Vol. A57 (1980) *ACTA PHYSICA POLONICA* No 2

SOFT PHONONS AND MAGNETIC PHASE TRANSITIONS

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(Received July 17, 1979)

A correlation between the structural and magnetic phase transitions due to the interaction of soft phonons with magnetic subsystem is discussed. On the basis of a model Hamiltonian equations for order parameters of structural and magnetic phase transitions are obtained. The possibility of magnetic transition of the type easy axis–easy plane induced by a structural transition and the appearance of a weak ferromagnetism, observed in $KMnF_3$, is considered.

1. Introduction

Recently a great attention has been paid to the investigation of magnetic crystals which undergo structural transitions. In some of them a mutual correlation between magnetic and structural transitions is observed (e.g. crystals with ferroelectric and magnetic properties [1], Jahn–Teller crystals [2], ferro- and antiferromagnets with a consecutive sequence of structural transitions, e.g. $KMnF_3$ [3]). This correlation can be explained as an effect of the interaction of a soft lattice mode describing the structural transition, with the spin subsystem. The theoretical investigations in this field, to the best of our knowledge, have principally phenomenological (e.g. [4]) or model (e.g. [5]) character. At the same time there exists the theory of structural phase transitions based on the concept of local normal coordinates [6], which reasonably describes the lattice dynamics, and the theory of the spin-phonon interaction in the highly anharmonic crystals [7], including these, which undergo structural transitions.

In the present paper we join the above mentioned two approaches and we propose a microscopic theory for description of structural and magnetic transitions with a self-

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consistent account of their mutual influence. The strictional interaction (the interaction with acoustic phonons), which plays an important role in the determination of the character of magnetic and structural phase transitions, in the present paper is not considered, although it can be also taken into account in the framework of proposed theory.

In the next Section the model Hamiltonian for the system undergoing structural and magnetic phase transitions is introduced. In Section 3, on the basis of this Hamiltonian the uniaxial ferro- and antiferromagnets are considered. In Section 4, the transition from antiferromagnetic state to the state with weak ferromagnetism, induced by a structural transition is considered and the qualitative explanation of the similar transition in $KMnF_3$ is proposed.

2. *Spin-soft phonons interaction*

We consider an insulating crystal with magnetic atoms and we assume that the potential energy of the lattice, the exchange interaction and the parameters of the crystal field depend on the instantaneous positions of atoms. Expanding these functions in Taylor series with respect to the displacements of atoms from their equilibrium positions, we obtain the Hamiltonian of magnetic crystal with spin-phonon interaction (cf. [7]). Taking further into account the soft phonons, the most important for the structural transition, we can write the Hamiltonian of the crystal in the model form

$$H = H_L + H_S + H_{LS}, \tag{1}$$

$$H_L = \tfrac{1}{2} \sum_{l\lambda, l'\lambda'} P_\lambda(l)\theta^{-1}_{\lambda\lambda'}(l, l')P_{\lambda'}(l') + \tfrac{1}{2} \sum_{l\lambda, l'\lambda'} v_{\lambda\lambda'}(l, l')Q_\lambda(l)Q_{\lambda'}(l')$$
$$+ \tfrac{1}{4} \sum_{l_1\lambda_1, \ldots, l_4\lambda_4} \Gamma_4(l_1\lambda_1, \ldots, l_4\lambda_4)Q_{\lambda_1}(l_1)Q_{\lambda_2}(l_2)Q_{\lambda_3}(l_3)Q_{\lambda_4}(l_4), \tag{2}$$

where we have introduced local normal coordinates $Q_\lambda(l)$ and their conjugated momenta $P_\lambda(l)$ for the lattice normal mode which describe local distortion in the l-th elementary cell. The parameters $\theta^{-1}_{\lambda\lambda'}(l, l')$, $v_{\lambda\lambda'}(l, l')$ and $\Gamma_4(l_1\lambda_1, \ldots, l_4\lambda_4)$ are used for the model description of the phase transition (cf. [6]).

