A general model of MnSi-like spiral magnets

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A general, symmetry-allowed model of nearest-neighbour interactions for MnSi-like magnets is presented. A left-handed helical magnet phase occurs within a large parameter space of the model, which is explored via numerical simulation. The relations between microscopic features of the spiral structure and various model parameters, including an external magnetic field, are determined and show good agreement with predictions from free energy considerations. A skyrmion structure is stabilized near the boundary.

I. INTRODUCTION

The B20 structure type of magnetic crystals is renowned for displaying unusual magnetic structures and for applications in a number of different fields. These diatomic materials belong to the non-centrosymmetric space group P2$_1$3 which supports helimagnetic phases, arising from the absence of centrosymmetry. As such, B20 materials have been at the forefront in the study of helical magnets where they were among the first to be experimentally observed [1,3]. In recent years there has been a resurgence of interest in these materials, MnSi in particular, due to the finding of non-Fermi liquid behaviour accompanied by partial magnetic order in the magnetic field-pressure-temperature phase diagram [3–12] and of a skyrmion crystal phase [13].

MnSi, an intermetallic compound, undergoes a phase transition at $T_c = 29$ K into a left-handed helical spin structure with wavevector $k$ oriented along one of the ⟨111⟩ directions with a wavelength of 18 nm [1,3]. Under an applied magnetic field greater than 100 mT $k$ rotates to align with the field and a conical spin structure is realized, where the cone angle decreases with field strength [3–14]. A field-induced ferromagnetic state appears above approximately 600 mT. A skyrmion crystal phase has been reported in ‘Phase A’, a small pocket in the phase diagram just below $T_c$ for small magnetic fields ($\approx 100$ to 250 mT) [13,15]. A quantum phase transition occurs under pressure with $P_c = 14.6$ kbar accompanied by non-Fermi liquid behaviour over a wide range of temperature [13,16,17].

As shown over sixty years ago, spiral magnetism arises from competing ferromagnetic (FM) and antiferromagnetic (AFM) interactions, which occur when there are more than one kind of exchange path [18] or from anti-symmetric exchange interactions (known as the Dzyaloshinskii-Moriya (DM) interaction) that exist in non-centrosymmetric crystals [19,20]. Over the years these phenomenological models of MnSi have been augmented by various additions, including gradient terms, same-site anistropy, generalized forms of the DM interaction, and coupling to external fields, in order to quantitatively account for details of the helical structures (such as the wavenumber and orientation) and the nature of the phase transition to this state [21–25]. The earliest studies employed a continuum approach to the magnetization which was later extended to lattice spin models for general three-dimensional crystals [26] and finally to the actual spin lattice for MnSi-type crystals [25,27]; the latter studies describe quantitatively not only the wavenumber of the helical spin state, but also canting of the spins and field/pressure dependence.

Recently, muon spin rotation ($\mu$SR) studies have revealed more details of the magnetic structure in MnSi, including canting and rotation of spins within the spiral structure [28,29]. The main objective of this paper is to describe these details within a completely general model for MnSi-type crystals, constructed using only nearest-neighbour (NN) exchange interactions and single ion anistropy. This model will be analyzed via numerical simulations using the “effective field method” (EFM) [30].

II. THE MODEL

The magnetic ions of B20 crystals occupy the 4a Wyckoff position of the space group P2$_1$3 ($T^4$, No. 198), forming a trillium lattice. The four spin sites within a cubic cell are:

$$
\begin{align*}
\mathbf{r}_1 &= (x, x, x) \\
\mathbf{r}_2 &= (-x + \frac{1}{2}, -x, x + \frac{1}{2}) \\
\mathbf{r}_3 &= (-x, x + \frac{1}{2}, -x + \frac{1}{2}) \\
\mathbf{r}_4 &= (x + \frac{1}{2}, -x + \frac{1}{2}, -x)
\end{align*}
$$

(1)

where the parameter $x \approx 0.138$ for Mn in MnSi. In the following, a spin located at site $\mathbf{r}_i$ in any cubic cell will be called a $\#i$ spin.

