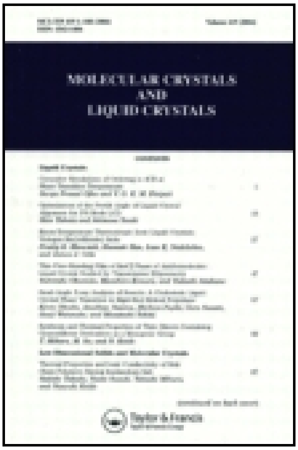

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Reorientation Transitions

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Reorientation Transitions

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Phase transitions of a quantum spin-1 Ising-Heisenberg model with uniaxial and single-ion anisotropy and with quadrupolar interactions are investigated by mean-field approximation. After the determination of the free energy, a Landau expansion is performed in order to analytically identify the critical temperatures. In some cases, for non-zero values of the anisotropy terms, first order reorientation transitions have been found. The influence of the quadrupolar interaction term on them is analyzed.

Keywords: spin-1 models; reorientation transitions

1. INTRODUCTION

Spin-1 models have been the subject of interest in last years as capable to describe the critical properties of many physical systems as ^{3}He–^{4}He solutions,[1] liquid crystals, fluid mixtures,[2–4] magnetic materials.[5] They are characterized by two kinds of order parameters: dipolar and quadrupolar. The phase diagram has a variety of critical properties in particular when anisotropy terms are present in the Hamiltonian.[6] In this paper we analyze a spin-1 quantum Ising-Heisenberg model with uniaxial and single-ion anisotropy and quadrupolar interaction terms. The relevance of such a model is to exhibit not only usual order-disorder transitions but also reorientation type order-order transitions. A mean-field approach has been adopted in order to determine the free energy, then a Landau expansion is carried out to analytically derive second order critical surfaces. First order critical surfaces are identified by numerical investigation. The paper is organized as follows. In section 2 the model Hamiltonian is introduced and the free energy evaluated. In section 3 the critical properties of the system are investigated. A conclusion is drawn in section 4.

2. MODEL AND PROCEDURE

The physical system we deal with consists of N quantum spin-1 objects arranged on a three-dimensional lattice, whose Hamiltonian is

$$H = -\sum_{\langle i,j\rangle}\{J_{ij}[\eta(S_i^x S_j^x + S_i^y S_j^y) + S_i^z S_j^z] + G_{ij}(S_i^z)^2(S_j^z)^2\}$$

$$-\sum_{i=1}^{N}\sum_{\mu=x,y,z}[B_\mu S_i^\mu + D_\mu(S_i^\mu)^2], \quad (2.1)$$

S_i^μ, ($\mu = x,y,z$) are the components of the spin-1 operator at site i ($S_i^\mu = I_{3^{i-1}} \otimes S_\mu \otimes I_{3^{N-i}}$, $i = 1, \ldots, N$). J_{ij} and G_{ij} are dipolar and quadrupolar nearest neighbor coupling strengths respectively; η is a non-negative parameter measuring the degree of anisotropy of the dipolar interaction; B_μ and D_μ, ($\mu = x,y,z$) are the external field components and single-ion anisotropy constants, respectively. Following the mean-field procedure, we introduce the dipolar δS_i^μ and quadrupolar $\delta\,(S_i^\mu)^2$ spin-fluctuation operators by

$$S_i^\mu = p_\mu + \delta S_i^\mu, \qquad (S_i^\mu)^2 = q_\mu + \delta(S_i^\mu)^2, \qquad \mu = x,y,z \quad (2.2)$$

where p_μ and q_μ, ($\mu = x,y,z$) are parameters to be determined in the sequel by some suitable conditions. The Hamiltonian is then decomposed into two parts $H = H_o + H'$, H' bilinear in the fluctuations. We assume the fluctuations small enough to approximate H with H_o. H_o turns out to be a sum of one-body terms only

$$H_o = \sum_{i=1}^{N} H_{oi}, \qquad H_{oi} = I_{3^{i-1}} \otimes \mathcal{H}_o \otimes I_{3^{N-i}}, \quad (2.3)$$

with

$$\mathcal{H}_o = \frac{1}{2}[\mathcal{J}(\eta p_o^2 + p_z^2) + \mathcal{G}q_z^2] - \sum_{\mu=x,y,z}(M_\mu S_\mu + W_\mu S_\mu^2). \quad (2.4)$$

In (2.4) the quantities

$$\mathcal{J} = \sum_j J_{ij}; \qquad \mathcal{G} = \sum_j G_{ij}; \qquad p_o^2 = p_x^2 + p_y^2; \quad (2.5)$$

$$M_\mu = \mathcal{J}\eta p_\mu + B_\mu, \quad W_\mu = D_\mu, \quad \mu = x,y;$$

$$M_z = \mathcal{J}p_z + B_z, \quad W_z = \mathcal{G}q_z + D_z, \quad (2.6)$$

have been introduced; for the definition (2.5) cyclic boundary condition were assumed.