We write the spin Hamiltonian in general form

$$H_S = \sum_{l\kappa\alpha} h^\alpha_\kappa S^\alpha_{l\kappa} + \sum_{l\kappa\alpha} K^\alpha_\kappa (S^\alpha_{l\kappa})^2 + \sum_{l\kappa\alpha, l'\kappa'\beta} D^{\alpha\beta}_{\kappa\kappa'}(l, l')S^\alpha_{l\kappa}S^\beta_{l'\kappa'} + \tfrac{1}{2} \sum_{l\kappa, l'\kappa'\alpha} J_{\kappa\kappa'}(l, l')S^\alpha_{l\kappa}S^\alpha_{l'\kappa'}, \tag{3}$$

where $S^\alpha_{l\kappa}$ is the effective spin operator for the atom of the type κ in the l-th elementary cell, $\alpha = x, y, z$. $h^\alpha_\kappa = g_\kappa \mu_\kappa \mathscr{H}^\alpha$ is the Zeeman energy. K^α_κ are the parameters of the single ion anisotropy. $D^{\alpha\beta}_{\kappa\kappa'}$ and $\mathscr{J}_{\kappa\kappa'}$ are the parameters of anisotropic and isotropic exchange interactions. For the sake of simplicity we have assumed that the crystal has noncubic symmetry (e.g. a tetragonal one) and that the effective spin of a magnetic atom $S_\kappa \geqslant 1$, so it is sufficient to take into account only the bilinear terms in the spin operators.

The terms in the magnetic energy depending on the local normal coordinates lead to the spin-phonon interaction

$$H_{LS} = \sum_{l\kappa\alpha} V^\alpha_{l\kappa}(S^\alpha_{l\kappa})^2 + \sum_{l\kappa\alpha, l'\kappa'\beta} V^{\alpha\beta}_{l\kappa, l'\kappa'}S^\alpha_{l\kappa}S^\beta_{l'\kappa'}, \tag{4}$$

where $V^{\alpha}_{l\kappa} = V^{\alpha}_{\kappa}(\{Q_\lambda(l)\})$, $V^{\alpha\beta}_{l\kappa,l'\kappa'} = V^{\alpha\beta}_{\kappa\kappa'}(\{Q_\lambda(l), Q_{\lambda'}(l')\})$ are the polynomials with respect to the variables $Q_\lambda(l)$. The explicit form of these expressions can be determined from the symmetry requirements for a specific model of the crystal. We have assumed that the coupling between lattice and spin subsystems arises due to the dependence of the crystal--field and exchange anisotropy energy on the positions of atoms and therefore on the local normal coordinates. Since the Hamiltonian is a bilinear form of the spin operators, so the time reversal symmetry requirements are fulfilled.

The Hamiltonian (1)–(4) has a quite general form which is convenient for the description of the various structural and magnetic phase transitions. To consider the most important features of the proposed model, it is sufficient to investigate only some particular cases of the Hamiltonian (1)–(4). This will be done in the next Sections.

3. The uniaxial ferro- and antiferromagnets

To describe the structural phase transition connected with lattice instability with respect to the nondegenerate soft optic mode described by one-component local normal coordinate Q_l, the Hamiltonian (2) can be written in the simple form

$$H_L = \sum_l \left\{ \frac{1}{2M} P_l^2 - \frac{A}{2} Q_l^2 + \frac{B}{4} Q_l^4 \right\} + \tfrac{1}{4} \sum_{l,l'} \varphi_{ll'} (Q_l - Q_{l'})^2, \tag{5}$$

where M is the effective mass for the soft optic mode under consideration. A, B and $\varphi_{ll'} = \varphi(l-l')$ are constants of the model which determine a character of the structural transition. In the case of displacement-type phase transition, the anharmonicity of lattice vibrations is small and $\varphi_0 = \sum_{l'} \varphi(l-l') \gg A$ [8].

In description of the magnetic phase transition we confine ourselves to the discussion of the simple model of the uniaxial ferro- or antiferromagnet with the Hamiltonian

$$H_S = \sum_{l\kappa} h_\kappa S^z_{l\kappa} - \sum_{l\kappa} K_\kappa (S^z_{l\kappa})^2 + \tfrac{1}{2} \sum_{l\kappa,l'\kappa'} J_{\kappa\kappa'}(l-l') \vec{S}_{l\kappa} \vec{S}_{l'\kappa'}, \tag{6}$$

where we will assume, that $K_\kappa > 0$. In the spin-phonon interaction, we take into account only single-ion contribution

$$H_{LS} = \sum_{l\kappa} \{ a_\kappa Q_l + \tfrac{1}{2} b_\kappa Q_l^2 \} (S^z_{l\kappa})^2 \tag{7}$$

which allows us to consider in the simplest way the mutual influence of magnetic and lattice subsystems.

