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LETTER TO THE EDITOR

Theory of helical magnetic structures and phase transitions in MnSi and FeGe

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Abstract. The long-period helical magnetic structures in MnSi and FeGe are shown to be consequences of a ferromagnetic Dzyaloshinskiĭ instability. Renormalisation group theory predicts the transition to be first order, in agreement with experiments on MnSi.

A few years ago Dzyaloshinskiĭ (1964) proposed a mechanism for describing long-period structures, in which the superstructure is caused by an instability of a ferromagnetic structure with respect to small 'relativistic' spin–lattice or spin–spin interactions. The instability may occur only in certain crystal structures lacking inversion symmetry. Until now, no realisations of such structures in real magnetic systems have been identified. In this paper it will be shown that the helical magnetic structures in MnSi and FeGe (cubic phase) can be explained by the Dzyaloshinskiĭ mechanism. We also study the phase transition into the helical phase by means of renormalisation group theory. It turns out that the appropriate Landau–Ginzburg–Wilson (LGW) Hamiltonian has no stable fixed point with the proper symmetry. This leads to a first-order transition in agreement with experiments on MnSi (Ishikawa *et al* 1977, Hansen 1977).

There have been reported several neutron diffraction experiments showing a helical magnetic structure in MnSi (Ishikawa *et al* 1976, Hansen 1977). The wavevector is found to be in the $\langle 111 \rangle$ direction, and it is rather small ($\sim 0{\cdot}036\ \text{Å}^{-1}$), indicating a very long period (~ 175 Å). Magnetisation curves in FeGe show a similar magnetic structure (Lundgren *et al* 1970). As well as MnSi, FeGe crystallises in the tetrahedral $P2_13$ structure, in which there is no inversion symmetry (figure 1). This is important in understanding the magnetic behaviour.

As a starting point, the free energy is expanded in terms of a slow-varying spin density $\boldsymbol{S}(\boldsymbol{r})$ (Landau and Lifshitz 1977):

$$\begin{aligned} F(\boldsymbol{r}) = {} & \tfrac{1}{2}A(S_x^2 + S_y^2 + S_z^2) + b\boldsymbol{S}\cdot(\nabla \times \boldsymbol{S}) \\ & + \tfrac{1}{2}B_1[(\nabla S_x)^2 + (\nabla S_y)^2 + (\nabla S_z)^2] \\ & + \tfrac{1}{2}B_2\left[\left(\frac{\partial S_x}{\partial x}\right)^2 + \left(\frac{\partial S_y}{\partial y}\right)^2 + \left(\frac{\partial S_z}{\partial z}\right)^2\right] \\ & + C(S_x^2 + S_y^2 + S_z^2)^2 \\ & + D(S_x^4 + S_y^4 + S_z^4). \end{aligned} \tag{1}$$

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This is the most general expression up to fourth order in the spins and to second order in the gradients, which is invariant with respect to the symmetry operations of the $P2_13$ space group. The expansion is valid for magnetic structures, where the magnetisation is locally almost ferromagnetic. As we shall see, the b term, which is linear in the gradient, destabilises the ferromagnetic structure. Physically this term may be caused by relativistic interactions between the spins of the form $\boldsymbol{S}_i \times \boldsymbol{S}_j$. We expect this term to be small compared to the other second-order terms, which may originate from the usual symmetric Heisenberg interaction $\boldsymbol{S}_i . \boldsymbol{S}_j$. In the absence of the b term and for positive B_1 and B_2, F($\boldsymbol{r}$) is minimised by a uniform $\boldsymbol{S}(\boldsymbol{r})$ (a ferromagnet), and the transition takes place when $A = 0$. The spin direction is determined by the fourth-order coefficients C and D.