The underlying point group of P2$_1$3 is the tetrahedral group $T$, which has twelve symmetry elements. The corresponding operations in the space group include pure
rotations and screw axes, but notably no inversion or reflections. None of the four sites of the 4\(a\) Wyckoff position are invariant under any space group operation.

We will model magnetic interactions in B20 crystals by finding the most general form of the nearest neighbour exchange interaction that is invariant under all space group operations. Each site has six nearest neighbours (NN) separated by a distance \(d = a\sqrt{2x^2 - 4x + 1/2}\) which gives \(d \approx 3.2a\), where \(a = 4.558\ \text{Å}\) is the lattice parameter. By considering all bilinears of the form \(S_i^a S_j^b\) (where \(S_i^a\) is the \(a\) component of the magnetic moment at site \(i\), and \(j\) is a NN of \(i\)), it can be shown that these will combine to give 9 invariants consisting of 12 bilinears each. These are

\[
H^{xx} = \sum_n S_{1n}^x (S_{2n}^z + S_{3n}^z) + (S_{3n}^y + S_{5n}^y) S_{3n}^x + S_{1n}^z (S_{3n}^y + S_{5n}^y)
+ S_{2n}^z (S_{4n}^z + S_{6n}^z) + S_{1n}^y (S_{4n}^z + S_{6n}^z) + (S_{2n}^y + S_{4n}^y) S_{6n}^x
H^{yy} = \sum_n S_{1n}^y S_{2n}^y + S_{1n}^y S_{4n}^y + S_{3n}^y S_{3n}^y + S_{2n}^y S_{4n}^y + S_{1n}^x S_{4n}^x + S_{2n}^x S_{4n}^x
H^{zz} = \sum_n S_{1n}^z S_{2n}^z + S_{1n}^z S_{4n}^z + S_{1n}^z S_{5n}^z + S_{2n}^z S_{4n}^z + S_{1n}^x S_{4n}^x + S_{2n}^x S_{4n}^x
H_{s,a}^{xy} = \sum_n S_{1n}^x (S_{2n}^y + S_{3n}^y) + S_{1n}^y (S_{2n}^x + S_{3n}^x) - (S_{3n}^y + S_{5n}^y) S_{3n}^x - (S_{3n}^x + S_{5n}^x) S_{3n}^y
+ S_{1n}^y (S_{2n}^y + S_{3n}^y) + S_{1n}^x (S_{2n}^x + S_{3n}^x) - S_{2n}^x (S_{1n}^y + S_{3n}^y) - S_{2n}^y (S_{1n}^x + S_{3n}^x)
+ S_{1n}^y (S_{2n}^y + S_{3n}^y) + S_{1n}^x (S_{2n}^x + S_{3n}^x) - (S_{2n}^y + S_{2n}^y) S_{3n}^x - (S_{2n}^y + S_{2n}^y) S_{3n}^y
H_{s,a}^{yy} = \sum_n S_{1n}^y S_{2n}^y + S_{1n}^y S_{4n}^y + S_{3n}^y S_{3n}^y + S_{2n}^y S_{4n}^y + S_{1n}^x S_{4n}^x + S_{2n}^x S_{4n}^x
H_{s,a}^{zz} = \sum_n S_{1n}^z S_{2n}^z + S_{1n}^z S_{4n}^z + S_{1n}^z S_{5n}^z + S_{2n}^z S_{4n}^z + S_{1n}^x S_{4n}^x + S_{2n}^x S_{4n}^x
\]

(2)

where the DM vectors \(D_{ij}\) are constrained by the symmetry of the lattice. This interaction corresponds to the three antisymmetric (subscript \(a\)) terms in (2); in fact comparison with these terms yields the minimal constraint on the DM vectors. For example, examining the terms in \(H_{s,a}^{yy}\) yields \(D_{12}^{yy} = -D_{21}^{yy} = -D_{34}^{yy} = D_{65}^{yy} = D_{56}^{yy}\). The DM vectors are often further constrained by taking the DM term to be \(H_{s,a}^{xy} + H_{s,a}^{xx} + H_{s,a}^{yy}\). Also, the symmetric terms \(H_{s,b}^{xx,y}\) are usually omitted altogether.