First let us consider the equation for the order parameter in the structural phase transition, which is defined as the average value of the local normal coordinate

$$\eta = \langle Q_l \rangle, \quad Q_l = \eta + u_l, \tag{8}$$

where

$$\langle \ldots \rangle = \mathrm{Tr} \left\{ \ldots e^{-\frac{H}{T}} \right\} / \mathrm{Tr} \left\{ e^{-\frac{H}{T}} \right\}$$

and $H = H_L + H_S + H_{SL}$ is the total Hamiltonian (5)–(7) of the system. From the minimum condition for the free energy, we get

$$\frac{\partial F}{\partial \eta} = -T \frac{\partial}{\partial \eta} \ln \mathrm{Tr} \left\{ e^{-\frac{H}{T}} \right\} = \left\langle \frac{\partial H}{\partial \eta} \right\rangle = 0. \tag{9}$$

Next, taking into account (5)–(7) we obtain

$$-A\eta + B\langle(\eta + u_l)^3\rangle + \sum_{\kappa} (a_\kappa + b_\kappa \eta) \langle (S_\kappa^z)^2 \rangle = 0. \tag{10}$$

Neglecting the small cubic anharmonicity,

$$\langle u_l^3 \rangle / \eta \langle u_l^2 \rangle \sim (B/T)(T/\varphi_0)^2 \lesssim A/\varphi_0 \ll 1$$

and introducing the dimensionless variables

$$\xi = \sqrt{\frac{B}{A}}\, \eta, \qquad y = \frac{B}{A} \langle u_l^2 \rangle,$$

$$\bar{a} = \frac{1}{A} \sqrt{\frac{B}{A}} \sum_{\kappa} a_\kappa \langle (S_\kappa^z)^2 \rangle, \qquad \bar{b} = \frac{1}{A} \sum_{\kappa} b_\kappa \langle (S_\kappa^z)^2 \rangle, \tag{11}$$

we obtain the equation for the order parameter

$$\xi^3 = (1 - \bar{b} - 3y)\xi - \bar{a}. \tag{12}$$

As it can be seen, a nonzero solution of above equation $\xi \neq 0$ always exists, when $\bar{a} \neq 0$. The situation is similar as in the case of the system in an external field $-\bar{a}\xi$. However, in the case when $\bar{a} \ll 1$, the range of temperature $T > T_0$ exists where $\xi \ll 1$. At the same time for $T \ll T_0$, $\xi \sim 1$ and therefore we can consider T_0 as the temperature of structural phase transition. To evaluate this temperature and to determine the temperature dependence $\xi(T)$, it is necessary to consider the lattice dynamics of this model.

Introducing displacement-displacement Green function $\mathcal{D}_{ll'}(t-t') = \langle\langle u_l(t); u_{l'}(t') \rangle\rangle$ and using the standard procedure for setting up a set of equations for these functions, described for spin-phonon systems in [7], we get

$$\mathcal{D}_{ll'}(\omega) = \frac{1}{NA} \sum_{\vec{q}} e^{i\vec{q}\cdot(\vec{l}-\vec{l}')} \frac{1}{\nu^2 - (\Delta + f_0 - f_q)}, \tag{13}$$

where $\nu^2 = \omega^2/(A/M)$, $f_q = \varphi(q)/A$. $\varphi(q)$ is the spatial Fourier transform of the interaction $\varphi(l-l')$. The gap in the spectrum of soft optic mode Δ is defined by the expression

$$\Delta = 3(\xi^2 + y) - (1 - \bar{b}). \tag{14}$$

The last equation has been obtained in the lowest order of the selfconsistent phonon field approximation (cf. [7], [8]). The displacement correlation function y in (12) is defined

by the equation

$$y = \frac{B}{A}\int_0^\infty d\omega \,\mathrm{cth}\,\frac{\omega}{2T}\left[-\frac{1}{\pi}\,\mathrm{Im}\,\mathscr{D}_{ll'}(\omega+i\varepsilon)\right]$$

$$= \frac{B}{A}\,\frac{1}{NM}\sum_q \frac{1}{2\omega_q}\,\mathrm{cth}\,\frac{\omega_q}{2T}\,, \tag{15}$$

where $\omega_q^2 = (A/M)(\Delta + f_0 - f_q)$. Solving the system of selfconsistent equations (12), (14) and (15), we can determine the temperature dependence $\xi(T)$, $\Delta(T)$ and find the temperature T_0, corresponding to structural transition.

