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The magnetic structure of MnSi under an applied field

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Abstract

Below $T_C = 29$ K the weak itinerant ferromagnet MnSi becomes ordered in a left-handed spin helical structure as a result of the Dzyaloshinskii–Moriya (DM) interaction. We give a recipe for calculating the orientation of the helix under an applied field. The recipe is derived on a basis of a theory recently developed for cubic magnets with DM interaction. The theory evaluates the ground state energy and the spin wave spectrum. It is shown that in zero field the orientation of the helix depends solely on the anisotropic exchange interaction and cubic anisotropy. Under an applied field the helix possesses two types of magnetic susceptibility: one parallel and another perpendicular to the applied magnetic field. The perpendicular susceptibility is related to the fact that the helical structure itself is unstable with respect to the small magnetic field **H** applied perpendicularly to the wavevector **k**. The spin wave gap Δ provides the stability of the spin wave spectrum of the helix structure and its presence may be revealed in the magnetic field behaviour. Our calculations show the essence of the field-induced transformations of the magnetic structure related to the spin wave gap. The experimental data provide the evidence for its existence. On the basis of our findings we discuss a possible scenario for the quantum phase transition in MnSi.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

Below $T_C = 29$ K the weak itinerant ferromagnet MnSi becomes ordered in a left-handed spin helical structure with a propagation vector $2\pi/a(\xi, \xi, \xi)$ with $\xi = 0.017$ [1, 2]. The helicity is realized by an antisymmetric Dzyaloshinskii–Moriya (DM) exchange interaction caused by the lack of a centre of symmetry in the Mn atomic arrangement [3–5]. This DM interaction is isotropic itself, but anisotropic exchange (AE) and cubic anisotropy fix a direction of the magnetic spiral below T_C along the cube diagonals $\langle 111 \rangle$. The magnetic

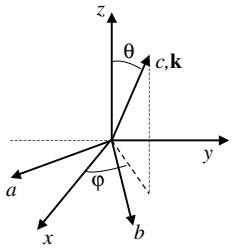

Figure 1. Mutual displacement of two coordinate systems: crystallographic frame with axes (x, y, z) along the edges of the cube, and systems related to the helix $\hat{a}, \hat{b}$ and $\hat{c}$ with $\hat{c}$ being parallel to the helix wavevector **k** and $\hat{a}, \hat{b}$ being in the plane perpendicular to $\hat{c}$.

properties of MnSi have attracted much attention in recent years because of the discovery of a quantum phase transition (QPT) to a magnetically disordered state, which is easily reached under applied pressure. As was found in [6–8] the magnetic transition temperature T_C decreases with increasing pressure and the magnetic ordering disappears at $T = 0$ and a critical pressure of $P_C \approx 14.6$ kbar. Accounting for the fact that the applied critical pressure changes the value of the effective moment insignificantly [9], one has to suppose that the magnetic system is close to ferromagnetic instability.

In this paper we show that the magnetic field susceptibility of the helix in MnSi has two components: perpendicular and parallel to the magnetic field. We demonstrate that the perpendicular susceptibility is caused by the presence of a small spin wave gap providing stability of the magnetic system with respect to the magnetic field perpendicular to the helix wavevector **k**. In our view the spin wave gap may become a source of ferromagnetic instability, and in conclusion we propose a scenario for the quantum phase transition under applied pressure.

2. Helix structure and its orientation at zero field

A theory was recently developed to describe the properties of a cubic helical magnet with DMI [10]. In this theory the following interactions are taken into account: conventional isotropic exchange, DM interaction D, AE interaction F, cubic anisotropy K and Zeeman energy. The ground state energy and the spin wave spectrum were evaluated. It is well known [3–5] that DM interaction is responsible for a magnetic helix structure with the wavevector

$$k = SD/A, \tag{1}$$

where D is the strength of the DM interaction and A is the spin wave stiffness at large momenta.