In our simulations, we consider a free energy constructed using all nine of the exchange terms (2) and the two same-site anisotropy terms (1), for a total of eleven independent interaction constants, as well as the Zeeman term (3):

\[
F = J^{xx} H^{xx} + J^{yy} H^{yy} + J^{zz} H^{zz} + J^{xy} H^{xy} + J^{yx} H^{yx} + J^{zz} H^{zz} + J^{xy} H^{yx} + \ldots + J_2 H_2 + J_4 H_4 + H_Z.
\]

(7)

III. MAGNETIC ORDER PARAMETERS

The helical magnet phase of MnSi is marked by the appearance of a left-handed spiral oriented along one of the four equivalent (111) directions. From here on, we will assume that the helices are oriented in the particu-
lar direction [111]. Perpendicular to [111] are alternating planes of #1 spins and of #2, 3 and 4 spins, which we label 1 and 2-3-4 respectively. Moving along the [111] direction, the distance between a 1-plane and the following 2-3-4-plane is \((1 - 4x)/\sqrt{3} = 0.259a\), and the distance between a 2-3-4-plane and the next 1-plane is \(4xa/\sqrt{3} = 0.319a\).

In order to classify magnetic structures we define magnetic order parameters associated with \(k \parallel [111]\). The little group of this wavevector is \(C_3\), a subgroup of the crystallographic point group \(T\). The three representations that belong to \(k \parallel [111]\), labelled \(F_1\), \(F_2\) and \(F_3\), are derived from the three representations of \(C_3\). All three are one-dimensional; \(F_2\) and \(F_3\) are related by time reversal.

The 12-dimensional basis of 4 spins within a unit cell and 3 spatial dimensions generates a (reducible) representation belonging to \(k \parallel [111]\). \(4F_1 \oplus 4F_2 \oplus 4F_3\) – that is, there are four copies of each irreducible representation. The basis is:

\[
\begin{align*}
F_1^{(1)} &= S_{1k}^x + S_{1k}^y + S_{1k}^z \\
F_2^{(1)} &= S_{1k}^x + \varepsilon S_{1k}^y + \varepsilon^2 S_{1k}^z \\
F_3^{(1)} &= S_{1k}^x + \varepsilon^2 S_{1k}^y + \varepsilon S_{1k}^z \\
F_1^{(2)} &= S_{2k}^x + S_{2k}^y + S_{2k}^z \\
F_2^{(2)} &= S_{2k}^x + \varepsilon S_{2k}^y + \varepsilon^2 S_{2k}^z \\
F_3^{(2)} &= S_{2k}^x + \varepsilon^2 S_{2k}^y + \varepsilon S_{2k}^z \\
F_1^{(3)} &= S_{3k}^y + S_{3k}^z + S_{3k}^x \\
F_2^{(3)} &= S_{3k}^y + \varepsilon S_{3k}^z + \varepsilon^2 S_{3k}^x \\
F_3^{(3)} &= S_{3k}^y + \varepsilon^2 S_{3k}^z + \varepsilon S_{3k}^x \\
F_1^{(4)} &= S_{4k}^y + S_{4k}^z + S_{4k}^x \\
F_2^{(4)} &= S_{4k}^y + \varepsilon S_{4k}^z + \varepsilon^2 S_{4k}^x \\
F_3^{(4)} &= S_{4k}^y + \varepsilon^2 S_{4k}^z + \varepsilon S_{4k}^x,
\end{align*}
\]

where \(\varepsilon = \exp 4\pi i/3 = -\frac{1}{2} - i\frac{\sqrt{3}}{2}\) and \(\varepsilon^2 = \varepsilon^*\). \(S_{ik}^n\) are the Fourier transforms of the spins,

\[
S_{ik}^n = \frac{1}{N^{1/2}} \sum_n \exp(-i \mathbf{k} \cdot \mathbf{r}_n) S_{in}^n
\]

where \(\mathbf{r}_n\) is the \(n\)-th lattice vector and \(N\) is the total number of cells. The physical spins are \(S_{in}^n\), that is

\[
\frac{1}{N^{1/2}} \sum_k S_{ik}^n \exp(i \mathbf{k} \cdot \mathbf{r}_n).
\]

There is no sum over wavenumber in this expression when \(\mathbf{k}\) is the only wavevector present in the structure.