It is useful for further discussion to estimate the constants of the spin-phonon interaction $\bar{a}$ and $\bar{b}$. To do this, we assume that the crystal field energy can be estimated as follows:

$$KS^2 \sim (a\eta + \tfrac{1}{2}\,b\eta^2)S^2 \sim \varepsilon J_0 S^2,$$

where $\varepsilon = K/J_0$ is the ratio of the anisotropy energy and the exchange energy $J_0 = \sum_{l'} J(l-l')$. Assuming, that the temperature of magnetic phase transition $T_c \sim J_0 S^2$ and the temperature of structural phase transition $T_0 \sim \varphi_0(A/B)$ (cf., e.g. [8]), we get the following estimations:

$$\bar{a} \sim \bar{b} \sim \varepsilon\,\frac{J_0 S^2}{(A^2/B)} \sim \varepsilon\,\frac{T_c}{T_0}\,\frac{\varphi_0}{A}\,. \tag{16}$$

Since for the displacement-type phase transition $\varphi_0 \gg A$ [8], the constants $\bar{a}$, $\bar{b}$ will be small only for sufficiently small anisotropy, $\varepsilon \lesssim 10^{-2}$. In this case, for $T > T_0$, where T_0 is determined from the equation

$$1 - \bar{b}(T_0) - 3\{y(T_0) + [\tfrac{1}{2}\,\bar{a}(T_0)]^{2/3}\} = 0, \tag{17}$$

the values of the order parameter are small:

$$\xi(T) < \xi(T_0) = [4\bar{a}(T_0)]^{1/3}.$$

The gap in the phonon spectrum $\Delta(T)$ attains its minimum value, $\Delta_{\min}(T_1) = (3/2)[2\bar{a}(T_1)]^{2/3}$ at the temperature T_1, determined from the equation

$$y(T_1) = \tfrac{1}{3}\{1 - \bar{b}(T_1) + 3[\tfrac{1}{4}\,\bar{a}(T_1)]^{2/3}\}. \tag{18}$$

It can be noticed that $T_1 > T_0$, but for small values of $\bar{a}$ and $\bar{b}$, these temperatures are close to $T_0^{(0)}$, which is determined neglecting the spin-phonon interaction (cf. (13) and (14) for $\bar{a} = 0 = \bar{b}$).

The influence of the magnetic subsystem on the structural transition, which we have considered above, may be expected in the case $T_c > T_0$, when the parameters of interaction $\bar{a}$, $\bar{b}$ depend essentially on temperature. In the opposite case, $T_c < T_0$, it is interesting to consider the influence of structural transition on the magnetic subsystem. In this case,

we use the molecular field approximation (MFA) to describe magnetic phase transition in the system with the Hamiltonian (6), (7). We write the trial Hamiltonian in the form

$$H_{S0} = \sum_{l\kappa} \{\mathcal{M}_\kappa S^z_{l\kappa} - \tilde{K}_\kappa (S^z_{l\kappa})^2\}, \tag{19}$$

where the sublattices magnetization $\mathcal{M}_\kappa$ and effective anisotropy constant $\tilde{K}_\kappa$ are determined from Bogolubov variational principle (cf. [7])

$$\frac{\delta \mathcal{F}}{\delta \mathcal{M}_\kappa} = 0, \qquad \frac{\delta \mathcal{F}}{\delta \tilde{K}_\kappa} = 0. \tag{20}$$

In this case, the trial free energy $\mathcal{F}$ has the form

$$\mathcal{F}(T) = \mathcal{F}_0(T) + \frac{1}{N} \langle H_S + H_{SL} - H_{S0} \rangle.$$

