, \zeta) \rangle$ and $\langle g_\alpha(\theta, \zeta) \rangle$ we have used the expansion technique for spin-1 Ising systems as follows[36]: Suppose one considers the general product

$\prod_{i=1}^N (\sum_{p=0}^2 (S_{iz})^{p1})$ that containing 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 $\{(S_i)^2, S_i\}_{N,p,q}$. For example, if $N=3$, $p=1$ and $q=2$, then

$$\{(S_j)^2, S_j\}_{3,1,2} = (S_{1z})^2 S_{2z} S_{3z} + (S_{2z})^2 S_{3z} S_{1z} + (S_{3z})^2 S_{2z} S_{1z} \quad (18)$$

Our aim is to expand the functions of eqs.(16) and (17) in terms of these

$\{(S_i)^2, S_i\}_{N,p,q}$. Thus, if one writes

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

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

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-1/2 representation

containing the Pauli operators $\sigma_{iz} = \pm 1$. This may be accomplished by setting

$S_{iz} = \tau_{iz} \sigma_{iz}$ with $\tau_{iz} = 0, 1$. In this representation, with $(\sigma_{iz})^2 = 1$ and $(\tau_{iz})^2 = \tau_{iz}$,

eqs.(19) and (20) become

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

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

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

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

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

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 $\binom{m}{n}$ are the binomial coefficients $m!/n!(m-n)!$. That is,

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

$$g_{\alpha}(\sum_{i=1}^r \sigma_{iz}, r) = \sum_{q=0}^r d^{(\alpha)}_q(r) (\sigma_z)_{r,q} \quad (26)$$

with

$$b^{(\alpha)}_q(r) = \sum_{p=0}^{r-q} A^{(\alpha)}_{pq}(N) \binom{r-q}{p} \quad (27)$$

$$d^{(\alpha)}_q(r) = \sum_{p=0}^{r-q} B^{(\alpha)}_{pq}(N) \binom{r-q}{p} \quad (28)$$

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.[38] for the spin-1/2 system. It may also be noted that whereas the coefficients $b^{(\alpha)}_q(r)$ and $d^{(\alpha)}_q(r)$ for the spin-1/2 problem depend on the total number of spins present, the coefficients $A^{(\alpha)}_{pq}(N)$ and $B^{(\alpha)}_{pq}(N)$ 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 S_{iz} spins equal to its zero value throughout. Specializing the results of ref.[38] to a single group of r spins, one has for the current problem

$$\binom{r}{q} b^{(\alpha)}_q(r) = \frac{1}{2^r} \sum_{i=0}^r \binom{r}{i} \epsilon_i(r,q) f_{\alpha}(r) \quad (29)$$

$$\binom{r}{q} d^{(\alpha)}_q(r) = \frac{1}{2^r} \sum_{i=0}^r \binom{r}{i} \epsilon_i(r,q) g_{\alpha}(r) \quad (30)$$

where

$$\epsilon_i(r,q) = \sum_{\mu=0}^i (-1)^{\mu} \binom{i}{\mu} \binom{r-i}{q-\mu} \quad (31)$$

and

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

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

3. Results and discussion.

Once the coefficients $b^{(\alpha)}_q(r)$ and $d^{(\alpha)}_q(r)$ have been calculated, and for getting the magnetizations m_z and m_x and the quadrupolar moments q_z and q_x , the coefficients $A^{(\alpha)}_{pq}$ and $B^{(\alpha)}_{pq}$ may be found by the following procedure. First, $A^{(\alpha)}_{0q}$ and $B^{(\alpha)}_{0q}$ are got by setting $r=q$ in eqs.(29) and (30), that is

$$A^{(\alpha)}_{0q} = b^{(\alpha)}_q(q) ; \quad B^{(\alpha)}_{0q} = d^{(\alpha)}_q(q) \quad (34)$$