In cubic crystals the DM interaction fixes the sense of the helix (right or left handed) but cannot determine its direction. Weak anisotropic interactions determine the orientation of the helix in zero field. The classical energy for them is given as [10]:

$$E_{\text{an}} = \frac{S^2 F k^2}{4} \sum_{i=x,y,z} \hat{c}_i^2(\hat{a}_i^2 + \hat{b}_i^2) + \frac{3S^4 K}{8} \sum_{i=x,y,z} (\hat{a}_i^2 + \hat{b}_i^2)^2 \tag{2}$$

where the first term is the anisotropic exchange contribution and the second term is cubic anisotropy. $\hat{a}, \hat{b}$ and $\hat{c}$ are mutually perpendicular unit vectors describing the helix: $\hat{c}$ is parallel to the helix wavevector **k** and $\hat{a}, \hat{b}$ are in the plane perpendicular to $\hat{c}$ (figure 1). It can be shown that

$$\sum_{i=x,y,z} \hat{c}_i^2(\hat{a}_i^2 + \hat{b}_i^2) + \sum_{i=x,y,z} (\hat{a}_i^2 + \hat{b}_i^2)^2 = 2. \tag{3}$$

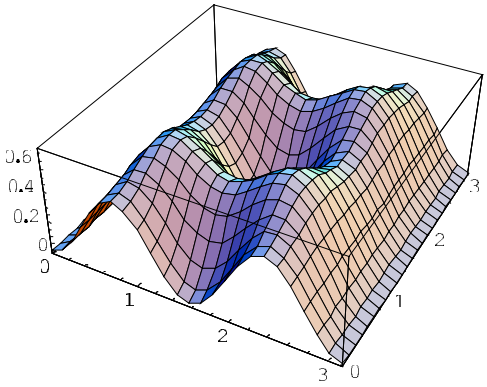

Figure 2. Two-dimensional surface of the angle-dependent factor L of the anisotropic energy $E_{\rm an}$ as a function of the angles θ and ϕ.

Then the anisotropic energy (equation (2)) is rewritten as:

$$E_{\rm an} = \left(\frac{S^2Fk^2}{4} - \frac{3S^4K}{8}\right)\sum_{i=x,y,z}\hat{c}_i^2(\hat{a}_i^2 + \hat{b}_i^2) + \frac{3S^4K}{4}. \tag{4}$$

Vectors $\hat{a}, \hat{b}, \hat{c}$ are related to the coordinate system of the crystallographic unit cell through angles θ and ϕ varying in intervals $(0, \pi)$ and $(0, 2\pi)$, respectively:

$$\begin{aligned} &\hat{c} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta) \qquad \hat{a} = (\sin\phi, -\cos\phi, 0) \\ &\hat{b} = (\cos\theta\cos\phi, \cos\theta\sin\phi, -\sin\theta). \end{aligned} \tag{5}$$

Thus, equation (4) may be represented as

$$E_{\rm an}(\theta,\phi) = \frac{1}{2}\left(S^2Fk^2 - \frac{3S^4K}{2}\right)\sin^2\theta(\cos^2\theta + \sin^2\theta\sin^2\phi\cos^2\phi) + \text{const}. \tag{6}$$

Figure 2 shows a two-dimensional surface for the angle-dependent factor L in equation (6) as a function of angles θ and ϕ, where due to ϕ-evenness we restrict the interval to $0 < \phi < \pi$. One can see from equation (6) and figure 2 that the function L has minima at (i) $\theta = 0, \pi$ and all ϕ, (ii) $\theta = \pi/2$ and $\phi = 0, \pi/2, \pi$, maxima at $\theta = \arccos(1/\sqrt{3}) \simeq 33°, \pi - \arccos(1/\sqrt{3})$ and $\phi = \pi/4, 3\pi/4$ and saddle points at (i) $\theta = \pi/2$ and $\phi = \pi/4, 3\pi/4$; (ii) $\theta = \pi/4, 3\pi/4$ and $\phi = 0, \pi/2, \pi$. In all minima we have $L = 0$ and in maxima $L = 1/3$. It is easy to see that if the prefactor in equation (6) is positive the helix vector $\boldsymbol{k}$ is directed along one of cubic edges as in Fe Ge in a high temperature phase [11]; otherwise it is along the cubic diagonals as in Mn Si [1, 2]. If this factor is close to zero or varies locally the helix is randomly oriented (Fe_x Co_{1-x} Si case [12]).

