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Magneto-elastic interaction in cubic helimagnets with $B20$ structure

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Abstract

The magneto-elastic interaction in cubic helimagnets with $B20$ symmetry is considered. It is shown that this interaction is responsible for a negative contribution to the square of the spin-wave gap Δ and it alone appears to disrupt the assumed helical structure. It is suggested that competition between the positive part of Δ_I^2 , which stems from magnon–magnon interaction, and its negative magneto-elastic part leads to the quantum phase transition observed at high pressure in MnSi and FeGe. This transition has to occur when $\Delta^2 \rightarrow 0$. For MnSi it was shown using rough estimations that at ambient pressure both parts Δ_I and $|\Delta_{ME}|$ are comparable with the experimentally observed gap. The magneto-elastic interaction is responsible for $2\mathbf{k}$ modulation of the lattice where \mathbf{k} is the helix wavevector and contributes to the magnetic anisotropy. Properties of the magnetic state above the quantum phase transition are also discussed.

Experimental observation of the lattice modulation by x-ray and neutron scattering allows the determination of the strength of the anisotropic part of the magneto-elastic interaction responsible for the above phenomena and the lattice helicity.

1. Introduction

As a rule long-range magnetic order is a result of strong exchange interaction. However, real magnetic structure is determined by weak interactions which break exchange symmetry. Interplay between them can lead to quantum phase transitions (QPT) between different structures. As the simplest example we can mention cubic ferromagnets. Changing the sign of cubic anisotropy leads to rotation of the magnetization from a cubic edge to its diagonal, or vice versa [1]. At the same time the spin-wave gap depends on this sign and the spin-wave spectrum remains stable on both sides of the transition. A similar situation occurs in tetragonal antiferromagnets in a magnetic field \mathbf{H} directed at 45° to the sublattices [2]. The field rotates them and a second order QPT occurs to the state where sublattices are perpendicular to the field. The critical field for this transition is determined by $H_C = \Delta$, where Δ is the spin-wave gap at $H = 0$ and $\Delta^2(H_C) = 0$, whereas on both sides of the transition we have $\Delta^2(H) > 0$. We also mention the field induced spin-wave gap in spin chains with the Dzyaloshinskii–Moriya interaction [3].

Competition of the low-symmetry Dzyaloshinskii–Moriya interaction with other more symmetrical weak interactions under external actions can lead to some new phenomena. In this paper we study the contributions of magneto-elastic

(ME) and Dzyaloshinskii (D) [4]¹ interactions to Δ^2 in cubic helimagnets with $P2_13(B20)$ structure and assert that their competition under pressure can lead to the QPT to a disordered state discovered in MnSi by magnetization and resistivity measurements [5–7] and neutron scattering [8, 9]. Recently a similar transition was observed in FeGe [10].

Non-centrosymmetric cubic helimagnets (MnSi, FeGe, FeCoSi) have been the subject of the intensive experimental and theoretical studies for several decades. Their helical structure was explained by Dzyaloshinskii [1, 4]. The full set of interactions responsible for the observed helical structure (the Bak–Jensen model) was established later in [11, 12] in agreement with existing experimental data (see for example [13] and references therein). The following set of interactions were considered: conventional ferromagnetic exchange, Dzyaloshinskii interaction in the form

$$V_D = D \int d\mathbf{x} (\mathbf{S}(\mathbf{x}) \cdot [\nabla \times \mathbf{S}(\mathbf{x})]), \quad (1)$$

where $\mathbf{S}(\mathbf{x})$ is the spin density, anisotropic exchange and cubic anisotropy. The first two interactions can explain the helical structure and the last two fix the direction of the helix

¹ An expression for antisymmetric exchange in cubic crystals was proposed by Dzyaloshinskii [1, 4] and we call it the Dzyaloshinskii (D) interaction.

wavevector \mathbf{k} relative the crystal axes [12]. As will be shown below, the ME energy plays the same role.

The renaissance of this field began with the discovery of a quantum phase transition to a disordered (partially ordered) state in MnSi. The following properties of this state attracted particular attention: (i) non-Fermi-liquid conductivity [5–7], and (ii) a spherical neutron scattering surface with weak maxima along the $\langle 110 \rangle$ axes [7, 8], whereas at ambient pressure Bragg reflections were observed along $\langle 111 \rangle$ [13]. These features and the structure of the partially ordered state have been discussed in several theoretical papers (see [14–16] and references therein). It should be noted that a spherical scattering surface with maxima along $\langle 111 \rangle$ was observed in MnSi at ambient pressure just above the critical temperature $T_C \simeq 29$ K and explained using the Bak–Jensen model [17]. It was demonstrated that this phase transition is of first order [18] in agreement with theory (see [19] and references therein). In [17] was also shown that the spherical scattering surface is a result of the D interaction and has to be above the critical pressure in the case of QPT. We discuss this problem further in section 6.

Low T spin-wave theory of these compounds was developed recently [20, 21]. Strong anisotropy of the spin-wave spectrum at low momenta was predicted: excitations with momentum along and perpendicular to the helical wavevector \mathbf{k} have linear and quadratic dispersion, respectively. At the same time there is a contradiction between these papers. In [20] was claimed that the spin-waves are gapless Goldstone excitations due to translation invariance along the helical axis, whereas in [21] the spin-wave gap was calculated in the $1/S$ approximation. This contradiction was discussed in [22]. In brief its essence is as follows. In [20] the $1/S$ corrections to the spin-wave energy were not evaluated and translation invariance was not proved. Meanwhile, if the authors did this they would meet the problem of how to consider the Dzyaloshinskii interaction: it contains two spin operators, and if they belong to a single lattice point as in the conventional expression given by equation (1), the translation invariance holds and the gap is zero. However, this interaction always acts between different spins, the lattice cannot be ignored and the translation changes the energy of the spin pairs². This generalized D interaction was used in [21] and $\Delta_I^2 \neq 0$ was evaluated.

The existence of a gap is very important for correct description of the behavior of the helix in a magnetic field H_\perp which is perpendicular to the helical vector \mathbf{k} . In the gapless case the spin-wave spectrum becomes unstable in infinitesimal H_\perp in contradiction to the well-known experimental findings [21] and predictions of the phenomenological Landau-like theory [23]. In [21] it was shown that the helical state remains stable if $H_\perp < \Delta\sqrt{2}$ and then \mathbf{k} begins to rotate toward the field. Recently this prediction was confirmed using small angle polarized neutron scattering, and it was found that $\Delta \simeq 13$ μeV for Mn Si [24–27].

² Infinitesimal translation of two different spins along vector \mathbf{k} leads to their rotation on angle $\vec{\varphi} \parallel \mathbf{k}$. It does not change the exchange energy but add $2D \sum_{1,2} (\nabla_1 - \nabla_2) [\mathbf{S}_1(\vec{\varphi} \cdot \mathbf{S}_2) - \mathbf{S}_2(\vec{\varphi} \cdot \mathbf{S}_1)] = 2Di \sum [(\mathbf{q} \cdot \mathbf{S}_q)(\vec{\varphi} \cdot \mathbf{S}_{-q}) - (\vec{\varphi} \cdot \mathbf{S}_q)(\mathbf{q} \cdot \mathbf{S}_{-q})] \neq 0$ to the Dzyaloshinskii interaction.

