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Behaviour of a Singlet Ground State System in the Presence of an External Magnetic Field

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Abstract. In a singlet ground state system the exchange interaction must exceed a critical value relative to the anisotropy energy to give magnetic order even at zero temperature. It is pointed out that a spin one Ising model with an uniaxial anisotropy energy Δ , which has the effect that the ground state of the system is a non-magnetic singlet, is able to show magnetic order in a transverse magnetic field, even if Δ is greater than the exchange interaction, so that the condition for ordering without the external field is not fulfilled. The molecular field theory is used to discuss the phase transition. The phase transition is of second order and the transition temperature is a monotonically increasing function of the applied field. The dynamical properties of the system are analysed on the basis of the Bogoliubov approximation.

I. Introduction

Phenomena of magnetic ordering in a spin one Ising model with a uniaxial anisotropy field of single ion type were extensively discussed by Capel [2], on the basis of a molecular field theory. He used the Hamiltonian:

$$\mathbb{H} = \sum_i \{ \Delta J_{iz}^2 - g\mu_B H J_{iz} \} - \sum_{\langle ij \rangle} G_{ij} J_{iz} \cdot J_{jz} \quad J = 1 \quad (1)$$

which reduces in the molecular field approximation to:

$$\mathbb{H}_m = \sum_i [\Delta J_{iz}^2 - g\mu_B H J_{iz} - 2G(0) \langle J \rangle J_{iz}] \quad (2)$$

where $G(0) = \sum_i G_{ij}$. The anisotropy energy was allowed to vary between $-\infty \leq \Delta \leq \infty$. Without an external magnetic field he found the possibility of the appearance of a first-order phase transition between the ordered and the paramagnetic state in the region of level crossing where one of the excited levels crosses under the ground state level ($\frac{1}{3} \ln 4 \leq \Delta/2G(0) \leq \frac{1}{2}$). In the other regions he got no phase transition ($\Delta/2G(0) > \frac{1}{2}$) or a phase transition of second order ($-\infty < \Delta/2G(0) < \frac{1}{3} \ln 4$) depending on the ratio $\Delta/2G(0)$ [2].

The purpose of this paper is to investigate a spin one Ising ferromagnet with a uniaxial anisotropy field of single ion type, whose ordering arises by induced moments, that is there is no magnetic moment in the ground state. Examples of such systems are

compounds of non-Kramers rare earth ions (J even). The Hamiltonian of the simplest system that shows this behaviour is:

$$\mathbb{H} = \sum_i [\Delta J_{iz}^2 - \mu \vec{H} \cdot \vec{J}] - \sum_{\langle ij \rangle} K_{ij} J_{ix} \cdot J_{jx} \quad J = 1. \quad (3)$$

Δ is called the zero field splitting. The second term is due to an applied external magnetic field \vec{H} , μ being the magnetic moment of the ion. The third term represents the exchange interaction between the x components of the spins of the ions i and j which are nearest neighbours. The symbol $\langle i, j \rangle$ indicates that the summation is over all pairs of neighbouring ions.

II. Molecular Field Approximation Without External Magnetic Field

We will use the molecular field approximation which leads at zero external field to the Hamiltonian

$$\mathbb{H}_m = \sum_i [\Delta J_{iz}^2 - 2K(0)\langle J \rangle J_{ix}] \quad J = 1, \quad (4)$$

where $K(0) = \sum_i K_{ij}$. In the following we assume that the exchange is ferromagnetic, $K(0) > 0$. The eigenfunctions of the anisotropy Hamiltonian are the $J = 1$ angular momentum functions:

$$J_z |m, 1\rangle = m |m, 1\rangle \quad m = 0, \pm 1 \quad \hbar = 1. \quad (5)$$

All matrix elements of the operator J_x between these functions disappear except the non-diagonal elements between the states $|\pm 1, 1\rangle$ and the state $|0, 1\rangle$:

$$\langle 1, 0 | J_x | \pm 1, 1 \rangle = \langle 1, \pm 1 | J_x | 0, 1 \rangle = c = 2^{-1/2}. \quad (6)$$

The anisotropy term has the effect of a crystal field. The triplet $J = 1$ splits into a singlet and a doublet separated by an energy gap Δ from the singlet. In the case $\Delta > 0$ the ground state is the singlet. It is known that a system with a singlet ground state shows no magnetic long-range order for exchange interactions which are not strong enough [1, 3]. The exchange interaction has to exceed a certain critical value to give magnetic order even at zero temperature. The magnetic moment which occurs in this case is essentially an induced moment corresponding to the temperature-independent van Vleck susceptibility [1], where the exchange field takes the place of an applied external magnetic field. Some rare earth compounds show this kind of ordering [3]. The condition for the existence of a spontaneous magnetization in our singlet ground state system is:

$$\eta = 4K(0)/\Delta \geq 1. \quad (7)$$

The sign of equality corresponds to the case $T_c = 0$. With growing ratios (7) we get higher values for the transition temperature T_c and higher values for the maximum of the spontaneous magnetization $\langle J \rangle_{T=0}$. The eigenvalues of the molecular field Hamiltonian (4) are given by:

$$E_0 = \frac{\Delta}{2} [1 \mp (1 + \eta^2 \langle J \rangle^2)^{1/2}]$$

$$E_2 = \Delta. \quad (8)$$

From (8) and the eigenfunctions corresponding to these eigenvalues we find the magnetization in thermal equilibrium and the critical value for magnetic ordering:

$$\langle J \rangle = \frac{\eta \langle J \rangle}{(1 + \eta^2 \langle J \rangle^2)^{1/2}} \frac{2 \sinh \left[\frac{\Delta}{2k_B T} (1 + \eta^2 \langle J \rangle^2)^{1/2} \right]}{2 \cosh \left[\frac{\Delta}{2k_B T} (1 + \eta^2 \langle J \rangle^2)^{1/2} \right] + \exp \left[-\frac{\Delta}{2k_B T} \right]}. \quad (9)$$

The spontaneous magnetization and the energy values at zero degree are:

$$\langle J \rangle_{T=0} = [1 - \eta^{-2}]^{1/2} \quad (10)$$

$$E_0 = \frac{\Delta}{2} (1 \mp \eta)$$

$$E_2 = \Delta. \quad (11)$$

If $\eta > 1$ the new ground state E_0 has a lower energy. From (9) follows at once: $\langle J \rangle = 0$ is always a solution of the self-consistent equation for the spontaneous magnetization, whereas $\langle J \rangle \neq 0$ follows only if $\eta > 1$. Another way to get these results is to calculate the free energy of the system similarly to [2]:

$$F = \frac{\Delta}{2} - k_B T \ln \left[2 \cosh \frac{\Delta}{2k_B T} (1 + \eta^2 \langle J \rangle^2)^{1/2} + \exp \left[-\frac{\Delta}{2k_B T} \right] \right] + K(0) \langle J \rangle^2. \quad (12)$$

The free energy of the paramagnetic phase results from (12) for $\langle J \rangle$ equal to zero. The condition of self-consistency (9) is obtained by minimizing (12) with respect to $\langle J \rangle$. The higher derivatives of F with respect to $\langle J \rangle$ determine the kind of the phase transition and the stability boundaries of the system. The stability boundary of the paramagnetic phase gives us a relation for the transition temperature:

$$\frac{k_B T_c}{\Delta} = \ln \frac{\eta - 1}{\eta + 2}, \quad (13)$$

in the case $\Delta = 0$ (no anisotropy energy) we get:

$$k_B T_c = \frac{4K(0)}{3}.$$

The phase transition from the paramagnetic to the ferromagnetic phase for $\eta \geq 1$ is of second order. The boundary of stability of the ordered phase gives the boundary of phases:

$$[1 + \eta^2 \langle J \rangle^2]^{1/2} = \eta L \left(\frac{\Delta}{2k_B T} [1 + \eta^2 \langle J \rangle^2]^{1/2} \right), \quad (14)$$

where $L(x) = \text{ctgh } x - (1/x)$ is the Langevin function.

III. Influence of the Transverse Magnetic Field

The Hamiltonian in the molecular field approximation in a transverse external magnetic field reads:

$$\mathbb{H} = \sum_i [\Delta J_{iz}^2 - hJ_{iz} - 2K(0)\langle J \rangle J_{ix}] \quad (15)$$

where $h = \mu H$ is the Zeeman energy. The transverse magnetic field has the effect of splitting the doublet of excited levels (Fig. 2) so that the gap between the ground state

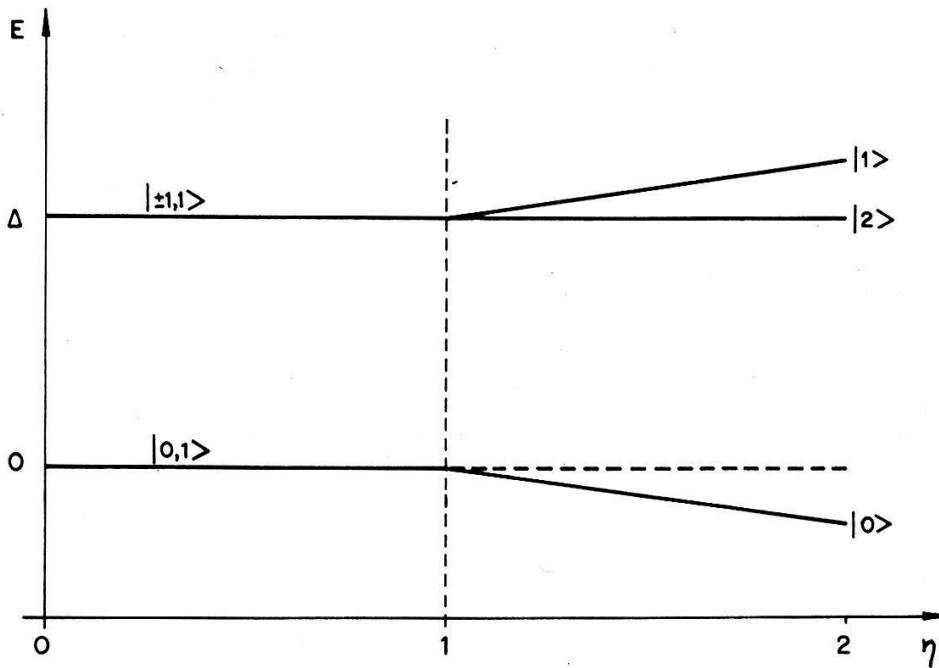


Figure 1

Energy eigenvalues in the molecular field approximation as a function of the exchange parameter η .