Then, the other $A^{(\alpha)}_{pq}$ and $B^{(\alpha)}_{pq}$ may be obtained by expressing eqs.(29) and (30) as a recurrence relations, namely as

$$A^{(\alpha)}_{r-q,q} = b^{(\alpha)}_q(r) - \sum_{p=0}^{r-q-1} A^{(\alpha)}_{pq} \binom{r-q}{p} \quad (35)$$

$$B^{(\alpha)}_{r-q,q} = d^{(\alpha)}_q(r) - \sum_{p=0}^{r-q-1} B^{(\alpha)}_{pq} \binom{r-q}{p} \quad (36)$$

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

$$m_\alpha = \sum_{q=0}^N \sum_{p=0}^{N-q} A_{pq}^{(\alpha)} \langle (S_z)^2, S_z \rangle_{N,p,q} \quad (37)$$

$$q_\alpha = \sum_{q=0}^N \sum_{p=0}^{N-q} B_{pq}^{(\alpha)} \langle (S_z)^2, S_z \rangle_{N,p,q} \quad (38)$$

Using the simplest approximation of the Zernike decoupling of the type

$$\langle S_{iz} S_{jz} \dots S_{kz} \dots \rangle \approx \langle S_{iz} \rangle \langle S_{jz} \rangle \dots \langle S_{kz} \rangle \dots \text{ for } ij \neq k \neq \dots,$$

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

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

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

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

$$m = am + bm^3 + \dots \quad (41)$$

where

$$a = N(A_{01}^{(z)} + \sum_{p=1}^{N-1} A_{p1}^{(z)} (\binom{N-1}{p}) (x_0)^p) \quad (42)$$

with x_0 the solution of the following equation

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

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

$$(m_x)^2 = \frac{1-a}{b} \quad (44)$$

At this temperature the transverse magnetization is given by

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

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

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

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

$$x = x_0 + x_1 m^2 \quad (47)$$

where x_1 is given by:

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

That is

$$x_1 = \frac{\sum_{p=0}^{N-2} B_{p2}^{(z)} \binom{N-2}{p} (x_0)^p}{1 - \sum_{p=1}^N p B_{p0}^{(z)} \binom{N}{p} (x_0)^{p-1}} \quad (49)$$

This yields

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

The dependence of the magnetizations m_z and m_x on the temperature for a fixed values of the biquadratic exchange interactions D and the transverse field Ω are represented in Fig.1 and Fig.2 respectively, for several values of the magnetic crystal field Δ . Fig.3 and Fig.4 give respectively the dependence of m_z and m_x on temperature for a fixed values of crystal field Δ and transverse field Ω , for several values of biquadratic exchange interactions D . While the dependence of m_z and m_x on temperature for fixed values of biquadratic exchange D and crystal field Δ are given in Fig.5 and Fig.6 respectively, for several values of transverse field Ω . First order transition is characterized by the gap of the longitudinal magnetization m_z (Fig.1, $\Delta=3.29$) and the transverse magnetization m_x (Fig.2, $\Delta=3.29$) at the transition

temperature. While the magnetization m_z decreases continuously in the vicinity of the second order transition temperature and vanishes at $T=T_c$. The longitudinal magnetizations decreases when increasing the crystal field Δ at fixed value of D and Ω (Fig.1) and when increasing the transverse field Ω , at fixed value of D and Δ (Fig.3), while it increases when increasing the biquadratic exchange interactions D (Fig.5). Contrary to the behavior of the transverse magnetization m_x , it increases when increasing crystal field Δ (Fig.2) and/or increasing transverse field Ω (Fig.4) and decreases when increasing the biquadratic exchange interactions D . On the other hand the transverse magnetization increases at low temperature and passes through a peak for the first order transition (Fig.2, $\Delta=3.29$) and through a cusp for the second order transition temperatures of m_x (Fig.2,4,6) and then falls off rapidly as determined by the relation (45). From the above it is seen that first order transition is favored by a small transverse field and/or small biquadratic exchange interactions coupling D for sufficiently large crystal field Δ . Then the tricritical behavior due to the presence of crystal field, disappears at sufficiently large transverse field Ω , and biquadratic exchange coupling D .