In this paper we demonstrate that the magneto-elastic (ME) interaction can provide a microscopical explanation of the nature of the QPT. We evaluate its contribution to the square of the spin-wave gap Δ and demonstrate that

$$\Delta^2 = \Delta_I^2 + \Delta_{\text{ME}}^2, \quad (2)$$

where Δ_I^2 was evaluated in [21] and $\Delta_{\text{ME}}^2 < 0$ appears due to magnon–phonon interaction stipulated by the ME interaction considered as the second order perturbation. It is important to note that if Δ_I^2 is zero the ME has to disrupt the helical magnetic order. Hence we speculate that the quantum phase transition at pressure is a result of competition between these two contributions to Δ^2 and occurs when $\Delta^2 = 0$.

Rough estimations for MnSi based on existing experimental data at ambient pressure (see section 5) give $|\Delta_{\text{ME}}| \sim 7.6$ μeV and $\Delta_I = 4.0$ – 28 μeV . Both contributions are comparable with the experimental value of $\Delta \simeq 13$ μeV determined in [24]. Hence at pressure two parts of Δ^2 have to compete and the quantum phase transition occurs when $\Delta = 0$. Besides we estimated the ME contribution to the magnetic anisotropy and demonstrated that it is not small in comparison to the experimental value. We also demonstrated that the ME leads to the lattice deformation with the wavevector $2\mathbf{k}$ and evaluated intensities of corresponding super-lattice reflections. An experimental study of this would allow one to determine both the strength of the anisotropic part of the ME interaction responsible for the above mentioned phenomena and the lattice helicity. It has to be noted that the ME interaction in the Landau theory was investigated in [28, 29] and lattice deformation was predicted at the wavevector \mathbf{k} . This result does not contradict ours as it was obtained for magnetized systems only.

The paper is organized as follows. In section 2 we consider the ME in cubic helimagnets. Classical ground state energy and the lattice deformation are studied in section 3. The spin-wave–phonon interaction and the ME contribution to Δ^2 are considered in section 4. Obtained results, numerical estimations and experimental consequences are discussed in section 5. In section 6 properties of the magnetic state above the QPT are discussed. The main results are summarized in section 7. In the appendices A and B some mathematical details are considered. Appendix C is devoted to a consideration of the super-lattice reflections near forbidden $\langle n00 \rangle$ Bragg peaks with odd ns .

2. Magneto-elastic interaction

In general form the magneto-elastic energy is given by (see for example [1])

$$V_{\text{ME}} = \sum_{\mathbf{R}} S_{\mathbf{R}}^\alpha S_{\mathbf{R}}^\beta B_{\alpha\beta\gamma\mu} U_{\gamma\mu}(\mathbf{R}), \quad (3)$$

where $S_{\mathbf{R}}^\alpha$ is the spin component at the lattice point \mathbf{R} , $U_{\gamma\mu} = (1/2)(\partial u_\gamma / \partial R_\mu + \partial u_\mu / \partial R_\gamma)$ is the deformation tensor and the lattice site displacement has well-known form

$$\mathbf{u}(\mathbf{R}) = \sum e^{i\mathbf{q}\cdot\mathbf{R}} \frac{1}{\sqrt{2NM\omega_{\mathbf{q}j}}} (\mathbf{e}_{\mathbf{q}j} b_{\mathbf{q}j} + \mathbf{e}_{-\mathbf{q}j} b_{-\mathbf{q}j}^\dagger), \quad (4)$$

where $\mathbf{e}_{\mathbf{q}j}$ are vectors of the phonon polarization, $b(b^+)$ their absorption (excitation) operators and $\mathbf{e}_{-\mathbf{q}j} = \mathbf{e}_{\mathbf{q}j}^*$ [30].

Tensor B is symmetric in $(\alpha\beta)$ and $(\gamma\mu)$ components. In cubic crystals there are the following non-zero components [1]:

$$\begin{aligned} B_{xxxx} &= B_{yyyy} = B_{zzzz} = B_1, \\ B_{xyxy} &= B_{yzyz} = B_{zxzx} = B_2, \end{aligned} \quad (5)$$

and $B_{xyxy} = B_{yxxy} = B_{xyyx}$ etc. In an isotropic medium we have

$$B_{\alpha\beta\mu\nu}^{\text{is}} = B_{\text{is}}(\delta_{\alpha\mu}\delta_{\beta\nu} + \delta_{\alpha\nu}\delta_{\beta\mu})/2, \quad (6)$$

$B_1 = B_{\text{is}}$, $B_2 = B_{\text{is}}/2$ and $B_1 - 2B_2 = 0$.

In non-collinear magnetic structures each lattice spin has to be considered in its local orthogonal frame. In the case of cubic helimagnets we have [21]

$$\begin{aligned} \mathbf{S}_{\mathbf{R}} &= \mathbf{A}e^{i\mathbf{k}\cdot\mathbf{R}}(S_{\mathbf{R}}^{\zeta}\cos\alpha + iS_{\mathbf{R}}^{\eta} - S_{\mathbf{R}}^{\xi}\sin\alpha) \\ &+ \mathbf{A}^*e^{-i\mathbf{k}\cdot\mathbf{R}}(S_{\mathbf{R}}^{\zeta}\cos\alpha - iS_{\mathbf{R}}^{\eta} - S_{\mathbf{R}}^{\xi}\sin\alpha) \\ &+ \hat{c}(S_{\mathbf{R}}^{\zeta}\sin\alpha + S_{\mathbf{R}}^{\xi}\cos\alpha) \\ &= \mathbf{A}S_{\mathbf{R}}^{\mathbf{A}} + \mathbf{A}^*S_{\mathbf{R}}^{\mathbf{A}^*} + \hat{c}S_{\mathbf{R}}^{\mathbf{C}}, \end{aligned} \quad (7)$$

where \mathbf{k} is the helical wavevector, $\mathbf{A} = (\hat{a} - i\hat{b})/2$, unit vectors \hat{a} , \hat{b} and \hat{c} form a right-handed orthogonal frame, $\langle S_{\mathbf{R}}^{\zeta} \rangle = \langle S \rangle \neq 0$ is an average value of the lattice spin which does not depend on \mathbf{R} . If $\alpha = 0$ we have a planar helix with rotation around \hat{c} . For $\alpha \neq 0$ the sample is magnetized along \hat{c} . Components $S_{\mathbf{R}}^{\eta,\xi}$ describe the perpendicular spin fluctuations and are responsible for the spin-wave excitations. In [21] was shown that $\sin\alpha = -H_{\parallel}/H_C$ where H_{\parallel} is the magnetic field component along the helical vector \mathbf{k} and H_C is the critical field for transition to the ferromagnetic state. According to [21] the vector $\mathbf{k} \parallel \hat{c}$ in an arbitrary field.