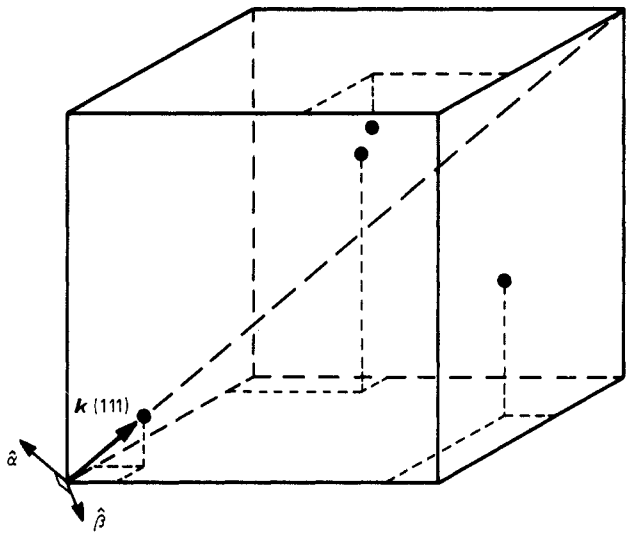

Figure 1. Crystal structure of MnSi and FeGe ($T^4 - P2_13$). There are four metal atoms in the positions (x, x, x), $(x + \frac{1}{2}, \frac{1}{2} - x, \bar{x})$, $(\bar{x}, x + \frac{1}{2}, \frac{1}{2} - x)$ and $(\frac{1}{2} - x, \bar{x}, x + \frac{1}{2})$. For MnSi, $x = 0{\cdot}137$.

Near T_c the free energy is generally minimised by periodic structures of the form

$$\boldsymbol{S}(\boldsymbol{r}) = (1/\sqrt{2})[\boldsymbol{S}_k \exp(i\boldsymbol{k} . \boldsymbol{r}) + \boldsymbol{S}_k^* \exp(-i\boldsymbol{k} . \boldsymbol{r})]. \tag{2}$$

When equation (2) is inserted into equation (1), the free energy density becomes (to second order in S_k)

$$\begin{aligned} F(k) = {} & \tfrac{1}{2}A\,|\boldsymbol{S}_k|^2 + ib\boldsymbol{k} . (\boldsymbol{S}_k \times \boldsymbol{S}_k^*) \\ & + \tfrac{1}{2}B_1\,k^2\,|\boldsymbol{S}_k|^2 \\ & + \tfrac{1}{2}B_2\,(k_x^2\,|S_{kx}|^2 + k_y^2\,|S_{ky}|^2 + k_z^2\,|S_{kz}|^2). \end{aligned} \tag{3}$$

By setting $\boldsymbol{S}_k = \boldsymbol{\alpha}_k + i\boldsymbol{\beta}_k$ we find that equation (3) is minimised when choosing $\boldsymbol{\alpha}_k \perp \boldsymbol{\beta}_k$, $|\boldsymbol{\alpha}_k| = |\boldsymbol{\beta}_k|$ and $\boldsymbol{k}$ antiparallel to $\boldsymbol{\alpha}_k \times \boldsymbol{\beta}_k (b > 0)$. In the case $b < 0$, $\boldsymbol{k}$ is then parallel to $\boldsymbol{\alpha}_k \times \boldsymbol{\beta}_k$. These two possibilities describe right-handed and left-handed spirals respectively. The b term has full rotational symmetry and gives no preferential direction for

the wavevector $\boldsymbol{k}$. The direction of $\boldsymbol{k}$ is fixed by the anisotropic second-order gradient term with coefficient B_2:

$$B_2 < 0: \boldsymbol{k} \| (111)$$
$$B_2 > 0: \boldsymbol{k} \| (001). \tag{4}$$

On the basis of the experimental results indicating $\boldsymbol{k} \| (111)$ (Lundgren *et al* 1970, Ishikawa *et al* 1976, Hansen 1977) we conclude that $B_2 < 0$. By applying a magnetic field, one may rotate the wavevector into any direction (Ishikawa *et al* 1977, Guy and Strom-Olsen 1979). This indicates that the anisotropic second-order term is relatively small. The potential (3) is now given by

$$F = (\tfrac{1}{2}A - |b|k)\,|\boldsymbol{S}_k|^2 + (\tfrac{1}{2}B + \tfrac{1}{6}B_2)\,k^2\,|\boldsymbol{S}_k|^2 \tag{5}$$

which is minimised by

$$k = |b|/(B_1 + \tfrac{1}{3}B_2). \tag{6}$$

The smallness of k follows from the smallness of b compared to $B_1 + \frac{1}{3}B_2$. This sum is assumed to be greater than zero in order to keep the k^2 term positive definite.