and the lower excited state in the field is reduced. It follows that even in the case where without the magnetic field no ordering is possible the system can show ferromagnetic order along the x direction as a consequence of a magnetic field applied along the z direction. In this section we deal with this problem.

The energy eigenvalues of the molecular field Hamiltonian (15) are given by

$$E_0 = \frac{1}{2} \left[\Delta(2 - \alpha) \mp \sqrt{\Delta^2(2 - \alpha)^2 + \frac{1}{\alpha} [4K(0)\langle J \rangle]^2} \right] \quad (16)$$

$$E_2 = \alpha\Delta,$$

where the parameter α has to satisfy the equation:

$$h^2 = \Delta^2(\alpha - 1)^2 - \frac{\alpha - 1}{\alpha} 4K^2(0)\langle J \rangle^2. \quad (17)$$

Instead of the magnetic field a parameter α is used which depends on the magnetic field and the spontaneous magnetization $\langle J \rangle$. Therefore we have another condition of self-consistency in addition to the normal one. We calculate the free energy of the system

depending on α , determine the spontaneous magnetization for the value of α and, at the end, we get the magnetic field strength belonging to the specific value of α . The parameter α varies for our problem between one and two. The value $\alpha = 1$ corresponds to the case $h = 0$, which we treated in Section I. $\alpha = 2$ corresponds to the case where, without any exchange interaction, the level crossing would appear. The exchange interaction has the effect of mixing the states and gives rise to the behaviour shown in Figure 2 [4].

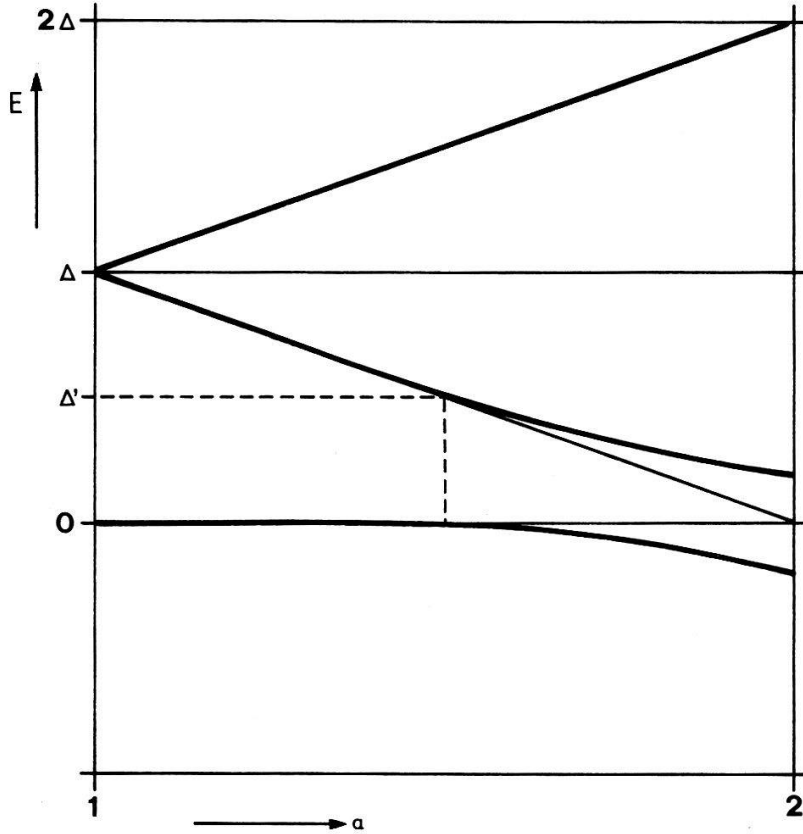


Figure 2

Dependence of the energy levels on the parameter α (--- without exchange interaction, — including the exchange field which gives rise to an energy gap at $\alpha = 2$).