Using the standard definition $\mathbf{S}_{\mathbf{q}} = N^{-1/2} \sum_{\mathbf{R}} \mathbf{S}_{\mathbf{R}}$ exp $(-i\mathbf{q} \cdot \mathbf{R})$ in momentum space we obtain [21]

$$\begin{aligned} \mathbf{S}_{\mathbf{q}} &= S_{\mathbf{q}}^{\zeta}\hat{c} + S_{\mathbf{q}}^{\mathbf{A}}\mathbf{A} + S_{\mathbf{q}}^{\mathbf{A}^*}\mathbf{A}^* \\ S_{\mathbf{q}}^{\zeta} &= S_{\mathbf{q}}^{\zeta}\sin\alpha + S_{\mathbf{q}}^{\xi}\cos\alpha, \\ S_{\mathbf{q}}^{\mathbf{A}} &= S_{\mathbf{q}-\mathbf{k}}^{\zeta}\cos\alpha - S_{\mathbf{q}-\mathbf{k}}^{\xi}\sin\alpha + iS_{\mathbf{q}-\mathbf{k}}^{\eta}, \\ S_{\mathbf{q}}^{\mathbf{A}^*} &= S_{\mathbf{q}+\mathbf{k}}^{\zeta}\cos\alpha - S_{\mathbf{q}+\mathbf{k}}^{\xi}\sin\alpha - iS_{\mathbf{q}+\mathbf{k}}^{\eta}, \end{aligned} \quad (8)$$

where $S_{\mathbf{q}}^{\zeta}$, $S_{\mathbf{q}}^{\mathbf{A}}$ and $S_{\mathbf{q}}^{\mathbf{A}^*}$ are functions of \mathbf{q} , $\mathbf{q} - \mathbf{k}$ and $\mathbf{q} + \mathbf{k}$, respectively.

The spin components in equations (8) have the well-known form

$$\begin{aligned} S_{\mathbf{q}}^{\zeta} &= N^{1/2}S\delta_{\mathbf{q},0} - (a^+a)_{\mathbf{q}}; \\ S_{\mathbf{q}}^{\eta} &= -i\sqrt{S/2}[a_{\mathbf{q}} - a_{-\mathbf{q}}^+ - (a^+a^2)_{\mathbf{q}}/2S] \\ S_{\mathbf{q}}^{\xi} &= \sqrt{S/2}[a_{\mathbf{q}} + a_{-\mathbf{q}}^+ - (a^+a^2)_{\mathbf{q}}/2S], \end{aligned} \quad (9)$$

where $a_{\mathbf{q}}$ and $a_{\mathbf{q}}^+$ are conventional spin-wave operators.

In momentum space equation (3) is given by

$$V_{\text{ME}} = N^{-1/2} \sum_{l,m=\mathbf{A},\mathbf{A}^*,\hat{c}} S_{\mathbf{q}_1}^l S_{\mathbf{q}_2}^m B U_{-\mathbf{q}_1-\mathbf{q}_2}. \quad (10)$$

This expression is divided into three parts: direct ($\hat{c}\hat{c}$ and $\mathbf{A}\mathbf{A}^*$) terms where the U tensor is \mathbf{k} independent, and first order ($\hat{c}\mathbf{A}$), ($\hat{c}\mathbf{A}^*$) and second order ($\mathbf{A}\mathbf{A}$ and $\mathbf{A}^*\mathbf{A}^*$) umklapp terms where the operator U depends on $\mathbf{q}_1 + \mathbf{q}_2 \pm \mathbf{k}$ and $\mathbf{q}_1 + \mathbf{q}_2 \pm 2\mathbf{k}$, respectively³.

In the case of uniform pressure P we have $U_{\alpha\beta} = -(P/3K)\delta_{\alpha\beta}$ where K is the bulk modulus and $U_{\mathbf{q}} \sim N^{1/2}\delta_{\mathbf{q},0}$. As a result the umklapp terms are zero as $\hat{c} \cdot \mathbf{A} = \mathbf{A} \cdot \mathbf{A} = 0$ and $V_{\text{ME}} \rightarrow -NB_1S(S+1)P/(3K)$. Hence the uniform pressure contributes to the classical part of the magneto-elastic ground state energy only and B_1 represents the isotropic part of the ME interaction. However, the pressure has to change basic parameters of the problem such as $B_{1,2}$, sound velocities etc.

For further analysis of equation (10) we use following identity:

$$\begin{aligned} mnBU_{\mathbf{Q}} &= iB_{\mathbf{A}} \sum_{p=x,y,z} m_p n_p Q_p u_p \\ &+ iB_2[(\mathbf{m} \cdot \mathbf{Q})(\mathbf{n} \cdot \mathbf{u}) + (\mathbf{m} \cdot \mathbf{u})(\mathbf{n} \cdot \mathbf{Q})], \end{aligned} \quad (11)$$

where $\mathbf{m}, \mathbf{n} = (\hat{c}, \mathbf{A}, \mathbf{A}^*)$, $B_{\mathbf{A}} = B_1 - 2B_2$ is an anisotropic part of the tensor B (see equation (6)) and $\mathbf{u} = \mathbf{u}_{\mathbf{Q}}$. As we will see below, the second order umklapps are important only for $\mathbf{Q} = 2\mathbf{k}$, $(\mathbf{m}, \mathbf{n}) \rightarrow (\mathbf{A}, \mathbf{A})$ or $(\mathbf{A}^*\mathbf{A}^*)$ and the second term is zero.

3. Ground state energy and lattice deformation

In zero magnetic field, $\sin\alpha = 0$ and we have a planar helix. Due to ME interaction it has to deform the lattice. In this case from equations (8)–(11) it follows that in the classical part of the ME interaction the first order umklapps are forbidden⁴ and we obtain

$$V_{\text{ME}} = -2iN^{1/2}S^2B_{\mathbf{A}}k[(\mathbf{g} \cdot \mathbf{u}) - \text{c.c.}], \quad (12)$$

where $g_p = A_p^2\hat{c}_p$ and $u_p = u_{-2\mathbf{k}}$.

For evaluation of the lattice deformation we must consider the elastic energy. Unlike [28, 29], for simplicity we ignore the cubic symmetry, as equation (12) is proportional to $B_{\mathbf{A}}$, i.e. this symmetry has been taken into account in the main order. In this case the unit cell elastic energy is given by [31]

$$F(\mathbf{r}) = W[U_{\alpha\beta}(\mathbf{r})U_{\beta\alpha}(\mathbf{r}) + \sigma U_{\alpha\alpha}^2(\mathbf{r})/(1-2\sigma)], \quad (13)$$

where $W = Ev_0/[2(1+\sigma)]$, v_0 is the unit cell volume and E and σ are the Young modulus and Poisson coefficient respectively. As a result we have

$$F_{2\mathbf{k}} = 2W[k^2(\mathbf{u} \cdot \mathbf{u}^*) + (\mathbf{k} \cdot \mathbf{u})(\mathbf{k} \cdot \mathbf{u}^*)/(1-2\sigma)]. \quad (14)$$

From equations (12)–(14) for the ME part of the ground state energy we obtain

$$\begin{aligned} E_{\text{ME}} &= (2NS^4B_{\mathbf{A}}^2/W)\{(\mathbf{w} \cdot \mathbf{w}^*) + (\mathbf{w} \cdot \hat{c})(\mathbf{w}^* \cdot \hat{c})/(1-2\sigma) \\ &- [(\mathbf{g} \cdot \mathbf{w}) + \text{c.c.}]\}, \end{aligned} \quad (15)$$

³ As in [21] we use term umklapp for processes mixing excitations with momenta \mathbf{q} and $\mathbf{q} \pm \mathbf{k}, \pm 2\mathbf{k}$ etc.