3. Effect of the magnetic field on helix orientation

If the magnetic field is applied along the helix axis $\mathbf{H} \parallel \mathbf{k}$ the classical energy depends on the product of $H_\parallel$ and the mean spin induced by the field, $S\sin\alpha$, where α is the inclination angle of the spin driven out of the plane perpendicular to $\mathbf{k}$ by the external field and determined by $\sin\alpha \simeq -H_\parallel/H_{C2}$ for $H < H_{C2}$ and $\sin\alpha = -1$ for $H > H_{C2}$ and H_{C2} is the critical field for the transition from the conical spin state to the ferromagnetic spin state. The critical field is determined through the major interactions as [10]:

$$g\mu_B H_{C2} = h_c = Ak^2 + SFk^2/3 \approx Ak^2. \tag{7}$$

From equations (1) and (7) one can estimate the major interaction of the system such as the high-momentum spin wave stiffness A and the DM constant D.

In the case of a magnetic field that is not parallel to the helix axis the field-dependent part of the ground state energy is given by [10]:

$$E_{\mathrm{h}} = -\frac{Sh_{\parallel}^2}{2h_{\mathrm{c}}} - \frac{Sh_{\perp}^2\Delta^2}{2h_{\mathrm{c}}(1+\cos^2\alpha)[\Delta^2 - (h_{\perp}^2/2)\cos^4\alpha]}. \tag{8}$$

Here $h_{\parallel}, h_{\perp}$ are the components of the magnetic field h parallel or perpendicular to the helix wavevector $\mathbf{k}$. The first term of this expression is the magnetic part of the classical energy mentioned above. The second term describes the interaction of the field, perpendicular to the helix vector, with the helix itself. Here the presence of the positive spin wave gap Δ is postulated, because otherwise the magnetic subsystem is unstable with respect to an infinitely small perpendicular magnetic field. According to experimental data [11, 13], the helix rotates toward the field direction at $g\mu H \ll h_{\mathrm{c}} = Ak^2$. Thus we can put $\cos^2\alpha \simeq 1$ and obtain from equation (8):

$$E_{\mathrm{h}} = -\frac{Sh^2}{2Ak^2}\left[\cos^2\Psi + \frac{\sin^2\Psi}{2(1 - h^2\sin^2\Psi/(2\Delta^2))}\right], \tag{9}$$

where Ψ is the angle between the helix axis $\mathbf{k}$ and the field $\mathbf{H}$

$$\cos^2\Psi = (\hat{c}\hat{h})^2 \qquad \text{and} \qquad \sin^2\Psi = 1 - (\hat{c}\hat{h})^2. \tag{10}$$

If the field is directed along the three principal directions:

(i) $h \parallel [111]$, $\hat{h} = (1/\sqrt{3})(111)$;
(ii) $h \parallel [110]$, $\hat{h} = (1/\sqrt{2})(110)$;
(iii) $h \parallel [001]$, $\hat{h} = (001)$;

the expressions for $\cos^2\Psi$ are given by:

$$\text{(i)}\ \cos^2\Psi = \tfrac{1}{3}(\sin\theta\cos\phi + \sin\theta\sin\phi + \cos\theta)^2 \tag{11}$$

$$\text{(ii)}\ \cos^2\Psi = \tfrac{1}{2}(\sin\theta\cos\phi + \sin\theta\sin\phi)^2 \tag{12}$$

$$\text{(iii)}\ \cos^2\Psi = \cos^2\theta. \tag{13}$$

Substituting equations (11)–(13) in equation (9) one obtains the magnetic energy as a function of the variables θ and ϕ. Figure 3 shows three-dimensional pictures of the ground state magnetic energy for $h \parallel [111]$ for $h = 0.1\Delta$ (a), $h = \Delta$ (b) and $h = 1.2\Delta$ (c). The surface shown in figure 3(a) has a minimum at $\theta = \arccos(1/\sqrt{3})$ and $\phi = \pi/4$, corresponding to the [111] axis and parallel to the field. As the field increases to $h = \Delta$ a new valley appears on this surface (figure 3(b)). The valley is displaced in the direction perpendicular to the field and reveals the presence of a new minimum. This valley is too shallow compared to the minimum provided by the parallel component of the field along the [111] axis. The valley becomes deeper than the minimum along the [111] axis at $\Delta < h < \sqrt{2}\Delta$ (figure 3(c)). In this range of the field one can expect that the vector $\boldsymbol{k}$ rotates from the [111] direction. Similar pictures may be drawn for $h \parallel [110]$ on the basis of equation (12) and for $h \parallel [001]$ on the basis of equation (13). In the latter case the pictures become two dimensional since the magnetic energy does not depend on ϕ (see equation (13)).

