Vol. 91 (1997) ACTA PHYSICA POLONICA A No. 2

Proceedings of the European Conference "Physics of Magnetism 96", Poznań 1996

MAGNETIC PROPERTIES OF THIN FILM WITH $S = 1$

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Blume–Emery–Griffiths model with single-ion anisotropy and biquadratic interactions has been applied for the description of thin magnetic films with $S = 1$. According to the Bogolyubov minimization principle, in the frame of molecular field approximation, the phase diagrams, magnetizations and quadrupolar moments in thin films have been calculated.

PACS numbers: 64.60.–i, 75.10.–b, 75.70.Ak

1. Introduction

The Blume–Emery–Griffiths (B–E–G) model for spin 1 takes into account the single-ion anisotropy and biquadratic terms [1]. When these terms are competitive to the usual bilinear exchange interactions they may lead to very interesting and varied phase diagrams. For instance, the occurrence of tricritical points, signalling the oneset of discontinuous phase transitions, as well as the existence of staggered quadrupolar phase can be predicted [2, 3].

The aim of the present paper is to study the thermodynamic properties of the B–E–G model in thin films. We will restrict ourselves to the case of a thin film with a simple cubic structure, consisting of two interpenetrating sublattices, in the molecular field approximation (MFA). We will consider only the stable solutions, for which the free energy minimizes.

2. Theory

The anisotropic B–E–G Hamiltonian in thin films is of the form

$$\mathcal{H} = -\frac{1}{2}J\sum_{\nu i,\mu j} S_{\nu i}S_{\mu j} - \frac{1}{2}A\sum_{\nu i,\mu j}(S_{\nu i}S_{\mu j})^2 - D\sum_{\nu i}(S_{\nu i})^2 - h\sum_{\nu i} S_{\nu i}, \qquad (1)$$

where by νi we denote the i-th lattice site in the ν-th layer ($\nu = 1, 2, \ldots, n$).

We introduce a trial Hamiltonian $\mathcal{H}^0$, with the scalar molecular fields for the bilinear and biquadratic parts, respectively. These fields are treated as variational parameters, characteristic for the ν-th layer and a particular sublattice. Next, we find a minimum of the Gibbs free energy with the help of Bogolyubov minimization principle

$$G(\mathcal{H}) \leq G(\mathcal{H}^0) + \langle \mathcal{H} - \mathcal{H}^0 \rangle_0. \tag{2}$$

In Eq. (2) $\langle \ldots \rangle_0$ means the statistical averaging with the trial Hamiltonian $\mathcal{H}_0$.

As a final result of minimization, we find the Gibbs potential as a function of the magnetizations $m_\nu = \langle S_{\nu i} \rangle_0$ and the quadrupolar moments $q_\nu = \langle (S_{\nu i})^2 \rangle_0$, whereas the thin film is in equilibrium.

3. Results and discussion

The phase diagrams have been obtained from the analysis of the Gibbs free energy for ferromagnetic (F), paramagnetic (P) and staggered quadrupolar (SQ) phases. As an example, the diagram calculated for the film with the thickness $n = 5$ and $D/J = -0.7$ is shown in Fig. 1. It is interesting to see in Fig. 1

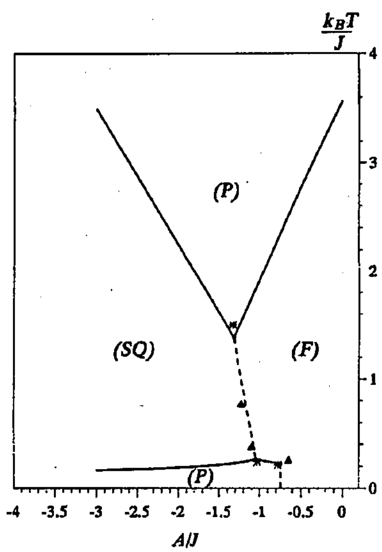

Fig. 1. Phase diagram for the thin film with $n = 5$ and $D/J = -0.7$.

that the P phase appears in some region of low temperatures, being energetically favourable. This low temperature phase does not exist in a pure B–E–G model, i.e. for $D/J = 0$ (comp. with Ref. [3]). When increasing the value of D/J we have observed that the low temperature P phase spreads up and pushes the SQ phase out. In the limiting case, for $A \to 0$, we can obtain the phase diagram of the pure Blume–Capel model, with no SQ phase present. The solid lines in Fig. 1 denote the continuous phase transitions, whereas the dashed lines stand for discontinuous ones. The points connecting the solid and dashed lines are the so-called tricritical points (TCPs) and for $n = 5$ they are marked with the square dots. It is worth noticing that changing the dimensionality of the system the phase diagram changes only quantitatively. For comparison, in Fig. 1 we denote with stars