⁴ They are allowed in magnetized state only [28].

where $\mathbf{w} = iWk\mathbf{u}_{-2\mathbf{k}}/(B_A S^2 N^{1/2})$. Minimum of this energy is evaluated in appendix A and we have

$$E_{\text{ME}} = -\frac{NS^4 B_A^2 (1 + \sigma)}{4E v_0} \left[(G_1 - G_2) + \frac{(1 - 2\sigma)}{2(1 - \sigma)} G_2 \right] \simeq -\frac{NE v_0 g_A^2}{4} (G_1 - G_2 + G_2/2), \quad (16)$$

$$\mathbf{u}_{-2\mathbf{k}} = \frac{-2iN^{1/2} S^2 B_A (1 + \sigma)}{E v_0 k} \left[\mathbf{g}^* - \frac{(\mathbf{g}^* \cdot \hat{c}) \hat{c}}{2(1 - \sigma)} \right] \simeq -(2ig_A/k) [\mathbf{g}^* - (\mathbf{g}^* \cdot \hat{c}) \hat{c}/2], \quad (17)$$

where $g_A = S^2 B_A / E v_0$, cubic invariants $G_1 = 16(\mathbf{g} \cdot \mathbf{g}^*)$ and $G_2 = 16(\mathbf{g} \cdot \hat{c})(\mathbf{g}^* \cdot \hat{c})$ are considered in appendix A and in the right-hand side of both equations we neglect σ as it is usually small [31].

4. Magnon–phonon interaction

We now consider the magnon–phonon interaction. We are interested in terms which survive at $\mathbf{q} = 0$ and contribute to the spin-wave gap as other terms are small corrections to the \mathbf{q} -dependent part of the magnon dispersion considered in [21] and [20]. To single them out we have to replace in equation (10) one of the S^c operators by $S\delta_{\mathbf{q}\pm\mathbf{k},0}$. As a result we obtain terms with phonon momenta \mathbf{q} , $\mathbf{q} \pm \mathbf{k}$, and $\mathbf{q} \pm 2\mathbf{k}$. The former disappear at $\mathbf{q} = 0$, the second are proportional to $a_{\mathbf{q}} + a_{-\mathbf{q}}^+$ and cannot contribute to the gap (see below). Using identity (11) for the last AA and A^*A^* terms in the case of planar helix we have

$$V_{2\mathbf{k}} = -(2S)^{3/2} ik B_A \sum [(a_{\mathbf{q}} - a_{-\mathbf{q}}^+) g_p u_{-2\mathbf{k}-\mathbf{q}}^p + (a_{-\mathbf{q}} - a_{\mathbf{q}}^+) g_p^* u_{2\mathbf{k}+\mathbf{q}}^p]. \quad (18)$$

From this equation for the magnon–magnon interaction we obtain

$$V_{\text{MM}} = 2(2kS^2 B_A)^2 / S \sum (a_{\mathbf{q}} - a_{-\mathbf{q}}^+) \times \left[\sum g_p D_{pr}(\Delta, 2\mathbf{k}) g_r^* \right] (a_{-\mathbf{q}} - a_{\mathbf{q}}^+), \quad (19)$$

where D is the phonon Green function and we neglect \mathbf{q} in comparison with $\pm 2\mathbf{k}$. It can be represented as

$$D_{pr}(\omega, \mathbf{Q}) = D_t(\delta_{pr} - \hat{Q}_p \hat{Q}_r) + D_l \hat{Q}_p \hat{Q}_r, \quad (20)$$

where $\hat{Q} = \mathbf{Q}/Q$ and $D_{l(t)} = [M(\omega^2 - s_{l(t)}^2 q^2)]^{-1}$, where $l(t)$ labels the longitudinal (transverse) phonon mode and $s_{l(t)}$ is a corresponding sound velocity. We neglect optical branches, as their contribution is of order $(sk/\theta_D)^2 \ll 1$ where θ_D is the Debye temperature.

In the linear spin-wave theory the Hamiltonian is given by

$$H_{\text{SW}} = \sum [E_{\mathbf{q}} a_{\mathbf{q}}^+ a_{\mathbf{q}} + B_{\mathbf{q}} (a_{\mathbf{q}} a_{-\mathbf{q}} + a_{-\mathbf{q}}^+ a_{\mathbf{q}}^+) / 2] \quad (21)$$

and the square of the spin-wave energy $\epsilon_{\mathbf{q}}^2 = E_{\mathbf{q}}^2 - B_{\mathbf{q}}^2$. As was shown in [21] $E_0 = B_0 = Ak^2/2$ where A is the spin-wave stiffness at $q \gg k$ and we have gapless excitations. We assume that the ME interaction (19) is weak and gives small corrections

δE_0 and δB_0 to E_0 and B_0 . In this case from equations (19)–(21) for the magneto-elastic contribution to the square of the spin-wave gap we obtain

$$\Delta_{\text{ME}}^2 = Ak^2(\delta E_0 - \delta B_0) = -\frac{Ak^2(B_A S^2)^2}{2SM} \times \left(\frac{G_1 - G_2}{s_t^2} + \frac{G_2}{s_l^2} \right) \simeq -\frac{Ak^2 E v_0 g_A^2}{4S} (G_1 + G_2) \quad (22)$$

where $g_A = S^2 B_A / E v_0$ and neglecting σ we have $M s_l^2 = E v_0$ and $s_t = s_l / \sqrt{2}$. Cubic invariants $G_{1,2}$ are defined below equation (17) and analyzed in appendix A. This expression is negative as it should be in the second order perturbation theory and $\Delta_{\text{ME}}^2 = 0$ in the $\langle 100 \rangle$ direction only (see appendix A). Consideration of $\mathbf{q} \pm \mathbf{k}$ terms lead to an expression similar to equation (19) with a replacement $a - a^+ \rightarrow a + a^+$ which does not contribute to the gap, as in this case we have $\delta E_0 = \delta B_0$.

The spin-wave interaction considered in the $1/S$ approximation leads to similar corrections and gives positive part of Δ^2 [21]⁵

$$\Delta_I^2 = \frac{(Ak^2)^2}{4SN} \sum \frac{D_{\mathbf{q}}}{D_0}, \quad (23)$$

where $D_{\mathbf{q}}$ is a form-factor of the Dzyaloshinskii interaction [21]. Hence Δ^2 is sum of both contributions and we obtain equation (2)⁶.

The helical structure can be stable if

$$\Delta^2 = \Delta_I^2 + \Delta_{\text{ME}}^2 > 0 \quad (24)$$

and if $\Delta_I = 0$ it can survive at $\mathbf{k} \parallel \langle 100 \rangle$ only where $\Delta_{\text{ME}} = 0$. Meanwhile it is well known that in MnSi and FeGe at low T the helix axis $\mathbf{k} \parallel \langle 111 \rangle$ and we have $\Delta_I > |\Delta_{\text{ME}}|$. Hence if $\Delta_I^2 = 0$ instead of the helical structure there are the chiral spin fluctuations and at $T = 0$ we have the chiral spin liquid considered briefly in section 6. It has to be noted that there are critical fluctuations in the range of very small Δ^2 as in the case of conventional phase transition but their study is out of scope of the paper.