The real orientation of the helix axis is determined by competition between the magnetic energy (equations (9) and (11)–(13)) and the anisotropic exchange energy along with the cubic anisotropy (equation (6)):

$$E_{\mathrm{g}} = E_{\mathrm{an}} + E_{\mathrm{h}}. \tag{14}$$

Minimizing this expression we are able to calculate the orientation of the helix wavevector $\mathbf{k}$ at any value of the field.

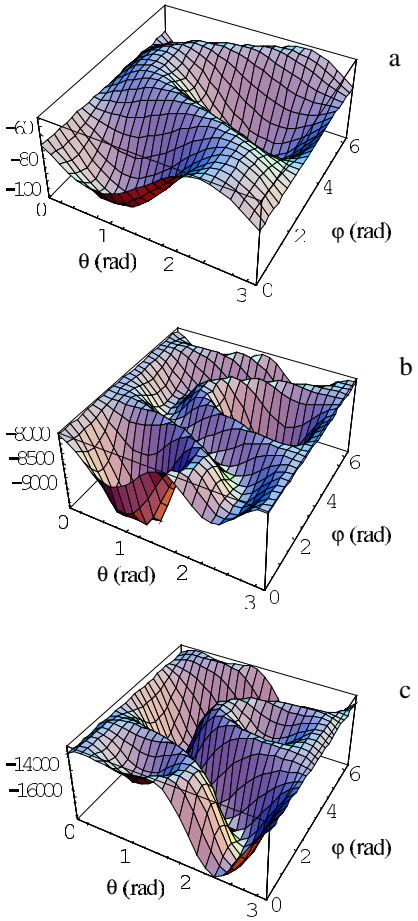

Figure 3. Two-dimensional surface of the ground state magnetic energy for $h \parallel [111]$ for $h = 0.1\Delta$ (a), $h = \Delta$ (b) and $h = 1.2\Delta$ (c).

4. Experimental evidence

The most intriguing feature in the behaviour of the magnetic system of MnSi under applied field seems to be the appearance of a minimum in the ground state energy in the direction **k** perpendicular to the magnetic field and to the [111] axis. Experimental evidence for this was recently obtained in [14], where the helix structure of MnSi under applied field was investigated near $T_C = 29$ K by small angle scattering of polarized neutrons. It was found that in zero field the magnetic structure of the MnSi consists of left-handed helices oriented along four ⟨111⟩ axes, so that four different domains coexist. The magnetic field, applied along the [111] axis, lifts the degeneracy of the magnetic system. The axis along the field becomes energetically more favourable as compared to the other three ⟨111⟩ axes. This single domain structure appears above the magnetic field H_{C1}, which in the critical range is of the order of 30 mT. Further increase of the field leads to the 90° reorientation of the spin helix from the [111] axis (also the field axis) to the $[1\bar{1}0]$ axis (perpendicular to the field) in the field range from 130 to 180 mT. Reverse rotation occurs at $H > 180$ mT. The helix transforms into a conical structure, which becomes the field-induced ferromagnet at $H_{C2} \simeq 350$ mT at $T = 28.5$ K. This 90°

rotation occurs in close vicinity to T_C only and elucidates the nature of the so called A-phase observed by different techniques in [15–17].

Thus we deal with the **k** rotation under applied field from one energetically favourable direction (parallel to the field) to the other (perpendicular to it). This phenomenon can be well described by equations (9) and (11) in combination with equation (6). This observation gives the experimental evidence for the spin wave gap $\Delta \sim g\mu_B H_{in}/\sqrt{2}$ that provides the stability of the spin wave spectrum with respect to the magnetic field perpendicular to **k**. Two contributions to the spin wave gap are considered in [10]. One contribution stems from the interactions between spin waves $\Delta^2_{SW} \sim h_c^2/(4S)$, which is always positive. The second contribution is determined by the cubic anisotropy: $\Delta^2_{cub} \sim S^3 K h_c$. It is seen that Δ^2_{cub} may have an arbitrary sign. So the different contributions to the gap may compete. Changing the sign and the strength of the cubic anisotropy, for example by pressure, may lead to a quantum phase transition from the ordered to a spin liquid state.

5. Conclusion

In conclusion, we give a recipe for calculating the helix wavevector orientation in MnSi under an applied field. The formulae derived are able to describe the experimental findings presented in [11, 13, 14].

Acknowledgments

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