# Exploring basis vectors and the different types of magnetic structure

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## 1 Overview

This pdf file contains hyperlinks that launch FullProf Studio with example files for different types of magnetic structure. By combining a tutorial directly with viewable structures, the reader is encouraged to explore the structure types and gain an understanding of how different types of basis vectors and values of the propagation vector correspond to the different types of magnetic structure.

### 1.1 File structure

The initial files are stored in the SARA*h* directory and temporary copies are made in the directory 'Magnetic Structures' on the desktop.

FullProf Studio must be installed and the extension '.fst' must be associated with it. (This may be done in Windows by right clicking on an fst file and changing the ¡Open with¿ options in the ¡Properties¿ area.) **You should close FullProf Studio when you have finished viewing a file.** Opening up several Studio windows will slow down your computer!

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# 2 Editing the FST file

The complete manual for Studio can be found in the FullProf documents directory. In this set of exercises only a few instructions and variables need to be changed. All variables are space delimited:

- The limits for the number of unit cells displayed along the a- b- and c-axes. In the example cells are drawn from 0 to 3 (a-axis), 0 to 3 (b-axis), 0 to 1 (c- axis)
  BOX 0.000 3.000 0.000 3.000 0.000 1.000

- The propagation vector of the magnetic structure
  K 0.0000 0.1470 0.0000

- The magnetic basis vector.
  The important parts for this exercise if is 3)-9): the real and imaginary basis vector components. Note that these are defined with respect to the space group axes, the natural axis system.
  SKP 1 1 1.000 0.000 0.000 0.000 1.000 0.000 0.000

- if the command GROUP is present, the contribitions from the different basis vectors for a site will be added together. If it is not present, they will be displayed separately.

# 3 The propagation vector

Magnetic structures can be described by the periodic repetition of a magnetic unit cell, just as crystal structures are described by translation of a nuclear unit cell. For convenience, rather than building a complete magnetic unit cell (which could contain thousands of magnetic atoms) we use a description based on the nuclear unit cell and a 'propagation vector', $\mathbf{k}$, that describes the relation between moment orientations of equivalent magnetic atoms in different nuclear unit cells. This provides a simple and a general formalism for the description of a magnetic structure.

We illustrate this for the moment distribution $m_j$ associated with the atom $j$ of a magnetic structure. This can be Fourier expanded, whatever the nature of the ordering, according to:

$$\mathbf{m}_j = \sum_k \mathbf{\Psi}_j^{\mathbf{k}} e^{2\pi i \mathbf{k}\cdot\mathbf{t}} \tag{1}$$

The summation can be made over several wave vectors that are confined to the first Brillouin zone of the Bravais lattice of the nuclear cell. If only one wave vector is involved, this simplifies to:

$$\mathbf{m}_j = \mathbf{\Psi}_j^{\mathbf{k}} e^{2\pi i \mathbf{k}\cdot\mathbf{t}} \tag{2}$$

This equation describes the translation properties of the vector, $\mathbf{\Psi}_j$, in direct space, which at present we can think of as the projections of the (complex) basis vector along the $a$, $b$, $c$ crystallographic axes with relation to the atomic site in the *zero*th (nuclear) cell.

At another atomic site (of the same type) in the crystal that is related by a lattice translation vector $\mathbf{t}$, the projections of the moment on the 3 crystallographic axes are related to those in the nuclear cell by Equation 2.

The following structure has the moments along the c-axis and has the propagation vector $\mathbf{k} = (0\ 0\ 0.5)$:

- Open k=0 0 0.5.fst

Exercises:

- Change the number along the c-axis, the direction of the modulation by the k-vector
- Change the number of cells along the a- and b- axes

Note how the k vector causes the moments to change along a specific direction. If the k vector is along $\mathbf{c}^*$, then cells displaced along a- or b- are unchanged. *The effect of the k vector is not to rotate the moments. It only phases them.*

If we know the basis vector that describes the moment orientation in the *zero*th cell and the propagation vector, we can use Equation 2 to calculate the basis vector and moment orientation, of any equivalent atom in the crystal structure.

## 3.1 The propagation vector in centred cells

A word of warning must be given when determining and using the propagation vector in centred cells, *i.e.* non-primitive cells. While the limits of the propagation vector are normally taken to be from 0 to 1 along the reciprocal axes, this **only** applies to primitive cells. In centred cells these limits may be exceeded.

It is recommended that indexing be carried out in the primitive cell to prevent confusion, or that primitive k vectors be generated and converted to the conventional centred cell where they can be used.