The helical magnet phase of MnSi is marked by the appearance of a left-handed spiral, which corresponds to a order parameter that transforms as \(F_3\) i.e., one or more of the \(F_3^{(i)}\) are non-zero while \(F_2^{(i)} = 0\). That is, the spins precess in a clockwise direction with respect to the [111] direction. Since \(F_1\) is compatible with \(F_3\) (in the sense that no additional symmetries are broken by \(F_1\)) there is no requirement that \(F_1^{(i)}\) be vanishing.

The spin arrangements associated with a \(F_3\) order parameter are in general quite complicated; here we make some simplifying assumptions based on experimental observations. First, we assume that the magnitude of individual spins is fixed. If \(F_1^{(1)}\) is present and not \(F_2^{(1)}\) then this constraint forces \(F_1^{(i)}\) to be absent in order for spin #1 to have fixed length. This means that spin #1 must be perpendicular to the [111] axis - i.e., no canting of this spin toward [111] is expected, as seen in experiment.

If we also assume that spins #2, 3, and 4 have the same magnitudes then the relative magnitudes of the various order parameters will be constrained, but there is no requirement that \(F_1^{(i)}\) must vanish if \(F_3^{(i)}\) is present and not \(F_2^{(i)}\) for \(i = 2, 3, 4\). However, in experiments it is observed that spins #2, 3, and 4 lie perpendicular to \(k\) in ferromagnetic arrangements within each 2-3-4-plane [28]. In this arrangement, if \(F_2^{(i)}\) vanishes then \(F_1^{(i)}\) also vanishes and the components of \(F_3^{(i)}\) are related by \(F_3^{(2)} = \varepsilon^2 F_3^{(3)} = \varepsilon F_3^{(4)}\).

Even with all these constraints imposed there remains a free parameter accessible by experiment: the relative orientation of spins in a 1-plane with respect to the nearest 2-3-4-plane [28]. The spins precess in a left-handed sense for a distance \(d\) along the [111] direction by an angle \(kd\) rad, where \(k = 0.35\) nm\(^{-1}\). The precession angle between planes of the same type is therefore \(ka/\sqrt{3}\) rad or 5.28\(^\circ\). According to this simple picture, the precession angle between a 2-3-4-plane and the next 1-plane would be 2.913\(^\circ\); however this angle is measured to be only 0.86\(^\circ\) [28]. The phase difference \(\phi = -2.04\(^\circ\)\) (-0.0356 rad) can be considered as a model-dependent parameter.

The only constraint we enforce in our numerical simulations is that all four spins have constant, equal magnitudes. We find that spins in the 2-3-4-planes do not always lie perpendicular to \(k\). Generally, they precess within a different plane, which gives rise to another model-dependent parameter, the angle \(\gamma\), which we define as the angle between the [111] plane and the plane of the of the spins precession. Since there are two kinds of planes, there are two angles, \(\gamma^{(1)}\), for the 1-plane and \(\gamma^{(2)}\), for the 2-3-4-plane. These angles have not been measured in experiment, but they have been predicted in quantitative analysis [27]. Furthermore, the individual spins are not ferromagnetically aligned, instead each #1 spin will cant towards the axis \(\tau_i\), where

\[
\begin{align*}
\tau_1 &= [111] \\
\tau_2 &= [111] \\
\tau_3 &= [111] \\
\tau_4 &= [111].
\end{align*}
\]
IV. RESULTS