5. Experimental consequences

For discussion of the experimental consequences of the magneto-elastic interaction we have to know the Young modulus E and the anisotropic part of the ME interaction $S^2 B_A$. For MnSi the bulk modulus $K = 1.37 \times 10^6$ bar [18, 32] and neglecting the Poisson coefficient σ we obtain $E = 3K = 4.11 \times 10^6$ bar and $E v_0 = 240$ eV ($v_0 = 95 \times 10^{-24}$ cm³).

Unfortunately the value of $B_A S^2$ is unknown. As we will see below, it may be determined by x-ray and neutron scattering. The isotropic part of the ME interaction was studied by an indirect method in [33]. Its contribution to the lattice constant $\Delta a/a \simeq -1.1 \times 10^{-4}$ at $T = 0$ K was determined

⁵ As the Dyson–Maleyev interaction is non-Hermitian the $1/S$ correction appears in the aa term in equation (21) only [21].

⁶ At $H = 0$ cubic anisotropy does not contribute to Δ^2 and equations (52)–(53) in [21] are erroneous.

and the sum of the isotropic part of the ME and elastic energies can be represented as

$$B_1 S^2 (\Delta a/a) + K v_0 (3 \Delta a/a)^2 / 2. \quad (25)$$

This expression is minimal at $g_1 = S^2 B_1 / E v_0 = -3.3 \times 10^{-4}$ and from equations (15) and (22) we obtain

$$E_{\text{ME}} = -6.5 \mu\text{eV} \{56 \text{ mT}\} (g_A/g_1)^2 (G_1 - G_2/2), \quad (26)$$

$$\Delta_{\text{ME}}^2 = -(17 \mu\text{eV} \{0.15 \text{ T}\})^2 (g_A/g_1)^2 (G_1 + G_2), \quad (27)$$

where we used $S = 1.6$, $Ak^2 = H_C = 0.6 \text{ T}$ and H_C is a critical field for transition to the ferromagnetic state [21].

Let us estimate now the value of Δ_I given by equation (23). We do not know the real form of the ratio $r = D_q/D_0$ in equation (23). For $r = 1$, $Ak^2 = 0.6 \text{ T}$ and $S = 1.6$ we get a maximum value $\Delta_I^2_{\text{max}} = (0.24 \text{ T} \{27 \mu\text{eV}\})^2$. The minimum value of Δ_I^2 may be estimated assuming that in equation (23) $q_{\text{max}} = 2.4 \text{ nm}^{-1}$ is equal to a border of the Stoner continuum [34]. In this case we have $\Delta_I^2_{\text{min}} = (35 \text{ mT} \{4.1 \mu\text{eV}\})^2$.

In equation (27) for $\langle 111 \rangle$ we have $G_1 + G_2 = 4/9$ (see equation (A.5)) and $\Delta_{\text{ME}} \simeq 0.10 (g_A/g_1) \text{ T}$. So we see that at ambient pressure both contributions to the gap are comparable with the observed $\Delta \simeq 0.11 \text{ T}$ (see below). Hence we can do make a plausible assumption that the quantum phase transition at 14.6 kbar [5–8] is a result of vanishing Δ^2 . At higher pressure Δ^2 becomes negative and the helical structure is unstable (see section 6).

It is not easy to measure the spin-wave gap $\Delta \sim 10 \mu\text{eV}$ by conventional neutron spectroscopy. It was done in [24] by an indirect method using polarized neutron scattering in a magnetized sample. We outline here main idea of this method and compare corresponding results with above estimation of the ME energy.

As was shown in [21] the ground state energy of the helical structure in magnetic field is given by

$$E_G = E_A + E_{\text{ME}} - \frac{SH_{\parallel}^2}{2H_C} - \frac{SH_{\perp}^2 \Delta^2}{4H_C(\Delta^2 - H_{\perp}^2/2)}, \quad (28)$$

where $H_{\parallel(\perp)}$ is a field component along (perpendicular to) the helical wavevector \mathbf{k} , $E_A = (S^2 F_0 k^2 - 3S^4 K)L/4$ is the energy of magnetic anisotropy, F_0 and K are constants of the anisotropic exchange and cubic anisotropy, respectively [12, 21]. The cubic invariant $L = (4\mathbf{g} \cdot \hat{\mathbf{c}})$ is considered in appendix A. It should be noted that growth of the last term in equation (28) when $H_{\perp} \rightarrow \Delta\sqrt{2}$ is restricted by condition $\Delta^2/(\Delta^2 - H_{\perp}^2/\sqrt{2}) \ll (H_C/\Delta)^2$ [21].

Evolution of the helical structure in a magnetic field was studied by small angle polarized neutron scattering in MnSi near T_C [25] at low T [24] and in FeCoSi compounds [26, 27]. Two new characteristic fields were determined. In zero field the sample is in a multidomain state with \mathbf{k} along all $\langle 111 \rangle$ directions. Then for the field along one of $\langle 111 \rangle$ axes at H_{C1} the single domain state appears. With further increase in field the Bragg intensity demonstrates a cusp at H_{in} . In [24] it was interpreted as instability of the \mathbf{k} direction connected with the second term in equation (28). Indeed if H is slightly

below $\Delta\sqrt{2}$ this term predominates if $\mathbf{k} \perp \mathbf{H}$ and this vector has to rotate perpendicular to the field but is blocked by the anisotropy. Just below T_C , where the anisotropy is weak, this rotation was observed in [25]. In MnSi we have $H_{C1} \simeq 80 \text{ mT}$, $H_{\text{in}} \simeq 160 \text{ mT}$ and $\Delta \simeq 110 \text{ mT} = 13 \mu\text{eV}$ [24].

It is obvious that the single domain state can be realized if $SH_{C1}^2/2H_C \simeq 9 \text{ mT}$ is of the order of $E_A + E_{\text{ME}}$. For $\langle 111 \rangle$ directions we have $E_{\text{ME}} \simeq -25 (g_A/g_1)^2 \text{ mT}$ (see equation (A.5)). So this condition is roughly fulfilled. More detailed analysis is impossible as we do not know E_A and g_A .

The invariant L has two extrema $L = 2/3$ and 0 at \mathbf{k} along $\langle 111 \rangle$ and $\langle 100 \rangle$ directions, respectively, and a saddle points at $\langle 110 \rangle$ directions. Hence if one neglects the ME interaction the configuration with $\mathbf{k} \parallel \langle 110 \rangle$ is forbidden [12]. The same holds for maxima of the critical fluctuations above $T_C \simeq 29 \text{ K}$ [17]. Meanwhile in MnSi at high pressure above the quantum critical point $P_C \simeq 14.6 \text{ kbar}$ maxima of the neutron scattering at $\langle 110 \rangle$ directions were observed [8]. In appendix B we show that the ME interaction cannot resolve this problem, i.e. that $\langle 111 \rangle$ and $\langle 100 \rangle$ remain the only possible \mathbf{k} directions in zero magnetic field.