In our case we assume $\Delta/4K(0) > 1$, that is the case where an external field is necessary to induce spontaneous magnetization. The critical field is given by:

$$h_{cr} = \Delta(\alpha_{cr} - 1). \quad (18)$$

α_{cr} is the greatest value for which even at zero degree no spontaneous magnetization appears. This value is obtained from the critical condition for ordering at $T = 0$:

$$16K^2(0)/[\alpha_{cr}(2 - \alpha_{cr})^2 \Delta^2] = 1 \quad \alpha_{cr} \in [1, 2]. \quad (19)$$

The physical solution $\alpha_{cr} \in [1, 2]$ of equation (19) is given by:

$$\alpha_{cr}(\eta) = \frac{4}{3} \left[1 + \cos \left(\frac{\pi}{3} + \frac{1}{3} \arccos \left[1 - \frac{27}{16} \eta^2 \right] \right) \right]. \quad (20)$$

The critical magnetic field reads:

$$h_{cr}/\Delta = \frac{1}{3} \left[1 + 4 \cos \left[\frac{\pi}{3} + \frac{1}{3} \arccos \left(1 - \frac{27}{16} \eta^2 \right) \right] \right]. \quad (18')$$

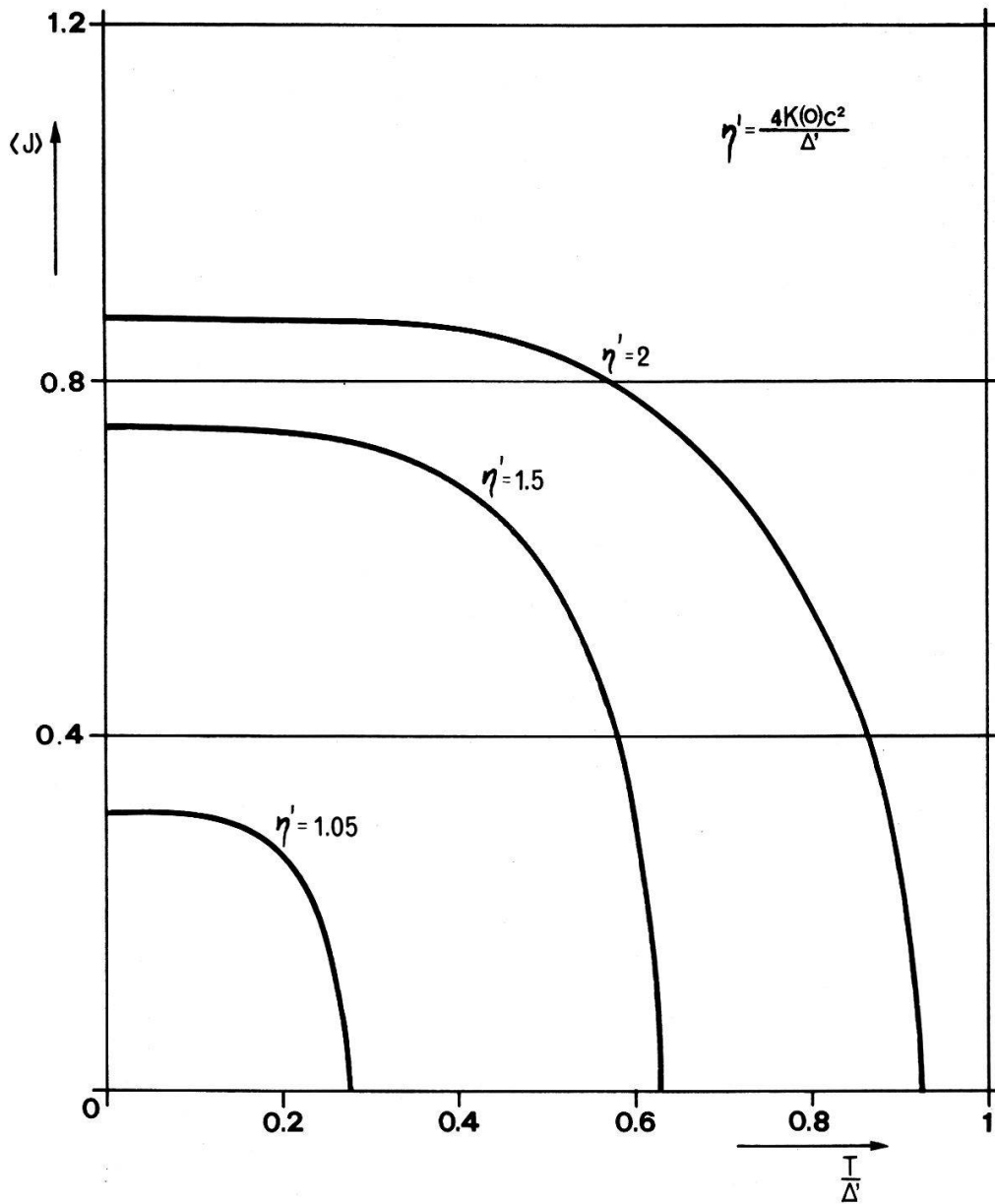


Figure 3

Spontaneous magnetization (in dimensionless form) versus temperature for varying values of η' .