The EFM is a computational method used for determining the spin configuration of a system as \( T \rightarrow 0 \) by finding local minima of the free energy in classical and semi-classical systems with pairwise interactions. The method uses an iterative algorithm which, in each step, scans all spins in a random order. For each spin site, a local field is calculated,

\[
H_i^\alpha = - \sum_{j,\beta} J_{ij}^{\alpha,\beta} S_j^\beta
\]

(22)

where \( S_j \) are the spins with which \( S_i \) interacts and \( J_{ij}^{\alpha,\beta} \) is the total of all interaction constants for \( S_i^\alpha \) and \( S_j^\beta \). The spin located at \( i \) is then reoriented, either fully or partially, in the direction of this field. This process is repeated many times until a local minimum is found. Since the algorithm has no process by which a given spin can increase its interaction energy, it is likely that the final lattice configuration will not be the global minimum. This is remedied by running the algorithm a large number of times with randomly generated starting configurations. From this set of simulations, only those which produce the lowest energy are selected.

Since we are primarily interested in modelling the helical phase, we begin by considering a set of interaction constants which yields such a configuration, and then we vary those parameters in order to discern their individual effect on the magnetic structures. For each simulation, we measure the wavenumber \( k \), the phase difference \( \phi \), the out-of-plane canting angle \( \gamma \) (with respect to the \([111]\) plane) and the relative size of the magnetic order parameters \( |F_i^{(j)}| \). All simulations were performed on a system with \( 23 \times 23 \times 23 \) cells (large enough to contain one full wavelength of the helix) with 48668 spins in total. In order to find an incommensurate \( k \), periodic boundary conditions were not imposed.

A. Reduced Model

We begin by examining a model with only two parameters, \( J \) and \( D \), defined by

\[
J = J_{xx} = J_{yy} = J_{zz}
\]

(23)

\[
D = J_{a}^{xy} = J_{a}^{yz} = J_{a}^{zx},
\]

(24)

corresponding to the Heisenberg exchange interaction and a simplified DM interaction where all components of the DM vector are \( \pm D \). In all simulations, we used \( J_2 = -J/2 \), \( J_3 = J/2 \) with all other constants zero. The sign of \( D \) is negative, yielding a left-handed spiral.

The wavelength was measured using the average rotation between unit cells along \([111]\). As shown in Fig. 1 for small \( |D| \), we find a linear relationship between wavenumber \( k \) and \( |D| \), as predicted from free energy considerations \[21\]. Non-linear deviations occur for \( |D|/J \gtrsim 0.6 \).

The measured wavelength is \( \lambda = 18 \text{ nm} = 22.8\sqrt{3}\alpha \), that is 22.8 unit cells along the \([111]\) direction. The corresponding wavenumber is \( k = 0.276/(\sqrt{3}\alpha) \), which occurs for \( |D|/J \approx 0.3 \).

Fig. 2 shows the phase difference \( \phi \) (defined at the end of Section III) as a function of \( |D|/J \). \( \phi \) is the average of phase differences measured between a 1-plane and a 2-3-4-plane. For small \( |D|/J \), there is a linear relation between \( \phi \) and \( |D|/J \), as predicted from free energy considerations \[27\].

The value of \( |D|/J \approx 0.3 \) yields a phase difference \( \phi \approx -0.07 \text{ rad} \), which is approximately twice as large as the measured value \[28\].

Fig. 3 shows the angle \( \gamma \) (defined at the end of Section III) for each kind of plane as a function of \( |D|/J \). In our simulations, \( \gamma \) is measured by assuming that all spins associated with a given position rotate within the same plane and measuring the angle between the \([111]\) axis and the normal vector of this plane. \( \gamma \) is the average of angles measured for each spin. The canting of spins in a 1-plane is always small, which correlates with a vanishing \( F_1 \) order parameter, as shown in Fig. 3. However,
the canting of the spins in a 2-3-4-plane increases with |D|/J, as expected from the free energy considerations [27]. Using the value |D|/J ≈ 0.3 (determined from our measurements of k), we estimate that γ ≈ 4.6° for the 2-3-4-plane in MnSi.