For more precise estimations, experimental measurements of the magneto-elastic anisotropy constant $S^2(B_1 - 2B_2)$ are important. We now demonstrate that it can be directly extracted from intensities of satellite peaks near nuclear Bragg reflections. Indeed, using equation (17) we obtain⁷

$$\delta I_{\pm}(\mathbf{K}) = (2g_A/k)^2 |\mathbf{K}_{\pm} \cdot [\mathbf{g} - (\mathbf{g} \cdot \hat{\mathbf{c}})\hat{\mathbf{c}}/2]|^2 |F(\mathbf{K}_{\pm})|^2, \quad (29)$$

where $F(\mathbf{Q})$ is the nuclear structure factor, \mathbf{K} is a reciprocal lattice point, $\mathbf{K}_{\pm} = \mathbf{K} \pm 2\mathbf{k}$ and $g_A = S^2(B_1 - 2B_2)/E v_0$. Relative satellite intensities are given by

$$\delta I_{\pm}(\mathbf{K})/I(\mathbf{K}) \simeq (2g_A/k)^2 |\mathbf{K} \cdot [\mathbf{g} - (\mathbf{g} \cdot \hat{\mathbf{c}})\hat{\mathbf{c}}/2]|^2. \quad (30)$$

In zero magnetic field vectors \mathbf{k} are along all $\langle 111 \rangle$ directions. If $\mathbf{K} \parallel \mathbf{k}$ we have $\delta I_{\pm} = 0$. If, however, $\mathbf{k} \parallel (1, 1, 1)$ but $\mathbf{K} = (2\pi n/a)(1, 1, -1)$ we obtain

$$\frac{\delta I_{\pm}}{I} = \left(\frac{4\pi n g_A}{9\sqrt{3}ka} \right)^2 = 2.2 \times 10^{-5} \left(\frac{n g_A}{g_1} \right)^2, \quad (31)$$

where we used $ka = 0.17$ [21]. For $\mathbf{K} \parallel (1, \pm 1, 0)$ this expression has to be multiplied by $1/4$.

Similar results can be obtained for other \mathbf{K} directions, with one exclusion. We are interested in crystals with $P2_13(B20)$ symmetry, where $\langle n, 0, 0 \rangle$ Bragg reflections are forbidden if n is odd and observation of very weak super-lattice reflections would be much easier⁸. Hence this case has to be considered separately. We restrict ourselves to the case $\mathbf{k} \parallel (1, 1, 1)$ only. First of all for even n we have equation (31) with the replacement $2.2 \rightarrow 2.2/4 \simeq 0.55$. For odd n the Bragg intensities of the satellites are given by

$$I_{\pm}(\mathbf{K}) = 0.55 \times 10^{-5} \left(\frac{n g_A}{g_1} \right)^2 |F_{\text{Mn}}(\mathbf{Q}) + F_{\text{Si}}(\mathbf{Q})|^2, \quad (32)$$

⁷ The equations presented below are correct if the lattice and the helical structure have the same mosaic. For MnSi the magnetic mosaic is greater than the lattice one [24] and an additional small factor has to be introduced in expressions for the relative intensities.

⁸ I am grateful to D Yu Chernyshov for providing this explanation.

where form-factors $F_j(\mathbf{Q})$ are given in appendix C. They are not zero due to $2\mathbf{k}$ modulation only and equation (32) has an additional small factor of order $(2ka)^2 \ll 1$ in comparison with the even- n case. Observation of these odd reflections provides a possibility to determine the lattice chirality (see equation (C.6)) and its connections with the spin chirality studied by polarized neutrons [13, 24–27]. It has to be noted that the lattice chirality in some cases was determined by anomalous x-ray scattering [13, 35] and electron diffraction [36].

There are six domains in a virgin sample corresponding to \mathbf{k} along $\langle 111 \rangle$ directions. In a magnetic field $H_{C1} \simeq 0.08 \text{ T} \ll H_C$ the single domain state is realized with \mathbf{k} along the field and the satellite intensity increases. However, further increase in the field suppresses the helical structure and it disappears at $H_C \simeq 0.6 \text{ T}$ [24]. In the intermediate region at $H_{C1} < H < H_C$ the lattice modulation with the wavevector \mathbf{k} also appears [28]. Along with the discussed $2\mathbf{k}$ lattice modulation at low field $H < \Delta\sqrt{2}$ the second order helical harmonic appears [21]. This was observed in [24, 37].

6. Beyond QPT

This paper is not devoted to an analysis of the paramagnetic state above QPT. According to [7, 8] this has a very complex structure. We present here a short and very preliminary consideration of this problem using the mean-field approach which is not applicable very close to the critical pressure P_C . However, it tackles correctly the symmetry of the problem.

It is a natural assumption that just below the critical pressure we have

$$\Delta^2 = \Delta_0^2(-x), \quad (33)$$

where $x = (P - P_C)/P_C$. Above P_C we can write the effective action density in the form similar to the free energy in [17]

$$S_{\mathbf{q}} = \left[\frac{A}{2S} (q^2 + \kappa_0^2) \delta_{\alpha\beta} + iD \epsilon_{\alpha\beta\gamma} q_\gamma \right] S_{\mathbf{q}}^\alpha S_{-\mathbf{q}}^\beta + \frac{F_0}{2} (q_x^2 |S_{\mathbf{q}}^x|^2 + q_y^2 |S_{\mathbf{q}}^y|^2 + q_z^2 |S_{\mathbf{q}}^z|^2), \quad (34)$$

where the first term describes ferromagnetic fluctuations, the second is the D interaction and the last one is the anisotropic exchange which is very small. Similar action without the F_0 term has been used in [14]. We restrict ourselves here to the simplest form of cubic anisotropy as we have seen above that other contributions do not change the final results. We assume that in this equation the non-renormalized square of the inverse correlation length $\kappa_0^2 = Cx_0$, where $C \sim \Delta_0^2/(Ak^2)$, has the correct dimensionality, $x_0 = (P - P_{C0})/P_{C0}$ and P_{C0} is the non-renormalized critical pressure. By the same way as in [17], above T_C (see also [14]) for static susceptibility we obtain⁹

$$\chi_{\alpha\beta}(\mathbf{q}) = \left\{ S[(q^2 + k^2 + \kappa_1^2) \delta_{\alpha\beta} + 2ikq(D/|D|) \epsilon_{\alpha\beta\gamma} \hat{q}_\gamma - (2qk)^2 \hat{q}_\alpha \hat{q}_\beta / (q^2 + k^2 + \kappa_1^2)] \right\} \left\{ A[(q+k)^2 + \kappa_1^2] \times \{(q-k)^2 + \kappa_1^2 + 4q^4 k^2 (SF_0 \{\hat{q}^4\} / A) (q^2 + k^2 + \kappa_1^2)^{-1} \times [(q+k)^2 + \kappa_1^2]^{-1} \} \right\}^{-1} \quad (35)$$

⁹ In [17] signs of the terms linear in D and F have to be changed. The wrong sign is given in the definition of κ_1^2 below equation (5) in [17] also.

where $k = |SD|/A$ is the pitch of the helix, renormalized $\kappa_1^2 = \kappa_0^2 - k^2 = C(P - P_1)/P_1$ with $P_1 = P_{C0} + k^2/C$, $\hat{q} = \mathbf{q}/q$ and $\{\hat{q}^4\} = \hat{q}_x^4 + \hat{q}_y^4 + \hat{q}_z^4$ is a cubic invariant responsible for anisotropy of the critical fluctuations. In the numerator the first term is responsible for isotropic part of the susceptibility, and the second and the last one are chiral and longitudinal contributions, respectively.