The spin structure can be expressed in terms of the real vectors in the following way:

$$\boldsymbol{S}(\boldsymbol{r}) = \boldsymbol{\alpha}_k \cos(\boldsymbol{k}\,.\,\boldsymbol{r}) - \boldsymbol{\beta}_k \sin(\boldsymbol{k}\,.\,\boldsymbol{r}) \tag{7}$$

which indeed describes left-handed or right-handed spirals with a long period. Figure 2 shows the free energy for left-handed ($b < 0$) and right-handed ($b > 0$) structures. Clearly, the ferromagnetic $\boldsymbol{k} = 0$ structure is unstable. For comparison, the free energy for a system with inversion symmetry ($b = 0$) is also shown.

In principle, one may also have helical structures in systems with inversion symmetry, as seen for example in several rare earth compounds. In such systems $F(k)$ has two symmetric minima at some finite k, in addition to the extremum at $k = 0$. There is no

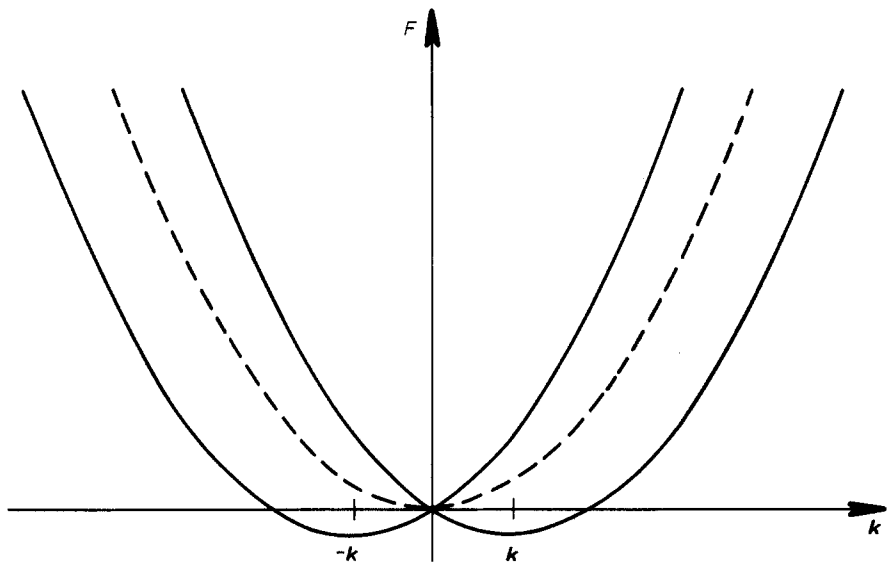

Figure 2. Free energy as a function of wavevector for left-handed and right-handed spirals. The broken curve shows the free energy for a system with inversion symmetry ($b = 0$).

reason to expect k to be small in this case, and generally it is not. In MnO_2 (Dzyaloshinskiĭ 1964) the simple *antiferromagnetic* up–down structure is unstable, but there is no symmetry which forbids the structure to be ferromagnetic. Indeed, the wavevector is not small: $q = (2/a)(2/7)$ (Yoshimori 1959).

To study the nature of the phase transition we first identify the order parameter. Since the paramagnetic space group is $P2_13$, the star of the ordering wavevector consists of four vectors $\boldsymbol{k}_1 = (k/\sqrt{3})(1, 1, 1)$, $\boldsymbol{k}_2 = (k/\sqrt{3})(-1, -1, 1)$, $\boldsymbol{k}_3 = (k/\sqrt{3})(-1, 1, -1)$ and $\boldsymbol{k}_4 = (k/\sqrt{3})(1, -1, -1)$. For each wavevector there are two equivalent perpendicular directions in the plane normal to $\boldsymbol{k}_i$, $\hat{\boldsymbol{\alpha}}_i$ and $\hat{\boldsymbol{\beta}}_i$. These define altogether eight independent *left*-handed spirals described by the order parameters η_i and $\bar{\eta}_i$ (Bak and Mukamel 1976):