### 3.1.1 k=(000)

As an example of this difficulty, consider a body-centred structure. The diffraction pattern displays magnetic intensity on some of the nuclear peaks. It is a frequent assumption that the propagation vector of the magnetic structure is therefore $\mathbf{k} = (0\ 0\ 0)$. Below is a structure file for this value of the propagation vector. Equation 2 indicates that for all values of the translation vector $\mathbf{t}$, the exponential is null. It follows that all atoms in the crystal structure that are related to the first by **primitive lattice translations** have the same orientation as it.

- Open k=000.fst

### 3.1.2 k=(001)

Now look as the corresponding structure with propagation vector $\mathbf{k} = (0\ 0\ 1)$:

- Open k=001.fst

Exercises:

- Consider the phase in the exponential of Equation 2 for this k vector and the centring translation $\mathbf{t} = (0.5\ 0.5\ 0.5)$
- When converted to the primitive setting the value of the k vector is $\mathbf{k} = (0.5\ 0.5\ 0.5)$. The lattice translation is $\mathbf{t} = (1\ 0\ 0)$. What is the exponential phase?

*It does not matter whether a structure is defined in a primitive or non-primitive setting. However, it is important to state the setting (centred or non-centred) used to define the propagation vector. When dealing with centred systems, consider the primitive k vector.*

# 4 A linear combination of basis vectors

The general basis function, $\mathbf{\Psi}_j$, in Equation 1 is made up from contributions from several basis vectors defined by the weighting coefficients, $C_n$, where $n$ is the index of the basis vector:

$$\mathbf{\Psi}_j = \sum_n C_n \psi_n \tag{3}$$

or written in an alternative form:

$$\mathbf{\Psi}_j = C_1\psi_1 + C_2\psi_2... \quad (4)$$

It is important to remember that $C_n$ may be real, imaginary or complex.

*Whether basis vectors, $C_n$ and $\mathbf{\Psi}_j$, and the coefficients $C_n$ are real or imaginary defines how the moments of the magnetic structure change as you go from one cell to another. Using this description (in terms of Bloch waves) apparently complicated structures, like helices or cycloids, can be simply defined.*

## 4.1 Example- an Umbrella structure

In the following example the magnetic structure is made by adding (weighted) components from two basis vectors:

1. The first basis vector involves components that are in the *ab* plane: Open umbrella 1.fst
2. The second basis vector involves only components that are perpendicular to the *ab* plane(*i.e.* along the *c*-axis of this hexagonal system): Open umbrella 2.fst

The following fst file shows how these basis vectors can be combines to create an 'umbrella' structure.

- Open umbrella 3.fst

Exercise:

- Change the canting angle of the moments from the *ab* plane by changing the contribution from the second basis vector

*Understanding how basis vectors combine to make a magnetic structure is very important. If you look at components separately and think how they will combine, you will learn to read the basis vector space and understand the possible structures and their degrees of freedom*

# 5 Different types of magnetic structure

The previous section showed how basis vectors combine to describe a magnetic structure within the nuclear unit cell (more specifically, within the primitive unit cell which is the asymmetric unit). In this chapter we will see how this structure can be extended to propagate through the crystal structure using the propagation vector **k**. The role of the propagation vector and the importance of the different types of propagation vector will be emphasised.

## 5.1 Simple structures

As we have seen, the translation properties of a magnetic structure may be described by:

$$\mathbf{m}_j = \mathbf{\Psi}_j^{\mathbf{k}} e^{2\pi i \mathbf{k}\cdot\mathbf{t}} \tag{5}$$

Expanding the exponential we have:

$$\mathbf{m}_j = \mathbf{\Psi}_j^{\mathbf{k}} \left[\cos(2\pi\mathbf{k}\cdot\mathbf{t}) + i\sin(2\pi\mathbf{k}\cdot\mathbf{t})\right] \tag{6}$$

We will now consider various possibilities for the basis vector $\mathbf{\Psi_j}$ and the propagation vector **k** and some of the different types of magnetic structure that they can lead to.

### 5.1.1 $\Psi$ is real and the k is such that the sine component is null

This is the simplest situation and occurs when $\mathbf{\Psi}_j^{\mathbf{k}}$ is a not a complex basis vector (this is the case when $\mathbf{\Psi}_j^{\mathbf{k}}$ is real, or purely imaginary and so can be made real by multiplication by $i$).