Using (6), (7) and (19) we get

$$\mathcal{F}(T) = \mathcal{F}_0(T) + \tfrac{1}{2} \sum_{\kappa\kappa'} J_{\kappa\kappa'} \langle S^z_\kappa \rangle \langle S^z_{\kappa'} \rangle$$

$$+ \sum_\kappa (h_\kappa - \mathcal{M}_\kappa) \langle S^z_\kappa \rangle - \sum_\kappa (K_\kappa - \bar{V}_\kappa - \tilde{K}_\kappa) \langle (S^z_\kappa)^2 \rangle, \tag{21}$$

where

$$\mathcal{F}_0(T) = -T \sum_\kappa \ln \Psi_{S_\kappa} \left(\frac{\mathcal{M}_\kappa}{T}, \frac{\tilde{K}_\kappa}{T} \right), \tag{22}$$

$$\Psi_{S_\kappa}(\alpha, \beta) = \sum_{m=-S_\kappa}^{S_\kappa} \exp(-\alpha m + \beta m^2), \tag{23}$$

$$J_{\kappa\kappa'} = \sum_{l'} J_{\kappa\kappa'}(l - l'), \tag{24}$$

$$\bar{V}_\kappa = a_\kappa \langle Q_l \rangle + \tfrac{1}{2} b_\kappa \langle Q_l^2 \rangle. \tag{25}$$

Using the equations (20)–(23), we obtain following expressions for the variational parameters:

$$\mathcal{M}_\kappa = h_\kappa + \sum_{\kappa'} J_{\kappa\kappa'} \langle S^z_{\kappa'} \rangle, \tag{26}$$

$$\tilde{K}_\kappa = K_\kappa - \bar{V}_\kappa. \tag{27}$$

The magnetization $\langle S^z_\kappa \rangle$ and the mean value of square of the spin operator $\langle (S^z_\kappa)^2 \rangle$ are determined by the equations:

$$\langle S^z_\kappa \rangle = \frac{\partial \mathcal{F}_0}{\partial \mathcal{M}_\kappa}, \qquad \langle (S^z_\kappa)^2 \rangle = \frac{\partial \mathcal{F}_0}{\partial \tilde{K}_\kappa}. \tag{28}$$

As it can be seen the adopted approximation leads to the usual results of MFA, but the anisotropy constant $\tilde{K}_\kappa$ depends on temperature via the order parameter $\eta = \langle Q_l \rangle$, accord-

ing to (25) and (27). As a result an additional temperature dependence of $\langle S_\kappa^z \rangle$ and $\langle (S_\kappa^z)^2 \rangle$ arises and the renormalization of the temperature of magnetic phase transition appears.

The possibility of change of sign of the effective constant of anisotropy $\tilde{K}_\kappa(T)$, due to the temperature dependence of the order parameter $\eta(T)$, attracts a special interest. This effect may lead to the reconstruction of a whole magnetic structure of the crystal. For a ferromagnet the change of sign of the anisotropy constant leads to the transition: easy axis ($\tilde{K}_\kappa > 0$)-easy plane ($\tilde{K}_\kappa < 0$). For an antiferromagnet the last transition can be accompanied by the appearance of a weak ferromagnetism, if in the basal plane of the crystal there arises an additional anisotropic interaction. We will discuss this problem in some detail.

4. The weak ferromagnetism

In many crystals the sequence of structural and magnetic phase transitions is observed. For example, in $KMnF_3$ crystal two successive structural phase transitions at $T_1 = 186$ K and at $T_2 = 91.5$ K occur [3]. These transitions are connected with the condensation of soft phonons at the point R (the mode of the symmetry Γ_{25}) and at the point M (the mode of the symmetry M_3) of the Brillouin zone at T_1 and T_2, respectively. The condensation of these phonons corresponds to the rotations of MnF_6 octahedra around the tetragonal axis (common in both transitions) in the opposite directions in adjacent planes (mode Γ_{25}) and in the same direction (mode M_3), respectively [3]. In this crystal one observes also two consecutive magnetic phase transitions: an antiferromagnetic (AF) with the antiferromagnetic axis along the tetragonal axis at $T_N = 88.3$ K and the transition to a weak ferromagnetic state at $T_c = 81.5$ K. The proximity in the temperature scale of magnetic and structural phase transitions (at T_2) allows us to suppose that the strong influence of the structural phase transition on the character of magnetic ordering in AF phase may exist. Indeed, the rotations of MnF_6 octahedra in structural transition are connected with their deformation and with the breaking of the cubic symmetry of the crystal field. This deformation can be described as a single-ion magnetocrystal field of anisotropy, which depends on the order parameter of the corresponding phase transition. In this case a uniaxial anisotropy along z-axis appears in the temperature region $T_2 < T < T_1$, and additionally at $T < T_2$, a nonsymmetric in the basal plane field of the single-ion anisotropy arises.