The free energy per site is given by

$$f = -\frac{1}{\beta}\,ln[Tr\,\exp(-\beta\mathcal{H}_o)] = -\frac{1}{\beta}\,ln\left[\sum_{i=1}^{3}\exp(-\beta\lambda_i)\right], \quad (2.7)$$

where λ_i, ($i = 1,2,3$) are the eigenvalues of $\mathcal{H}_o$ and β is the inverse temperature in units $k_B = 1$. It is convenient to introduce units such that $\mathcal{J} = 1$ as well: we shall denote by lower-case symbols the quantities expressed in such units (i.e. d_μ for D_μ, b_μ for B_μ, m_μ for M_μ, w_μ for W_μ, g for $\mathcal{G}$).

In order to simplify the treatment and in view of the determination of critical behavior we assume $d_z - d_x = d_z - d_y = d$ and the external field $\mathbf{B} = 0$. In a previous paper[6] the author analyzed the model in the case in which no quadrupolar terms where present. In this paper the quadrupolar interaction has required the introduction of quadrupolar order parameters q_μ, nevertheless from a purely formal point of view, the diagonalization of our Hamiltonian leads to the same 3rd order algebraic equation as in Reference 6, in the new variables υ, if the parameter d_μ of Reference 6 is replaced by the parameter w_μ and

$$\lambda_i = \frac{1}{2}\left[\eta p_o^2 + p_z^2 + g q_z^2\right] - \frac{2}{3}(w_x + w_y + w_z) + \upsilon_i,$$

$$w = g q_z + d. \tag{2.8}$$

It is

$$\upsilon_1 = 2\rho\cos(\psi/3 - 2\pi/3); \qquad \upsilon_2 = 2\rho\cos(\psi/3);$$

$$\upsilon_3 = 2\rho\cos(\psi/3 + 2\pi/3); \tag{2.9}$$

with

$$\rho = \frac{[w^2 + 3(\eta^2 p_o^2 + p_z^2)]^{1/2}}{3},$$

$$\tau = \frac{w(2w^2 - 18p_z^2 + 9\eta^2 p_o^2)}{54}, \quad \cos\psi = \frac{\tau}{\rho^3}. \tag{2.10}$$

The resulting free energy depends on three order parameters p_o, p_z and q_z. They will be determined by the requirement of absolute minimum free energy. The first order derivatives are

$$\frac{\partial f}{\partial p_o} = \eta p_o\left[1 + \frac{\eta\upsilon_o}{3\rho^2} + \frac{\eta\zeta_o}{3\rho^2\sin\psi}\left(\frac{\tau}{\rho^2} - \frac{w}{3}\right)\right] = \eta p_o L_o, \tag{2.11}$$

$$\frac{\partial f}{\partial p_z} = p_z\left[1 + \frac{\upsilon_o}{3\rho^2} + \frac{\zeta_o}{3\rho^2\sin\psi}\left(\frac{\tau}{\rho^2} + \frac{2w}{3}\right)\right] = p_z L_z, \tag{2.12}$$

$$\frac{\partial f}{\partial q_z} = g\left[q_z - \frac{2}{3} + \frac{w\upsilon_o}{9\rho^2} + \frac{\zeta_o}{9\rho^2\sin\psi}\left(\frac{w\tau}{\rho^2} - \frac{2w^2 - 6p_z^2 + 3\eta^2 p_o^2}{6}\right)\right] = g\,\Omega_z. \tag{2.13}$$

with

$$\upsilon_o = \frac{1}{Z_n}\sum_{i=1}^{3} \upsilon_i \exp(-\beta\upsilon_i);$$

$$\zeta_o = \frac{1}{Z_n}\sum_{i=1}^{3} \zeta_i \exp(-\beta\upsilon_i); \quad Z_n = \sum_{i=1}^{3} \exp(-\beta\upsilon_i). \qquad (2.14)$$

and

$$\zeta_1 = -2\sin(\psi/3 - 2\pi/3); \quad \zeta_2 = -2\sin(\psi/3);$$

$$\zeta_3 = -2\, sin(\psi/3 + 2\pi/3). \qquad (2.15)$$

Free energy minimum requires the expressions (2.11), (2.12), (2.13) to be zero, together with the usual conditions on the Hessian matrix. To do that one of following necessary conditons must be satisfied:

$$1)\ p_o = 0, \quad p_z = 0, \quad \Omega_z = 0; \qquad (2.16)$$

$$2)\ p_o = 0, \quad L_z = 0, \quad \Omega_z = 0; \qquad (2.17)$$

$$3)\ L_o = 0, \quad p_z = 0, \quad \Omega_z = 0; \qquad (2.18)$$

$$4)\ L_o = 0, \quad L_z = 0, \quad \Omega_z = 0; \qquad (2.19)$$

A numerical analysis in the range of parameters examined in this paper (see Figure 1) has shown that no solution comes from the condition 4). It follows that if we refer to the space of the order parameters (p_o,p_z,q_z) the minimum of f is only on the plane $p_o = 0$ or on the plane $p_z = 0$. In the case $p_o = 0$, in which the significant dipolar order parameter is p_z, the minimum will be denoted as "p_z type"; similarly in the case $p_z = 0$, the minimum will be denoted as "p_o type." For fixed values of model parameters d, η, g two possibilities must then be considered:

1) As the temperature T increases (from zero) the absolute minimum moves always on the same plane ($p_o = 0$ or $p_z = 0$) up to a critical temperature T_c, at which it falls into the axis q_z (either continuously or discontinuously).

2) As T increases (from zero) the absolute minimum moves initially on one plane (i.e. $p_z = 0$), then for a given critical temperature T^* it switches to the other plane ($p_o = 0$) and finally for a different critical temperature T_c it drops to the axis q_z. (At least in principle, one has also to consider the possibility that more than one switching from one plane to the other occurs.) At the temperature T_c an order-disorder transition takes place, while at the temperature T^* an order-order transition occurs; in latter case the dipolar order parameter changes orientation and for this reason this kind of transition may be defined as reorientation transition. In reference 6 in which only dipolar interactions were considered, the presence of

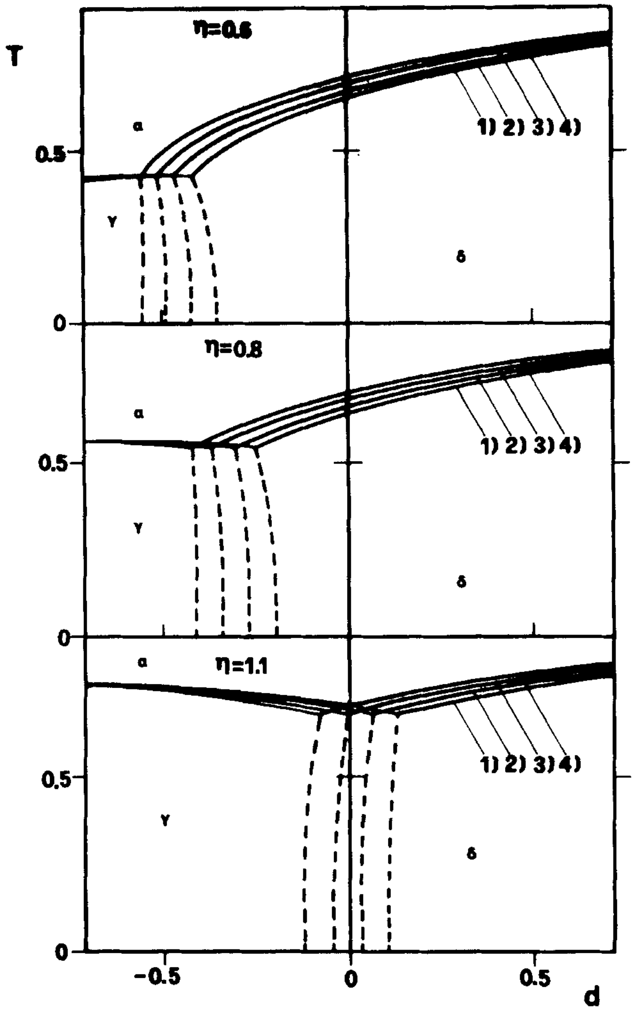

FIGURE 1 Sections (T,d) of the global phase diagram at $\eta = 0.6$, 0.8, 1.1. The lines 1),2),3),4) correspond to $g = 0$, 0.1, 0.2, 0.3 respectively. Tick lines refer to p_z critical lines, thin to p_o critical lines, broken to reorientation transition. α is a disorder region, γ a region with dipolar ordering in the plane (x,y), δ a region with dipolar ordering in the z direction.

such reorientation transitions was pointed out. Actually we want to analyze the influence of the quadrupolar interaction term on them.