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Figures Captions

Fig.1 The temperature dependence of the longitudinal magnetization when $\Omega/J=0.1$ and $D/J=0.1$. The number accompanying each curve denotes the value of Δ/J .

Fig.2 The temperature dependence of the transverse magnetization when $\Omega/J=0.1$ and $D/J=0.1$. The number accompanying each curve denotes the value of Δ/J .

Fig.3 The temperature dependence of the longitudinal magnetization when $\Omega/J=0.1$ and $\Delta/J=1.5$. The number accompanying each curve denotes the value of D/J .

Fig.4 The temperature dependence of the transverse magnetization when $\Omega/J=0.1$ and $\Delta/J=1.5$. The number accompanying each curve denotes the value of D/J .

Fig.5 The temperature dependence of the longitudinal magnetization for $\Delta/J=1.5$ and $D/J=0.5$. The number accompanying each curve denotes the value of Ω/J .

Fig.6 The temperature dependence of the transverse magnetization for $\Delta/J=1.5$ and $D/J=0.5$. The number accompanying each curve denotes the value of Ω/J .

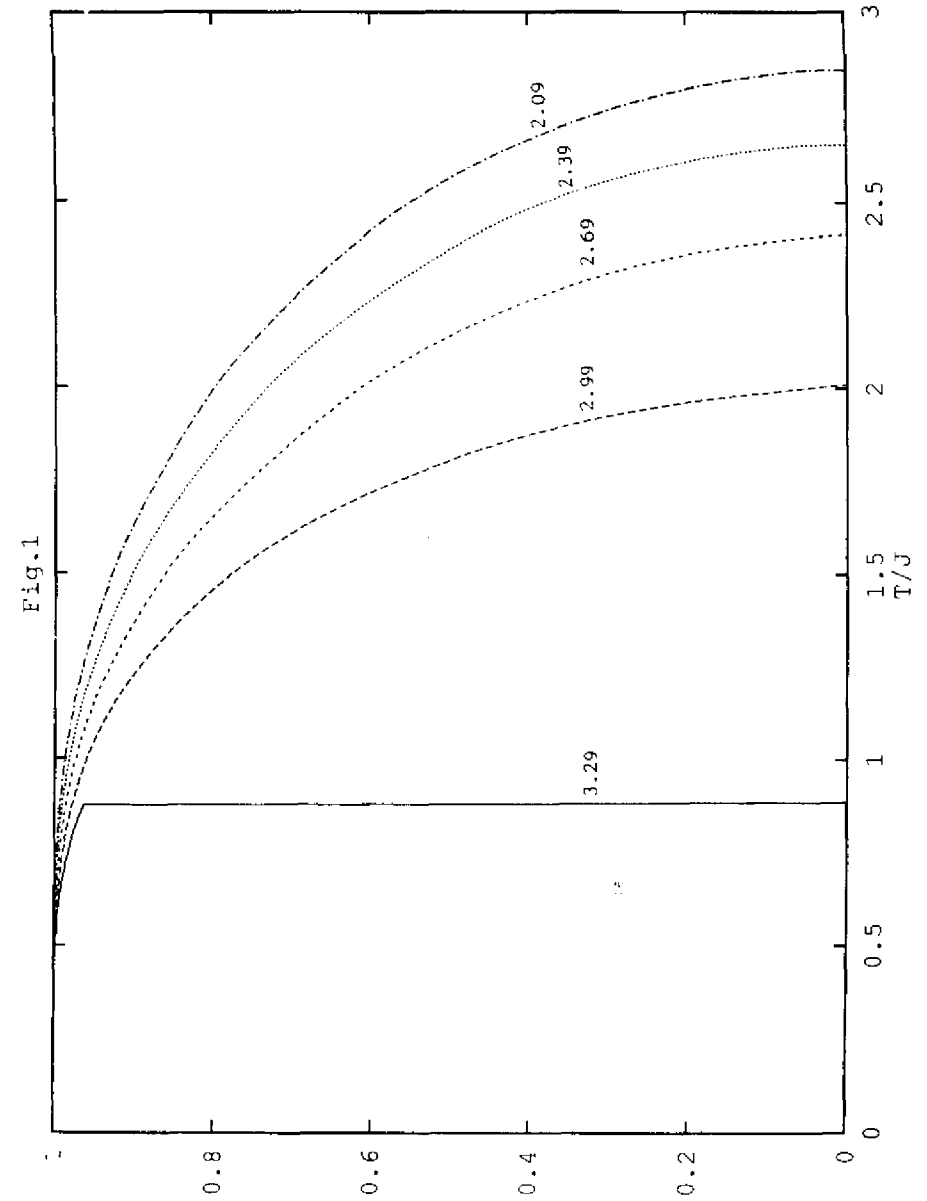


Fig.2

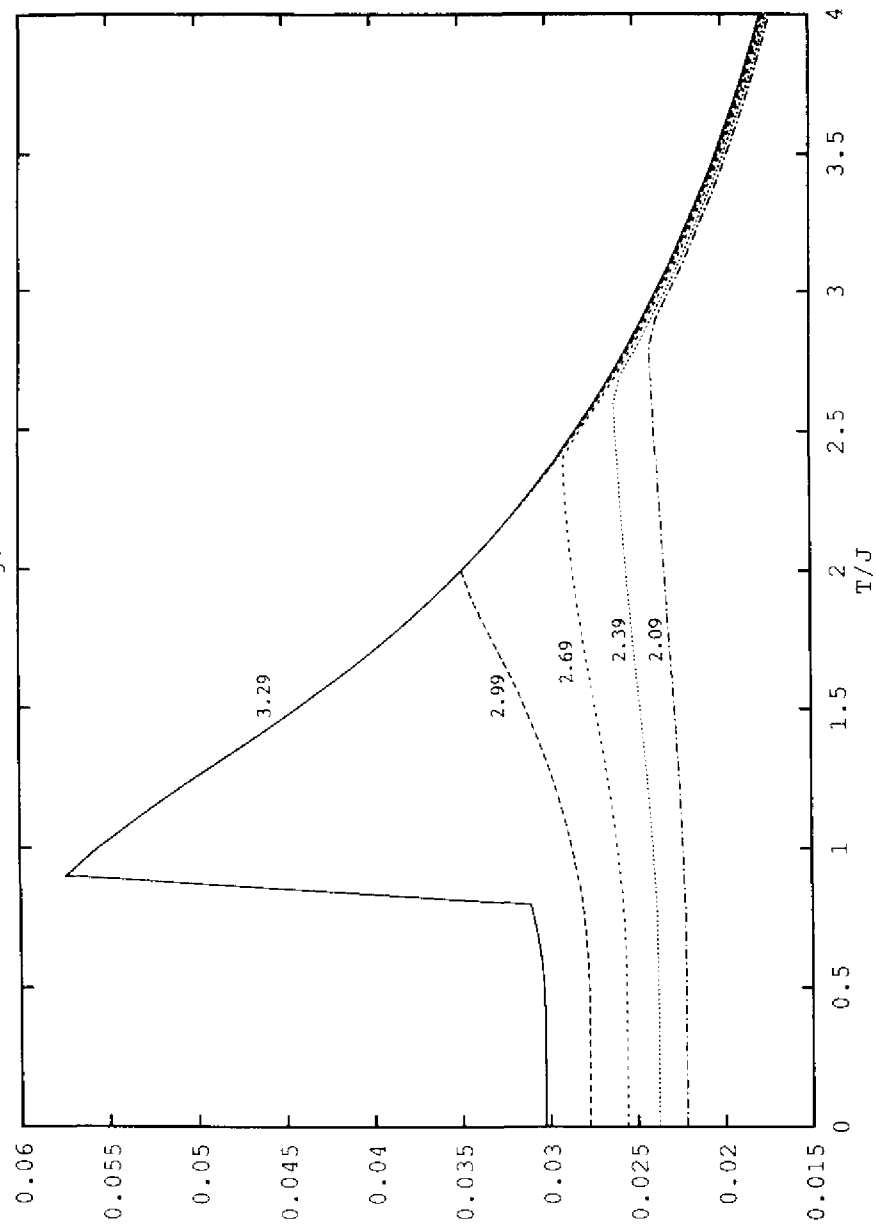


Fig.3

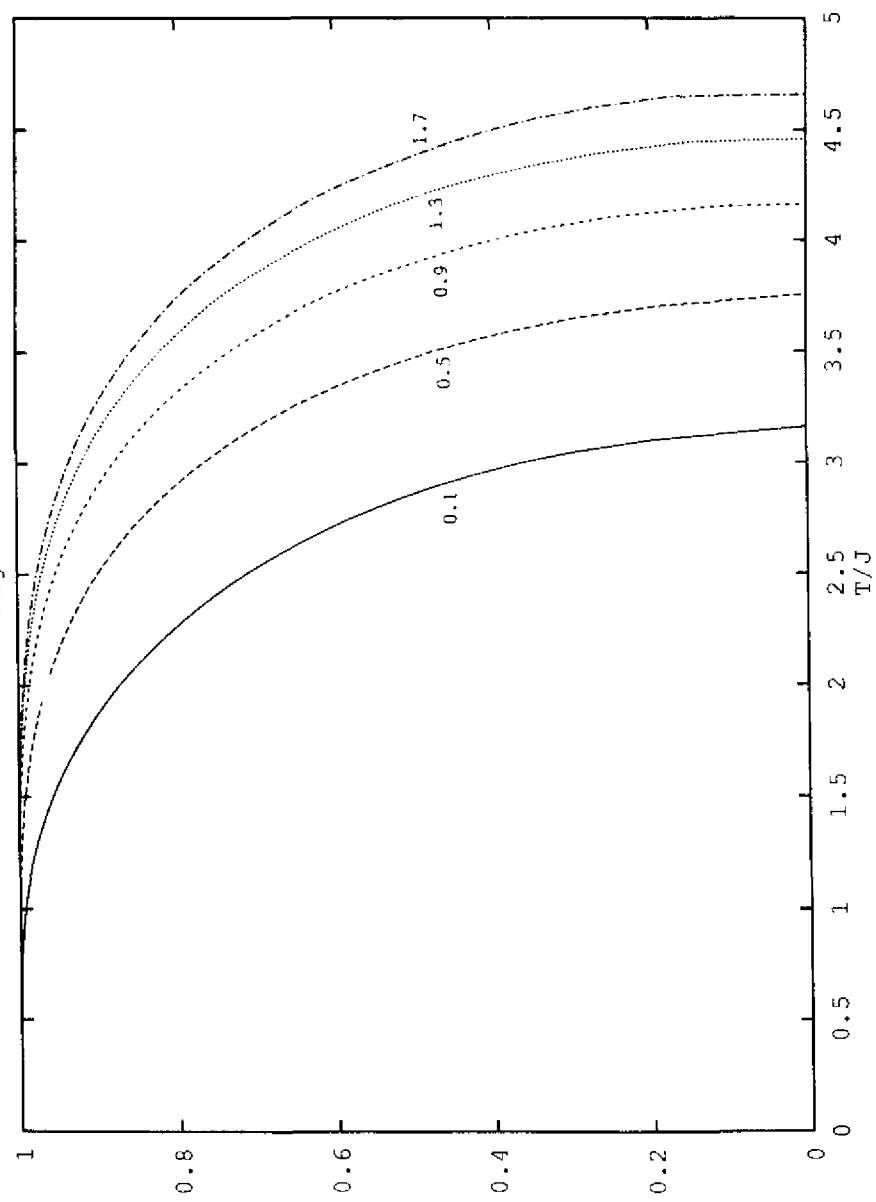


Fig.4

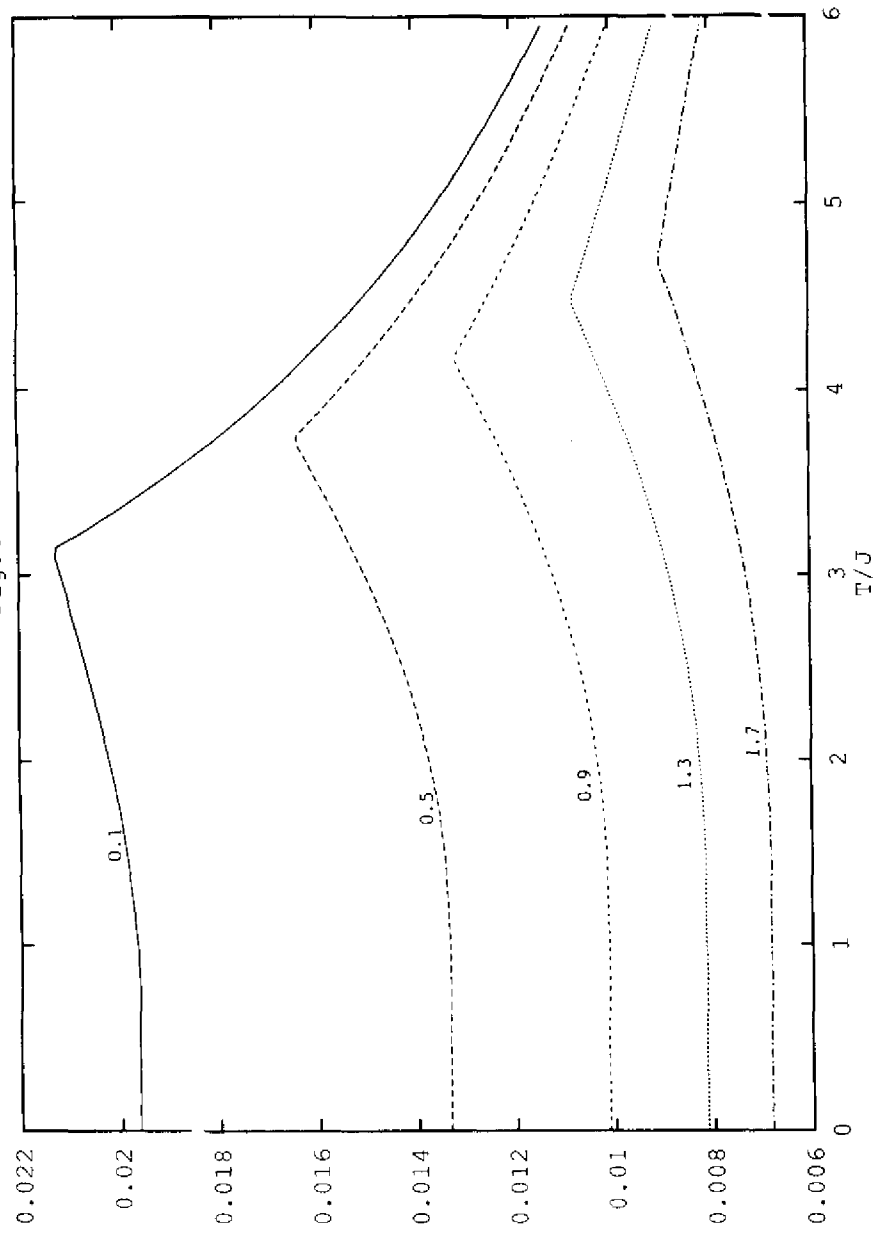


Fig.5