For the qualitative description of the magnetic phase transition at $T < T_2$, we consider the model of two-sublattices antiferromagnet ($\kappa = 1, 2$) with the Hamiltonian (6) and the energy of the spin-phonon interaction of the form

$$H_{SL} = \tfrac{1}{2} \sum_{l\kappa} b_\kappa Q_l^2 (S_{l\kappa}^z)^2 - \sum_{l\kappa} D_\kappa [(S_{l\kappa}^x)^2 - (S_{l\kappa}^y)^2], \tag{29}$$

where for simplicity we can assume, that $b_1 = b_2 = b$ and $D_1 = -D_2 = cQ_l$. Then using MFA, we introduce the trial Hamiltonian in the simple form

$$H_{S0} = \sum_{l\kappa} \vec{\mathcal{M}}_\kappa \cdot \vec{S}_{l\kappa}. \tag{30}$$

For the free energy, analogously to (21), we get

$$\mathscr{F}(T) = \mathscr{F}_0(T) + \tfrac{1}{2}\sum_{\kappa\kappa'\alpha} J_{\kappa\kappa'}\langle S_\kappa^\alpha\rangle\langle S_{\kappa'}^\alpha\rangle + \sum_{\kappa\alpha}(h_\kappa^\alpha - \mathscr{M}_\kappa^\alpha)\langle S_\kappa^\alpha\rangle - \sum_\kappa \tilde{K}_\kappa\langle(S_\kappa^z)^2\rangle$$
$$- \sum_\kappa \tilde{D}_\kappa[\langle(S_\kappa^x)^2\rangle - \langle(S_\kappa^y)^2\rangle], \tag{31}$$

where

$$\mathscr{F}_0(T) = -T\sum_\kappa \ln \mathrm{Tr}\left[\exp\left\{-\frac{1}{T}(\vec{\mathscr{M}}_\kappa\cdot\vec{S}_\kappa)\right\}\right]. \tag{32}$$

The effective anisotropy constants are equal to

$$\tilde{K}_\kappa = K_\kappa - \tfrac{1}{2}b_\kappa\langle Q_l^2\rangle = K_\kappa - \tfrac{1}{2}b_\kappa(\eta^2 + \langle u_l^2\rangle),$$
$$\tilde{D}_1 = -\tilde{D}_2 = \tilde{D}(T) = c\eta. \tag{33}$$

The magnetization of sublattices are determined by the vector $\langle S_\kappa^\alpha\rangle = \partial\mathscr{F}_0(T)/\partial\mathscr{M}_\kappa^\alpha$, where the molecular field is evaluated from the equations

$$\mathscr{M}_\kappa^\alpha = h_\kappa^\alpha + \sum_{\kappa'} J_{\kappa\kappa'}\langle S_{\kappa'}^\alpha\rangle - \frac{\partial}{\partial\langle S_\kappa^\alpha\rangle}\{\tilde{K}_\kappa\langle(S_\kappa^z)^2\rangle + \tilde{D}_\kappa[\langle(S_\kappa^x)^2\rangle - \langle(S_\kappa^y)^2\rangle]\}. \tag{34}$$

Complete analysis of the system of equations (31)–(34) with the account of corresponding equations for the order parameter $\eta = \langle Q_l\rangle$ and for the fluctuation $\langle u_l^2\rangle$, describing structural phase transition, needs numerical calculations. For a qualitative analysis of the type of magnetic structure for $T < T_N$, we can consider the expression for the free energy (31) in the low temperature limit ($T \ll T_N$). In this case we can neglect the contribution of magnetic excitations (spin waves) and take into consideration the ground state energy only

$$\mathscr{E}_0 = \lim_{T\to 0}\mathscr{F}(T) = \frac{1}{N}\langle H_S + H_{SL}\rangle|_{T=0}. \tag{35}$$