Figure 5 shows the critical field as a function of η . The free energy is calculated similar to (I):

$$F = \alpha\Delta + K(0)\langle J \rangle^2 - k_B T \ln \left[2 \exp \left(-\frac{\Delta}{k_B T} \left[1 - \frac{3}{2}\alpha \right] \right) \right] \tag{21}$$

$$\cdot \cosh \left[\frac{\Delta(2 - \alpha)}{2k_B T} (1 + \eta'^2 \langle J \rangle^2)^{1/2} \right] + 1 \tag{22}$$

where

$$\eta' = \frac{4K(0)}{\Delta(2 - \alpha)\alpha^{1/2}}$$

In principle we are able to calculate from (21) the thermodynamic properties of this system. In the case $\Delta \gg 4K(0)$ (dilute rare earth salt) we can neglect the highest level

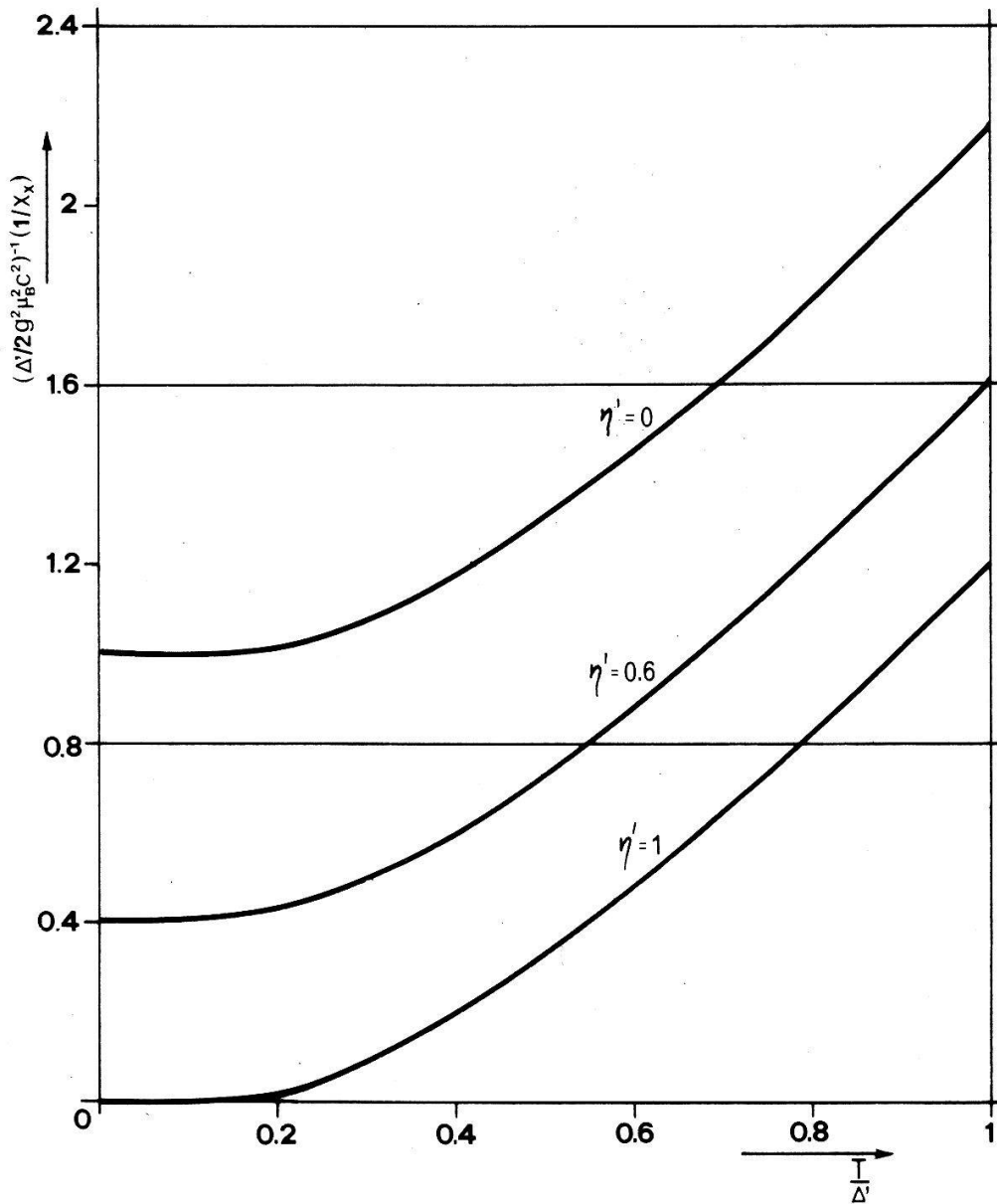


Figure 4
Inverse susceptibility versus temperature for several values of η' .

in the magnetic field, because there is only a very small influence of this level on the ordering. The error due to this approximation is of the order of $K(0)/(\Delta + h) \ll 1$. In this approximation we get an effective two-level system with the free energy given by:

$$F = \frac{\Delta'}{2} + K(0)\langle J \rangle^2 - k_B T \ln \left[2 \cosh \left[\frac{\Delta'}{2k_B T} (1 + \eta'^2 \langle J \rangle^2)^{1/2} \right] \right], \quad (23)$$

where $\Delta' = \Delta - h$.