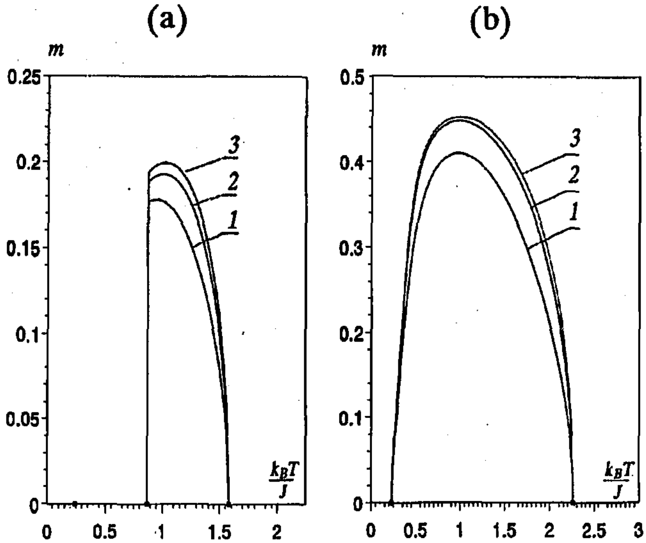

Fig. 2. Magnetization vs. temperature for the same film as in Fig. 1. (a) $A/J = -1.2$; (b) $A/J = -0.8$. Curves 1, 2 and 3 denote the surface, 2nd and 3rd layer, respectively.

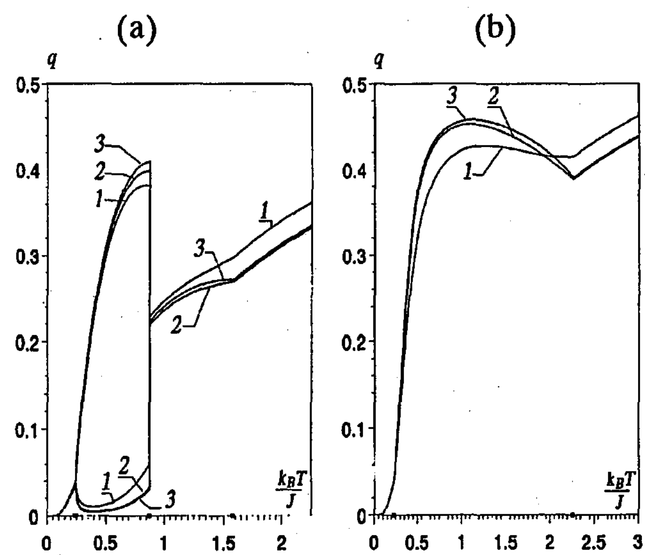

Fig. 3. Quadrupolar moment vs. temperature for the same film parameters as in Fig. 2.

the corresponding TCPs for the bulk system ($n = \infty$), whereas with triangles the TCPs positions for the 2D-monolayer ($n = 1$) are shown. With the change of D/J the position of each TCP changes, forming a trajectory in (T, A, D)-space.

As an illustration of such kind of phase diagram, the temperature dependence of magnetizations (Fig. 2) and corresponding quadrupolar moments (Fig. 3) have been plotted for the film with $n = 5$. The curves 1, 2 and 3 in both Fig. 2 and Fig. 3 correspond to the surface, second- and the third layer, respectively. Figures 2a and 3a are obtained for $A/J = -1.2$, whereas Figs. 2b and 3b are for $A/J = -0.8$. In Figs. 2a and 3a we can see a stepwise behaviour of the magnetization and quadrupolar moment, respectively, when the transition from SQ to F phase takes place. In Fig. 3a we note the splitting up of the quadrupolar moments in SQ phase into two branches, which correspond to two sublattices. In Figs. 2b and 3b only two (continuous) phase transitions are apparent between P and F phases, and the situation is then typical for the re-entrant phenomenon.

The numerical results presented in Figs. 1–3 show that the method based on the free energy analysis can be useful for studies of the thin films with $S = 1$. Other thermodynamic properties, for instance the susceptibility or specific heat can be calculated from the same expression for the free energy (in preparation).

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