$$\boldsymbol{S}(\boldsymbol{r}) = \eta_i[\hat{\boldsymbol{\alpha}}_i \cos(\boldsymbol{k}_i \cdot \boldsymbol{r}) - \hat{\boldsymbol{\beta}}_i \sin(\boldsymbol{k}_i \cdot \boldsymbol{r})] + \bar{\eta}_i[\hat{\boldsymbol{\alpha}}_i \sin(\boldsymbol{k}_i \cdot \boldsymbol{r}) + \hat{\boldsymbol{\beta}}_i \cos(\boldsymbol{k}_i \cdot \boldsymbol{r})]. \tag{8}$$

Near T_c, fluctuations in the order parameter become important. One way of taking this into account is by means of the Wilson and Fisher (1972) renormalisation group theory in $d = 4 - \epsilon$ dimensions. The starting point is the LGW Hamiltonian, which in our case has the form

$$H = \sum_{i=1}^{4} [(r/2)(\eta_i^2 + \bar{\eta}_i^2) + (\nabla\eta_i)^2 + (\nabla\bar{\eta}_i)^2] + u(\sum_{i=1}^{4} \eta_i^2 + \bar{\eta}_i^2)^2 + v \sum_{i<j} (\eta_i^2 + \bar{\eta}_i^2)(\eta_j^2 + \bar{\eta}_j^2). \tag{9}$$

The coefficients in equation (9) are related to those in equation (3). Near the transition point, u and v are replaced by renormalised coefficients, and at a second-order transition

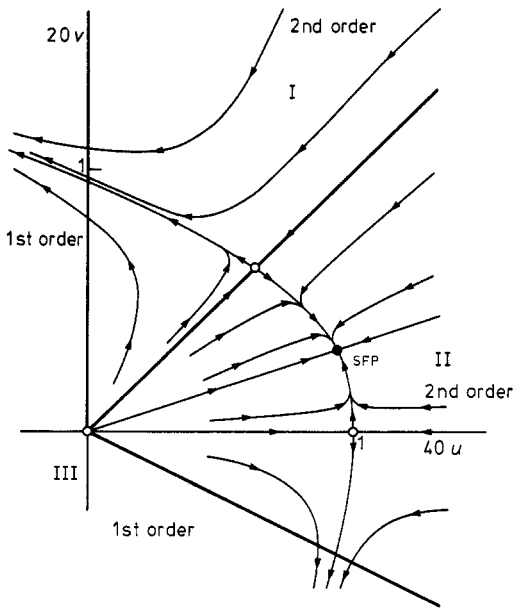

Figure 3. Renormalisation group flow diagram (to order ϵ) for $n = 8$ LGW Hamiltonian describing the phase transition in MnSi and FeGe.

(u, v) converges to a stable fixed point. The recursion relations for (u, v) have been studied by Mukamel and Krinsky (1976), and they found a stable fixed point. It is important, however, to study the flow diagram more globally. Figure 3 shows the flow diagram to order ϵ. The diagram has the same structure as the one discussed by Bak and Lebech (1978) related to the rare earth neodymium. The phase diagram consists of three regions I, II and III. The flow carries (u, v) *either* into the first-order regime III, where the fourth-order term is not positive definite, *or* to a fixed point in a region where the magnetic structure is described by a superposition of four helicals ('multiple q-structure' with $|S_{k_1}| = |S_{k_2}| = |S_{k_3}| = |S_{k_4}|$). A single-$q$ helical structure, as the one discussed here, is thus inconsistent with a second-order transition. Therefore the transition is predicted to be first order, in agreement with experiments on MnSi (Ishikawa *et al* 1977, Hansen 1977). The phase transition belongs to the class of transitions which are necessarily driven first order by fluctuations (Bak *et al* 1976). We find that neutron scattering experiments on FeGe would be of interest to check the magnetic structure and to study the phase transition.

In conclusion, we have demonstrated that the helical magnetic structures in MnSi and FeGe are caused by a ferromagnetic Dzyaloshinskiĭ instability. Renormalisation group theory predicts the transition to be first order, in agreement with experiments on MnSi.

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