We minimize this expression with respect to $\langle J \rangle$ and obtain the equation for the temperature dependence of the spontaneous magnetization (Fig. 3):

$$[1 + \eta'^2 \langle J \rangle^2]^{1/2} = \eta' \operatorname{tgh} \left[\frac{\Delta'}{2k_B T} (1 + \eta'^2 \langle J \rangle^2)^{1/2} \right] \quad (24)$$

where $\eta' = 4K(0)c^2/\Delta'$.

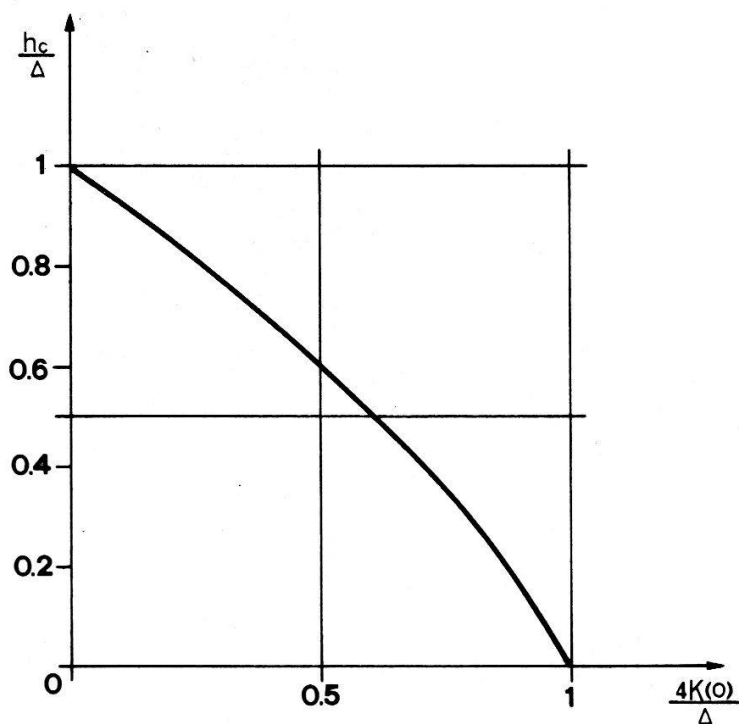


Figure 5
The critical magnetic field as a function of η .

From the condition that we have at zero degree a spontaneous magnetization we get the critical value for ordering which is very similar to (19):

$$4K(0) c^2 \geq \Delta' = \Delta - h. \quad (25)$$

That is, for all values of Δ and $K(0)$ we are able to induce a phase transition in a transverse magnetic field. It is easy to show that the phase transition from the paramagnetic to the ordered phase in the transverse field is of second order. The critical temperature is given by the expression (Fig. 6):

$$\frac{\Delta'}{2k_B T} = \text{ctgh}^{-1} \eta'. \quad (26)$$

A calculation analogous to that of Section I gives the boundary of phases of our system:

$$[1 + \eta'^2 \langle J \rangle^2]^{1/2} = c\eta' L \left(\frac{\Delta'}{2k_B T} [1 + \eta'^2 \langle J \rangle^2]^{1/2} \right), \quad (27)$$

where $L(x)$ is the Langevin function.

The inverse susceptibility in the paramagnetic phase in the x direction is (Fig. 4):

$$\chi_x^{-1} = \frac{\Delta'}{2\mu^2 c^2} \left[\text{ctgh} \frac{\Delta'}{2k_B T} - \eta' \right]. \quad (28)$$

The zero of χ_x^{-1} gives the transition temperature (26). For small values of Δ' we obtain from (26):

$$k_B T_c(\Delta') \simeq 2K(0) c^2 [1 - \frac{1}{3}\eta'^{-2}]. \quad (29)$$

Figure 7 shows the Curie temperature as a function of the applied external field for several values of η . The transition temperature increases monotonically with increasing strength of magnetic field.