3. CRITICAL BEHAVIOR

In order to determine the phase diagram we evaluate first the order-disorder critical temperatures. We have to consider separately the case $p_o = 0$ and the case $p_z = 0$.

When $p_o = 0$, the free energy becomes

$$f = \frac{1}{2}p_z^2 + \frac{1}{2}gq_z^2 - d^* + \frac{2}{3}d - \frac{1}{\beta}ln[1 + 2e^{\beta w}\cosh(\beta p_z)];$$

$$d^* = \frac{2}{3}(d_x + d_y + d_z). \quad (3.1)$$

It can be expanded in powers of p_z^2

$$f = \sum_{k=0}^{\infty} a_{2k}p_z^{2k} \quad (3.2)$$

with the coefficients a_{2k} depending in general on q_z. Assuming q_z be analytic in p_z^2, we expand q_z as power series of p_z^2, consequently

$$a_{2k} = \sum_{s=0}^{\infty} a_{2k}(s)p_z^{2s}. \quad (3.3)$$

The coefficients $a_{2k}(s)$ can be determined utilizing (2.13). We can then identify the second order critical surfaces by the relation[7] $a_2(0) = 0$, i.e.

$$1 - \beta\frac{2\exp(\beta w_o)}{1 + 2\exp(\beta w_o)} = 0 \quad \text{being} \quad \frac{2\exp(\beta w_o)}{1 + 2\exp(\beta w_o)} = \frac{w_o - d}{g}. \quad (3.4)$$

To assure the minimum, the (3.4) must then be coupled to the conditions on the second derivatives of f. As the order parameter characterizing the critical surfaces obtained from (3.4) is p_z, we denote them as "p_z critical surfaces."

The drawing of the global phase diagram of the system needs a four-dimensional space (T,d,η,g); in Figure 1 sections (T,d) of the p_z critical surfaces (thick lines) are given for significative values of the quadrupolar interaction parameter g and of the anisotropy parameter η.

We consider now the case $p_z = 0$. The free energy is

$$f = \frac{1}{2}\eta p_o^2 + \frac{1}{2}gq_z(q_z - 1) - d^* + \frac{d}{6} - \frac{1}{\beta}ln\left\{e^{bw/2} + 2\cosh\left[\frac{\beta}{2}(w^2 + 4\eta^2p_o^2)^{1/2}\right]\right\}. \quad (3.5)$$

Following the above procedure, an expansion in powers of p_o^2 is performed. The second order critical surfaces are given by

$$1 - \frac{2\eta[\exp(\beta w_o) - 1]}{w_o[1 + 2\exp(\beta w_o)]} = 0 \quad \text{being} \quad \frac{2\exp(\beta w_o)}{1 + 2\exp(\beta w_o)} = \frac{w_o - d}{g}. \quad (3.6)$$

Similarly to the previous case, these surfaces are denoted as "p_o critical surfaces." They are drawn in Figure 1 (thin lines).

In order to determine the reorientation critical surfaces one has to consider the region of the model parameters for which both the relations (2.17) and (2.18) have solutions and compare the two minima choosing the deepest. If for a fixed point of the parameter space (d,η,g) the absolute minimum is always of p_o type (or of p_z type) for all values of T, no order-order transitions are present; conversely if, varying T, the absolute minimum switches from p_o type to p_z type (or vice versa) we have a reorientation transition. The presence of this kind of transition was shown in reference 6 in the case of no quadrupolar interaction ($g = 0$). In this paper the influence of the quadrupolar interaction term is examined, considering the values $g = 0.1, 0.2, 0.3$ and comparing with the case $g = 0$. In Figure 1 dashed