The chiral term in the static susceptibility is a result of the D interaction in which the Dzyaloshinskii vector does not change sign under time reflection [21]. This interaction appears due to non-centrosymmetric lattice structure and the very existence of the chiral spin fluctuations cannot depend on the pressure. Hence the magnetic state at $T = 0$ and $P > P_C$ can be considered as the chiral spin liquid.

The expression for the ω -integrated neutron scattering is given by

$$\frac{d\sigma}{d\Omega} \sim \frac{q^2 + k^2 + \kappa_1^2 + 2k(D/|D|)(\mathbf{q} \cdot \mathbf{P})}{[(q+k)^2 + \kappa_1^2][(q-k)^2 + \kappa_1^2 + Fk^2\{\hat{q}^2\}/(2A)]}, \quad (36)$$

where \mathbf{P} is the neutron polarization and in the small F_0 term we put $q = k$ and neglect κ_1^2 . Completely neglecting the F_0 term we obtain that the scattering intensity is maximal on the sphere with $q = k$, as was observed in [8]. The invariant $\{\hat{q}^4\}$ has extrema at \mathbf{q} along $\langle 111 \rangle$ and $\langle 100 \rangle$ directions equal to $1/3$ and unity, respectively [12], and the scattering is maximal along one of these directions depending on the sign of F_0 . For example, if $F_0 > 0$ the maxima occur along the cubic diagonals and the second factor in the denominator has to be represented as

$$(q-k)^2 + \kappa^2 + (SF_0 k^2 / 2A) (\{\hat{q}^4\} - 1/3), \quad (37)$$

where $\kappa^2 = Cx$, $x = (P - P_C)/P_C$ and $P_C = P_1 + SF_0 k^2 / (6AC)$ is the mean-field critical pressure (cf [17]). Unfortunately we have here a disagreement with experiment where the intensity maxima were observed along $\langle 110 \rangle$ [8]. As was explained above, other anisotropic interactions with cubic symmetry cannot resolve this problem.

The last term in the numerator gives the chiral contribution to the cross section which is proportional to neutron polarization. This part depends on the sign of the D interaction and the angle between \mathbf{q} and \mathbf{P} . As a result, depending on the \mathbf{P} direction the scattering may be increased or suppressed as was observed in MnSi just above T_C [17].

7. Conclusions

We considered the magneto-elastic interaction in cubic helimagnets with $B20$ structure and demonstrated that it deformed the lattice and gave a negative contribution to the square of the spin-wave gap Δ^2 . Hence the helical structure is stabilized due to a positive contribution to Δ^2 which stems from the magnon–magnon interaction [21]. It was suggested that the quantum phase transition observed at pressure in MnSi and FeGe is a result of competition between these two parts of the gap and takes place when $\Delta^2 = 0$. This suggestion is supported by rough estimations at ambient pressure of both contributions to Δ^2 for MnSi which have the same order and are close to experimentally observed gap. It was also

discussed how to measure directly the anisotropic part of the ME interaction responsible for the considered phenomena using x-ray and neutron scattering. Section 6 gave preliminary discussion of the partly disordered state at pressures above the QPT and polarized neutron scattering in it. It was suggested that in this state we are dealing with a chiral spin liquid.

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Appendix A

In this appendix we calculate the deformation of the lattice by the ME interactions, cubic invariants $G_{1,2}$ and L and analyze their properties.

We begin with the classical energy (15). It is minimal if

$$w_p + (\mathbf{w} \cdot \hat{c})\hat{c}_p / (1 - 2\sigma) = g_p^*, \quad (\text{A.1})$$

where $p = x, y, z$ and $g_p = A_p^2 \hat{c}_p$ and we have

$$w_p = g_p^* - (\hat{c} \cdot \mathbf{g}^*)\hat{c}_p / [2(1 - \sigma)],$$

$$E_{\text{ME}} = -(2NS^4 B^2 / Q)[(\mathbf{g} \cdot \mathbf{g}^*) - (\mathbf{g} \cdot \hat{c})(\hat{c} \cdot \mathbf{g}^*) / (1 - \sigma)] \quad (\text{A.2})$$

where $16(\mathbf{g} \cdot \mathbf{g}^*) = G_1$ and $16(\mathbf{g} \cdot \hat{c})(\hat{c} \cdot \mathbf{g}^*) = G_2$.

In the cubic xyz frame we can write

$$\begin{aligned} \hat{a} &= (\cos \vartheta \cos \varphi, \cos \vartheta \sin \varphi, -\sin \vartheta); \\ \hat{b} &= (\sin \varphi, -\cos \varphi, 0); \\ \hat{c} &= (\sin \vartheta \cos \varphi, \sin \vartheta \sin \varphi, \cos \vartheta), \end{aligned} \quad (\text{A.3})$$

and for three principal \mathbf{k} -directions $\langle 111 \rangle, \langle 110 \rangle,$ and $\langle 100 \rangle$ we have: $\{\hat{a} = (1/\sqrt{6}, 1/\sqrt{6}, -\sqrt{2/3}); \hat{b} = (1, -1, 0)/\sqrt{2}; \hat{c} = (1, 1, 1)/\sqrt{3}\}, \{\hat{a} = (0, 0, -1); \hat{b} = (1, -1, 0)/\sqrt{2}; \hat{c} = (1, 1, 0)/\sqrt{2}\},$ and $\{\hat{a} = (0, 0, -1); \hat{b} = (0, -1, 0); \hat{c} = (1, 0, 0)\},$ respectively.

In this representation for G -functions we obtain

$$\begin{aligned} G_1 &= \sin^2 \vartheta [(\cos^2 \vartheta \cos^2 \varphi + \sin^2 \varphi)^2 \cos^2 \varphi \\ &\quad + (\cos^2 \vartheta \sin^2 \varphi + \cos^2 \varphi)^2 \sin^2 \varphi + \sin^2 \vartheta \cos^2 \vartheta] \\ G_2 &= \sin^4 \vartheta \{[\cos^2 \vartheta (1 + \sin^4 \varphi + \cos^4 \varphi) + 2 \sin^2 \varphi \cos^2 \varphi]^2 \\ &\quad + 4(\sin^2 \varphi - \cos^2 \varphi)^2 \cos^2 \vartheta \sin^2 \varphi \cos^2 \varphi\}. \end{aligned} \quad (\text{A.4})$$

From these equations follows that functions $G_1 - G_2$ and G_2 have extrema at $\langle 111 \rangle, \langle 110 \rangle$ and $\langle 100 \rangle,$ near which we have

$$\begin{aligned} G_1 - G_2 &= 4/9 - 20\delta\vartheta^2/9 - 40\delta\varphi^2/27; \\ G_2 &= 8\delta\vartheta^2/9 + 16\delta\varphi^2/27, \langle 111 \rangle; \\ G_1 - G_2 &= 13\delta\vartheta^2/4 + \delta\varphi^2; \\ G_2 &= 1/4 - 2(\delta\vartheta^2 + \delta\varphi^2), \langle 110 \rangle; \\ G_1 - G_2 &= \delta\vartheta^2 + \delta\varphi^2; \\ G_2 &= 4(\delta\vartheta^4 + \delta\varphi^4 + \delta\vartheta^2\delta\varphi^2), \langle 100 \rangle, \end{aligned} \quad (\text{A.5})$$

where $\delta\vartheta$ and $\delta\varphi$ are distances from corresponding extremal points. Hence in the considered directions both functions $G_1 - G_2$ and G_2 have extrema and one can show that they have no other extrema.