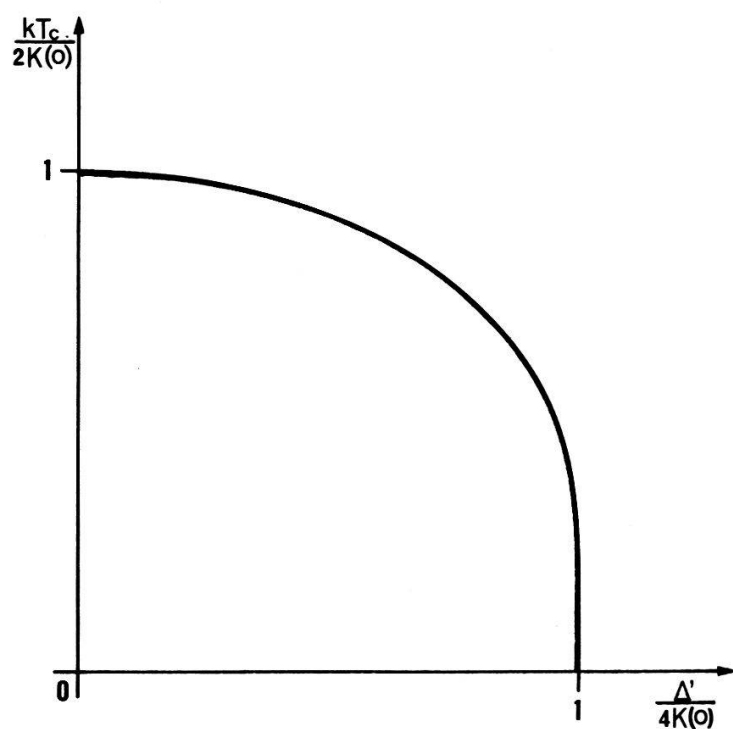


Figure 6
The transition temperature as a function of η' .

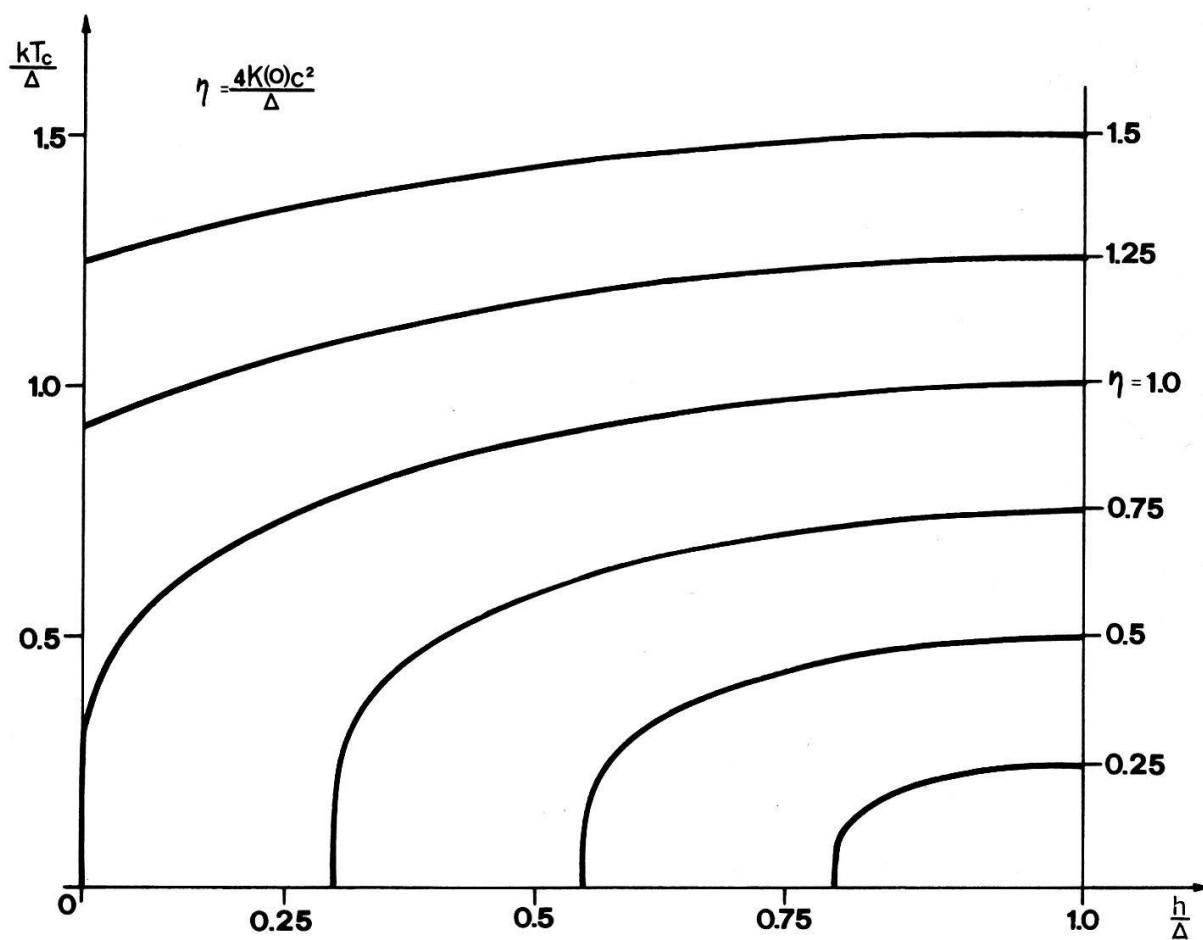


Figure 7
The transition temperature T_c as a function of the applied transverse field.