In order to make it easier to compare the relative sizes of the order parameters, the plots in Fig. 4 have been normalized at each value of |D|/J such that the highest value is one. In fact, the scale of each plot decreases with |D|/J, indicating a transfer of weight to other values of k with increasing |D|/J. This is most likely due to finite size and non-periodic boundary conditions of our simulation.

Fig. 4 shows that at larger wavelengths (small |D|/J) there is a mixture of F2 and F3 order parameters, corresponding to right-handed and left-handed structures, but the right-handed part quickly decreases with respect to the left-handed part as the wavelength decreases. At |D|/J ≈ 0.3, the left-handed component is five times larger than the right-handed component, and all four parts of the left-handed order parameter are present, but not equal.

There is a slight increase of F1 order parameters with larger values of |D|/J, which coincides with the appearance of isolated skyrmions in our simulations, such as the one shown in Fig. 5. When present, skyrmions always appear near the boundary as a small tunnel through a few layers.

FIG. 3: The average out-of-plane angle γ(1) for the 1-plane (black squares) and γ(2) for the 2-3-4-plane (purple circles). In the 2-3-4-planes, the individual spins in a given layer have the same orientation.

FIG. 4: The averaged magnetic order parameters derived from Eqs. 8–19 as a function of |D|/J. The plots are normalized such that the maximum size of any order parameter at each value of |D|/J is always 1.

B. Individual model terms

In this Section, we examine the effects of each independent interaction constant. As the starting point, we use a set of parameters which yield a left-handed helix: J = 1, D = −0.5, J2 = −1/2, J3 = 1/2, with all other constants vanishing. We vary the nine interaction constants around this point in order to examine the dependence of k, φ and γ on these parameters. In the following, we present those results where the dependence on individual parameters is most pronounced. Complete details of all
of the simulations may be found in Ref. [31].

Fig. 6 shows the dependence of the out-of-plane angles $\gamma^{(1)}$ and $\gamma^{(2)}$ on the three symmetric exchange parameters $J_{xx}$, $J_{yy}$ and $J_{zz}$. For both angles we note the strongest dependence on $J_{zz}$, while $J_{xx}$ yields nearly constant results. For $\gamma^{(1)}$, the slopes of the lines for $J_{zz}$ and $J_{yy}$ have the opposite sign.

![Graph 1: Out-of-plane angles $\gamma^{(1)}$ vs $|J_{xx}|$](image1)

![Graph 2: Out-of-plane angles $\gamma^{(2)}$ vs $|J_{xx}|$](image2)

**FIG. 6:** The out-of-plane angles $\gamma^{(1)}$ and $\gamma^{(2)}$ as a function of individual symmetric (Heisenberg-like) coupling constants. The black square represents the $|D| = 0.50$ result.

Fig. 7 shows the dependence of $k$, $\phi$ and $\gamma^{(2)}$ on the anti-symmetric exchange constants $J^a_{ij}$. The wavenumber results are similar to what are shown shown in Fig. 1, except for the variation of $J^a_{xx}$ which has a linear dependence of the opposite sign. The plots for $\phi$ and $\gamma^{(2)}$ also display linear dependence similar to what is shown in Figs. 2 and 3, except for the parameter $J^a_{zy}$, where the dependence is almost flat. It is clear from the plots that all three measurable quantities are sensitive to the tuning of the three anti-symmetric exchange constants, especially the phase difference $\phi$, which varies by as much as 50% in the (limited) range shown in the plot.

![Graph 3: Wavenumber $k$ vs $|J^a_{xx}|$](image3)

![Graph 4: Angle $\phi$ vs $|J^a_{xx}|$](image4)

**FIG. 7:** Wavenumber $k$, angle $\phi$, and out-of-plane angle $\gamma^{(2)}$ as functions of the antisymmetric coupling constants $J^a_{ij}$. The black square represents the $|D| = 0.50$ result. In the bottommost plot the error bars are too small to be seen.