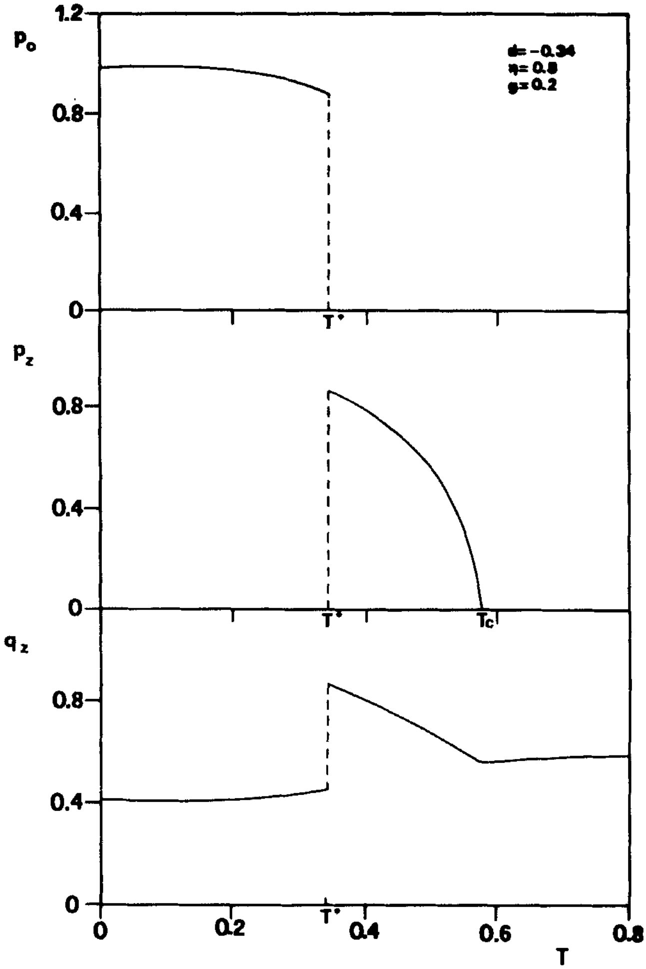

FIGURE 2 The order parameters p_o,p_z,q_z versus T in a point of the parameter space (d,η,g) characterized by reorientation transition. T^* is the order-order critical temperature, T_c the order-disorder critical temperature.

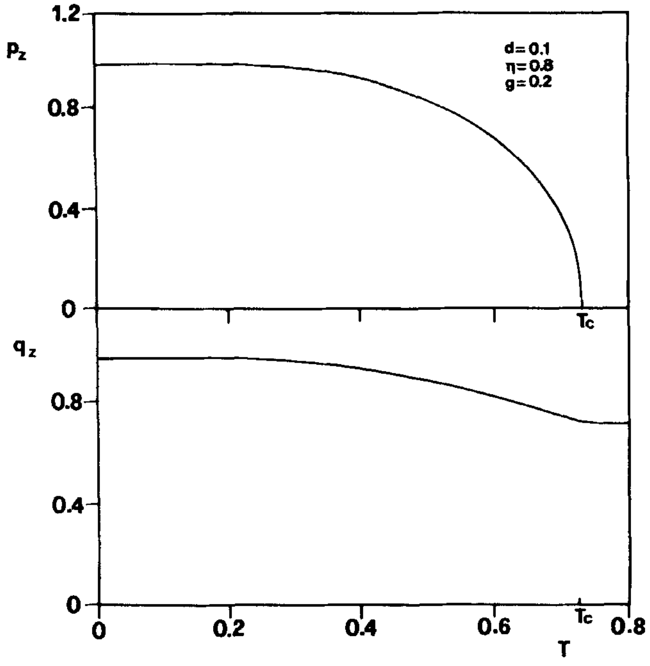

FIGURE 3 The order parameters p_z, q_z versus T (p_o is zero) for $d = 0.1$, $\eta = 0.8$, $g = 0.2$ characterized by an order-disorder transition at critical temperature T_c.

lines represent reorientation transitions. The role of the quadrupolar interaction term is to shift the region of the parameter space characterized by order-order transition to lower values of the single-ion anisotropy constant d. From a rough numerical investigation, it comes out that the presence of quadrupolar interaction seems not to modify significantly the extension of the region of the parameter space involved by reorientation transition, but only to move it in parameter space.

Figures 2 and 3 give the behavior of the order parameters p_o, p_z, q_z versus T for two typical points of the parameter space (d, η, g). In Figure 2 the case of reorientation transitions is shown. The dipolar order parameter p_o has its largest value at $T = 0$, when T increases it decreases and at T^* it goes suddenly at zero, at this same temperature T^* the dipolar order parameter p_z from zero jumps to a finite value and then as T increases it decreases becoming zero at the T_c order-disorder critical temperature. At the reorientation critical temperature T^* the dipolar ordering changes orientation from the plane (x,y) to the axis z. The quadrupolar order parameter q_z has a discontinuity at T^*, whereas it changes only slope at T_c. The case of Figure 3 refers to an usual order-disorder transition.

4. Conclusions

In this paper we have analyzed the critical properties of a quantum spin-1 model with dipolar and quadrupolar interactions and uniaxial and single-ion anisotropy terms. The presence of the anisotropy terms allow us to have reorientation transitions i.e. transitions at which the dipolar ordering changes direction. The influence of the quadrupolar interaction term on these transitions has been examined. It produces essentially a shifting of the parameter space region characterized by reorientation transitions to lower values of the single-ion anisotropy term. Work is in progress to perform a more detailed analysis of this region in order to give analytic expression of its extension.

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