IV. Elementary Excitations in the Bogoliubov Approximation

If we are not only interested in the thermostatic properties but also in the dynamics of our system (p.e. dependence of the specific heat and the spontaneous magnetization on the temperature T in the region of low temperatures) we have to consider the spectrum of low-lying elementary excitations of the system. Once this spectrum is known it is a simple matter to calculate the thermodynamic properties. To obtain the dispersion relations of the collective excitations, one can either use an equation of motion method or a method of second quantization. For simplicity we will use the latter in the Bogoliubov approximation [5]. The calculation starts with the Hamiltonian (3) (furthermore we will restrict ourselves to the case $4K(0) \ll \Delta$ and to the presence of an external transverse magnetic field). By definition [5]:

$$b_i^\dagger |0, 1\rangle = |1, 1\rangle, \quad (30)$$

b_i^\dagger, b_i are the creation and destruction operators of an electron in the state $|1, 1\rangle$ at the ion i and $b_i^\dagger b_i$ is the occupation number of the triplet state $|1, 1\rangle$. These operators satisfy, in the regime of low temperatures (occupation number of the excited state \ll occupation number of the ground state), the commutation relations for bosons. This leads in the paramagnetic regime after the Fourier transformation into the k -space:

$$b_i = N^{-1/2} \sum_k b_k \exp[i\vec{k}\vec{r}_i] \quad (31)$$

to the Hamiltonian:

$$\mathbb{H} = \sum_k [\Delta' - 2K(0) c^2 \gamma_k] b_k^\dagger b_k - K(0) c^2 \gamma_k [b_k b_{-k} + b_k^\dagger b_{-k}^\dagger]. \quad (32)$$

This Hamiltonian can be diagonalized by means of the Bogoliubov transformation

$$\begin{aligned} \alpha_k &= u_k b_k^\dagger - v_k b_{-k} \\ \alpha_k^\dagger &= u_k b_k - v_k b_{-k}^\dagger. \end{aligned} \quad (33)$$

This leads to the dispersion relations for these modes of Bose type:

$$\omega(k) = \Delta' [1 - \eta' \gamma_k]^{1/2}$$

with

$$\gamma_k = \gamma_{-k} = \sum_{\langle ij \rangle} \exp[-i\vec{k}(\vec{r}_i - \vec{r}_j)]. \quad (34)$$

For the case of a simple cubic lattice of lattice constant a we find in the limit of long wavelength for the paramagnetic phase:

$$\begin{aligned} \omega_p(k) &= \Omega' [1 + A'^2 a^2 k^2]^{1/2} \\ \Omega' &= \Delta' (1 - \eta')^{1/2} \quad A'^2 = \eta' / (1 - \eta'), \end{aligned} \quad (35)$$

whereas we receive for the ferromagnetic phase ($\eta' > 1$):

$$\begin{aligned} \omega_F(k) &= \Omega'' [1 + A''^2 a^2 k^2]^{1/2} \\ \Omega'' &= \Delta' (\eta'^2 - 1)^{1/2} \quad A''^2 = (\eta'^2 - 1)^{-1}. \end{aligned} \quad (36)$$

The contribution of these excitations to the specific heat of the crystal at low temperatures is easily calculated with the help of (35), (36):

$$C_v = \frac{Nk_B}{2\pi^2 A^3} \frac{\Omega}{k_B T} \sum_{n=1}^{\infty} \left[\frac{3k_B T}{n\Omega} K_1\left(\frac{n\Omega}{k_B T}\right) + \left(1 + \frac{12k_B^2 T^2}{n^2 \Omega^2}\right) K_2\left(\frac{n\Omega}{k_B T}\right) \right] \quad (37)$$

$K_\nu(x)$ are the modified Bessel functions of second kind and integer order [6]. We get the same temperature dependence of the specific heat in both phases, only the constants Ω and A have to be replaced by Ω', Ω'' and A', A'' respectively. In the limit of low temperatures formula (37) simplifies to [5]:

$$C_v = \frac{Nk_B}{(2\pi A^2)^{3/2}} \left(\frac{\Omega}{k_B T}\right)^{1/2} \cdot \exp[-\Omega/k_B T]. \quad (31)$$

Whereas in the ferromagnetic regime the spontaneous magnetization is given by

$$[\langle J \rangle_0 - \langle J \rangle_T] / \langle J \rangle_0 \cong \frac{\eta'(2\eta'^2 - 1)}{(2\pi)^{3/2}} \left(\frac{k_B T}{\Omega''}\right)^{3/2} \exp\left[-\frac{\Omega''}{k_B T}\right]. \quad (39)$$

From (38) and (39) we can conclude that in the ferromagnetic region for increasing transverse magnetic field the specific heat vanishes faster towards zero degree, and so do the difference between the maximum value of the magnetization $\langle J \rangle_0$ and the value at a certain temperature T because $\Omega''(h) \geq \Omega''(0)$. In the paramagnetic phase c_v vanishes slower for growing values of h ($\Omega'(h) \leq \Omega'(0)$).

V. Conclusion

We have shown that a transverse magnetic field is able to induce a phase transition of second order in a uniaxial spin one Ising model whose phenomena of ordering are a consequence of a kind of van Vleck magnetism. We found that the Curie temperature is a monotonically increasing function of the applied transverse field contrary to a normal magnetic system where in all cases T_c decreases with increasing strength of the applied field. This is, therefore, a very simple method to distinguish between magnetic ordering phenomena of normal and induced magnetic moments.

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