The independent variation of the anti-symmetric interaction constants was analyzed by Chizhikov and Dmitrienko [27], who used the notation $(D_x, D_y, D_z) \equiv (J_{a_{xx}}, J_{a_{xy}}, J_{a_{yz}})$. They found:

$$k = \frac{2(D_x - D_y - D_z)}{3J}$$

(25)

$$\phi \propto \frac{D_x + D_z}{J}$$

(26)

$$\gamma \propto -\frac{(D_x + D_z)}{J}$$

(27)

in rough agreement with the results shown in Fig. 7. In particular, these results predict the flatness of the plots.
for \(\phi\) and \(\gamma^{(2)}\) with respect to the parameter \(J^{zv}\), as well as the relative sizes and signs of the slopes of the plots for \(k\).

It is worth noting that the other six independent interaction terms also appear in Ref. 27 with associated interaction constants. First there is a small correction to the Heisenberg interaction constant \(-J \rightarrow -J + \frac{D_2}{2}\) with separate, additional contributions to each of the components in \((J^{xx}, J^{yy}, J^{zz})\): \(\frac{1}{6}(2D_x^2 - D_y^2 - D_z^2, 2D_y^2 - D_z^2 - D_x^2, 2D_z^2 - D_x^2 - D_y^2)\). The other symmetric interaction constants also appear as \((J^{yz}, J^{zx}, J^{xy}) \equiv -\frac{1}{3}(D_xD_y, D_yD_z, D_zD_x)\). However the analysis in Ref. 27 does not consider these contributions.

C. Applied Field

We also performed numerical simulations of the model under an applied magnetic field, where the field is scaled according to Eq. 3. Fig. 8 shows the out-of-plane canting of the spins as a function of an applied field in the [111] direction. As expected, with increasing field, canting toward the field direction increases as \(\arcsin(B)\) and there is little difference between \(\gamma^{(1)}\) and \(\gamma^{(2)}\). Extrapolating the fit, complete alignment of the moments with the field occurs when \(H \sim 1\).

![Fig. 8: The out-of-plane canting of individual sublattices as a function of applied field. The lines are fits to the function \(c + \arcsin(bH)\).](image)

Fig. 9 shows how the components of the order parameter evolve as a function of an applied field in the [111] direction. The \(F_1\) components increase with increasing field, until they become the dominant contribution, in rough correspondence with the out-of-plane canting shown in Fig. 8.

![Fig. 9: Magnetic order parameters vs applied field in the [111] direction. The magnitudes are normalized within a single value of \(H\) such that the maximum is always 1.0.](image)

V. DISCUSSION & CONCLUSION

The computational results of the simplified two-parameter model discussed in Section IV A provide a qualitative description of the helical magnet phase of MnSi, but fail to describe it in detail: the measured values of \(k\) and \(\phi\) cannot be consistently explained within a two-parameter model of symmetric and anti-symmetric interactions. Our numerical simulations using the full model, presented in Section IV B, demonstrate that an appropriate tuning of the parameters of the more general model could reproduce those experimentally measured values. Also, in our simulations, we have measured other features of the spin configuration in the helical phase that are potentially experimentally accessible - the out-of-plane angles \(\gamma^{(1)}\) and \(\gamma^{(2)}\). Our results are in good agreement with the free energy analysis of Ref. 27.

Furthermore, an additional measurement, the canting of individual spins towards their \(\tau_i\) axes (Eq. 21) could also be obtained from our results.

We have also shown - at least within the limits of our finite-sized simulation - the extent to which the helical phase is contained within a single kind of order parameter (the \(F_3\) OP), and the relative weight of the four separate contributions to \(F_3\). Their evolution under an applied field was also presented. These details can provide a different point of comparison for measurements on the helical phase.

To summarize, we have considered a general, symmetry-allowed model with eleven free parameters - nine interaction constants and two same-site anisotropy constants - to describe the helical magnet phase in MnSi-like crystals. Experimental observations greatly constrain the parameter space of this model, as shown in the earliest theoretical studies, which derived the relationship between symmetric and anti-symmetric (DM) interaction constants and the spiral wavelength. Recent experiments have uncovered details concerning the orientation of individual magnetic moments in the magnetic...
spirals; those findings can be explained by the more detailed model we have considered here.

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