Introducing for the sake of convenience the vectors

$$\vec{m} = \frac{1}{2S}(\langle\vec{S}_1\rangle + \langle\vec{S}_2\rangle), \quad \vec{l} = \frac{1}{2S}(\langle\vec{S}_1\rangle - \langle\vec{S}_2\rangle) \tag{36}$$

we write the ground state energy in the form

$$\mathscr{E}_0 = (\mathscr{A} - \mathscr{B})\vec{m}^2 + (\mathscr{A} + \mathscr{B})\vec{l}^2 - \beta(l_z^2 + m_z^2) - 2\gamma(l_x m_x - l_y m_y), \tag{37}$$

where we have used the following designations:

$$\mathscr{A} = (2S)^2 J_{12} > 0, \quad \mathscr{B} = -(2S)^2 J_{11} > 0,$$
$$\beta = (2S)^2 2\tilde{K} = (2S)^2 2(K - \tfrac{1}{2}b\eta^2),$$
$$\gamma = (2S)^2 2\tilde{D} = (2S)^2 2c\eta. \tag{38}$$

We have also assumed, that $K_1 = K_2 = K$. Taking into account the normalization condition (for $T \ll T_N$) $\vec{l}^2 + \vec{m}^2 = 1$, $\vec{l} \cdot \vec{m} = 0$ and introducing the angular variables determining the direction of the vectors $\vec{l}$ and $\vec{m}$, we find possible types of the ordering corresponding to the minimum of the energy (37) (cf., e.g. [9]). The calculations show, that for $\beta > 0$ the antiferromagnetic state with the vector $\vec{l}$ along z-axis and $\vec{m} = 0$ is stable. The energy of this state is given by

$$\mathscr{E}_0^{(z)} = -(\mathscr{A} + \mathscr{B} + \beta). \tag{39}$$

In the case when $\beta < 0$, the antiferromagnetic state with the vector $\vec{l}$ in the xy-plane $l_x = l_y = |\vec{l}|/\sqrt{2}$, $l_z = 0$ has lower energy. The presence of the anisotropy field γ in the basal plane leads to a weak non-collinearity of the vectors $\langle \vec{S}_1 \rangle$ and $\langle \vec{S}_2 \rangle$ and therefore to the weak ferromagnetism

$$|\vec{m}| \approx \frac{\gamma^2}{\mathscr{A}} = \frac{(2S \cdot 2\tilde{D})}{J_{12}}, \quad |\vec{l}| = \sqrt{1 - |\vec{m}|^2}. \tag{40}$$

The energy of this state is equal to

$$\mathscr{E}_0^{(x,y)} = -\left(\mathscr{A} + \mathscr{B} + \frac{\gamma^2}{\mathscr{A}}\right). \tag{41}$$

Comparing (41) with (39) we can conclude that for $(\gamma^2/\mathscr{A}) > \beta$, or with an account of (38), for the value of the order parameter

$$\eta^2(T) > \eta_c^2(T_c) = \frac{K}{(2c^2/J_{12}) + (b/2)} \tag{42}$$

the phase transition (of the first order) from the uniaxial AF state to WF state in the basal plane does occur.

Therefore, for appropriate relations between the parameters of the model, fulfilling the condition (42), the phase transition induced by the structural transition is possible. For a quantitative description of this type transition, occurring in $KMnF_3$, in the framework of proposed model it is necessary to evaluate more accurately the free energy (31), also taking into account the temperature dependence of magnetization vectors $\vec{l}(T)$, $\vec{m}(T)$ and of the order parameter $\eta(T)$ with appropriate description of the phase transition at T_2.

5. Final remarks

Model of the spin-phonon system based on concept of the local normal coordinate Q_1, proposed in the present paper allows one to consider the mutual interrelation between magnetic phase transition and structural phase transition, driven by a soft mode. The character of this coupling depends essentially on the form of the spin-phonon interaction (4) and its magnitude. In particular, an appearance of the terms linear in Q_l (cf. (7)) leads to the effective field for structural transition. However, the influence of this field is essential only for a sufficiently high magnitude of the coupling constants (16).

The reverse influence of structural transition (at T_0) on the magnetic one (at T_c) is essential only for $T_0 > T_c$ and $(T_0 - T_c) \ll T_c$. Since in the temperature range $(T_0 - T) \ll T_0$, the order parameter of the structural phase transition $\eta(T)$ strongly depends on the temperature, therefore the main change of the characteristics of the magnetic subsystem (e.g. anisotropy constants determining the type of magnetic structure) is possible. In particular, the model of the spin-phonon interaction (29) allows one to give a qualitative explanation of AF–WF transition, observed in $KMnF_3$. For a quantitative calculations and for a comparison with experimental data, it is necessary to take into account the interaction with acoustic phonons, describing lattice deformations. The latter problem will be considered elsewhere.

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