The contribution of the anisotropic exchange and cubic anisotropy to the classical energy is proportional to cubic invariant L given by [21]

$$\begin{aligned} L &= 4 \sum |A_p|^2 \hat{c}_p^2 = \sin^2 \vartheta [(\cos^2 \vartheta \cos^2 \varphi + \sin^2 \varphi) \cos^2 \varphi \\ &\quad + (\cos^2 \vartheta \sin^2 \varphi + \cos^2 \varphi) \sin^2 \varphi + \cos^2 \vartheta]. \end{aligned} \quad (\text{A.6})$$

As above, for the three principal directions we have

$$\begin{aligned} L &= 2/3 - 4\delta\vartheta^2/3 - 8\delta\varphi^2/9, \langle 111 \rangle; \\ 1/2 + \delta\vartheta^2 - 2\delta\varphi^2, \langle 110 \rangle; \quad &2(\delta\vartheta^2 + \delta\varphi^2), \langle 100 \rangle, \end{aligned} \quad (\text{A.7})$$

and L has a saddle point at $\langle 110 \rangle.$

Appendix B

We demonstrate now that in the presence of the ME contribution to the ground state energy $\langle 111 \rangle$ and $\langle 100 \rangle$ remain the only possible stable directions for the vector $\mathbf{k}.$

From equations (26) and (28) at $\mathbf{H} = 0$ it follows

$$E_G = \Phi L - \Psi(G_1 - G_2 + G_2/2) = \Psi f(y), \quad (\text{B.1})$$

where $\Psi > 0$ and $y = \Phi/\Psi.$

We have to study the behavior of $f(y)$ for three principal directions. For $\mathbf{k} \parallel \langle 111 \rangle$ we obtain

$$f(y) = (2/3)(y-2/3) + (4/3)(-y+4/3)(\delta\vartheta^2 + 2\delta\varphi^2) \quad (\text{B.2})$$

and E_G is stable if $\Phi < 4\Psi/3.$ In the $\langle 110 \rangle$ case we have

$$f(y) = (1/2)(y - 1/4) + (y - 9/4)\delta\vartheta^2 - 2y\delta\varphi^2. \quad (\text{B.3})$$

In this configuration there is a saddle point as coefficients at deviations $\delta\vartheta^2$ and $\delta\varphi^2$ cannot be positive simultaneously. Finally, if $\mathbf{k} \parallel \langle 100 \rangle$ we have

$$f(y) = 2(y - 1/2)(\delta\vartheta^2 + \delta\varphi^2). \quad (\text{B.4})$$

This configuration is stable if $\Phi > \Psi/2.$ However, comparing equations (B.2) and (B.4) we see that in the region $\Psi/2 < \Phi < \Psi/3$ the configuration $\langle 111 \rangle$ has the lower energy and the $\langle 100 \rangle$ configuration is metastable. Hence we see that the magneto-elastic energy cannot be responsible for the stability of the $\langle 110 \rangle$ configuration.

Appendix C

There are two different ions in compounds with $P2_13$ symmetry (Mn and Si; Fe and Ge etc) labeled below as 1 and 2, respectively. Each of them occupy four positions in the cubic unit cell: $\rho_1 = (x, x, x)$, $\rho_2 = (1/2 + x, 1/2 - x, 1 - x)$, $\rho_3 = (1 - x, 1/2 + x, 1/2 - x)$ and $\rho_4 = (1/2 - x, 1 - x, 1/2 + x)$ (right-handed structure) or $\rho_1 = (x, x, x)$, $\rho_2 = (1/2 - x, 1/2 + x, 1 - x)$, $\rho_3 = (1/2 + x, 1 - x, 1/2 - x)$, and $\rho_4 = (1 - x, 1/2 - x, 1/2 + x)$ (left-handed structure) [13]. For MnSi we have $x_1 = 0.138$ (Mn) and $x_2 = 0.846$ (Si). It is interesting to note that these numbers are very close to the ion positions in an 'ideal' $B20$ structure with $x_1 = 1/4\tau = 0.1545$ and $x_2 = 1 - x_1 = 0.8455$ where $\tau = (1 + \sqrt{5})/2$ [38].

We consider below the odd- n case only. As we have two different ions in the unit cell the total structure factor is a sum $F(\mathbf{Q}) = F_1(\mathbf{Q}) + F_2(\mathbf{Q})$ where

$$F_j(\mathbf{Q}) = f_j(\mathbf{Q}) \sum e^{i(\mathbf{Q} \cdot \rho_k(x_j))} \quad (\text{C.1})$$

and $f_j(\mathbf{Q})$ is a scattering amplitude for the j ion.

There are eight super-lattice reflections corresponding to $\mathbf{Q}_1 = (2\pi n + \kappa, \kappa, \kappa)$, $\mathbf{Q}_2 = (2\pi n - \kappa, \kappa, \kappa)$, $\mathbf{Q}_3 = (2\pi n + \kappa, -\kappa, \kappa)$, and $\mathbf{Q}_4 = (2\pi n + \kappa, \kappa, -\kappa)$ where $\kappa = \pm 2ka/\sqrt{3}$. Corresponding partial form-factors are given by

$$F_R(\mathbf{Q}_1) = F_L(\mathbf{Q}_1) = f e^{2\pi i n x} [e^{3i\kappa x} - e^{i\kappa(2-x)}] \simeq i f \kappa (4x - 2) e^{2\pi i n x}, \quad (\text{C.2})$$

$$F_R(\mathbf{Q}_2) = F_L(\mathbf{Q}_2) = f \{ e^{2\pi i n x} [e^{i\kappa x} - e^{i\kappa(1-3x)}] + e^{-2i\pi n x} [e^{i\kappa x} - e^{i\kappa(1+x)}] \} \simeq i f \kappa [(4x - 1) e^{2\pi i n x} - e^{-2\pi i n x}], \quad (\text{C.3})$$

$$F_R(\mathbf{Q}_3) = F_L(\mathbf{Q}_4) = f \{ e^{2\pi i n x} [e^{i\kappa x} - e^{i\kappa(1+x)}] + e^{-2\pi i n x} [e^{i\kappa(1-3x)} - e^{i\kappa x}] \} \simeq i f \kappa [-e^{2\pi i n x} + (1 - 4x) e^{-2\pi i n x}], \quad (\text{C.4})$$

$$F_R(\mathbf{Q}_4) = F_L(\mathbf{Q}_3) = f e^{-2\pi i n x} [e^{i\kappa(1+x)} - e^{i\kappa(1-3x)}] \simeq 4 f i \kappa x e^{-2\pi i n x}. \quad (\text{C.5})$$

From equations (C.4), (C.5) follows the intensity ratio

$$\frac{I_R(\mathbf{Q}_3)}{I_R(\mathbf{Q}_4)} = \frac{I_L(\mathbf{Q}_4)}{I_L(\mathbf{Q}_3)}, \quad (\text{C.6})$$

and from measurement of the $2k$ lattice deformation one can determine the lattice chirality.

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