The condition that $\mathbf{m}_j$ is real requires that the sine component is zero – this can occurs **only** for certain values of **k**, *i.e.* if $\mathbf{k} = (0\ 0\ 0)$ or if the vector has non-zero that are $\frac{1}{2}$, *e.g.* $\mathbf{k} = (0\ 0\ \frac{1}{2})$. Equation 6 then reduces to

$$\mathbf{m}_j = \mathbf{\Psi}_j^{\mathbf{k}} \cos(2\pi\mathbf{k}\cdot\mathbf{t}) \tag{7}$$

This is the situation in many simple ferromagnetic where the propagation vector is necessarily $\mathbf{k} = (0\ 0\ 0)$, ferrimagnetic where again it must be $\mathbf{k} = (0\ 0\ 0)$, and antiferromagnetic where the propagation vector is $\mathbf{k} = (0\ 0\ 0)$ or $\mathbf{k} = (0\ 0\ \frac{1}{2})$, $\mathbf{k} = (0\ \frac{1}{2}\ \frac{1}{2})$ *etc* structures.

Exercise:

- Open k=000.fst and change the k vector to $\mathbf{k} = (0\ 0\ 0.5)$ Look at how the moments in the second nuclear unit cell change from being in phase ($\mathbf{k} = (0\ 0\ 0)$) to being $\pi$ out of phase (*i.e.* reversed) for $\mathbf{k} = (0\ 0\ 0.5)$.

### 5.1.2 $\Psi$ is real and k is such that the sine component is non-zero

If the basis vector is real and the sine component is non-zero, Equation 6 leads to a magnetic moment that is complex – an unrealistic situation as the magnetic moment (or the spin density that creates it) is a real entity.

We are therefore left with the problem of how to relate our complex Fourier component to a real moment. Resolution of this problem in fact turns out to be very simple: the moment here cannot be described by a single propagation vector, but rather is described by contributions from 2 propagation vectors: the second propagation vector that is required in order to describe the magnetic moment distribution is the propagation vector -**k**. If **k** and -**k** are thought of as waves going in opposite directions, we see that their combination creates a standing wave that will be entirely real.

Using this approach the atomic vector for an atom in the $n$th cell related to that in the *zero*th cell by translation **t** is then given by:

$$\mathbf{m}_j = \mathbf{\Psi}_j^{\mathbf{k}} e^{2\pi i \mathbf{k}\cdot\mathbf{t}} + \mathbf{\Psi}_j^{-\mathbf{k}} e^{-2\pi i \mathbf{k}\cdot\mathbf{t}}, \tag{8}$$

where,

$$\mathbf{\Psi}_j^{-\boldsymbol{k}} = \mathbf{\Psi}_j^{\mathbf{k}^*} \tag{9}$$

Insertion of this relation into Equation 8 and expansion of the exponential leads to

$$\mathbf{m}_j = 2\mathrm{Re}(\mathbf{\Psi}_j^{\mathbf{k}})\cos(2\pi\mathbf{k}\cdot\mathbf{t}) + 2\mathrm{Im}(\mathbf{\Psi}_j^{\mathbf{k}})\sin(2\pi\mathbf{k}\cdot\mathbf{t}) \tag{10}$$

As we are considering real basis vectors, the imaginary component in Equation 10 is zero and this reduces to

$$\mathbf{m}_j = 2\mathrm{Re}(\mathbf{\Psi}_j^{\mathbf{k}})\cos(2\pi\mathbf{k}\cdot\mathbf{t}) \tag{11}$$

The resulting structure therefore has a cosine modulation. For historical reasons it is commonly referred to as a 'sine structure'. There are 2 limiting types of sine structure, these are detailed below.

Exercise:

- Open k=0 0 0.5.fst and look at how changing the k vector to $\mathbf{k} = (0\ 0\ 0.25)$, $\mathbf{k} = (0\ 0\ 0.2145)$, and corresponds to changing the periodicity with which the magnetic structure propagates through the crystal.

Small values of a component of **k** correspond to long wavelength component in direct space.

This example involved both commensurate and incommensurate k vectors. Changing the k value away from the symmetric **k** = (0 0 0.5) lead to a non-zero sine component in Equation 6. Adding the component of -k is required and this leads to a modulation in the size of the moments as the magnetic structure propagates through the crystal structure (this addition is performed automatically by FpStudio, so you do not need to worry about it. Just understand that it is happening in the background.). There is no intrinsic difference between **k** = (0 0 0.25) and **k** = (0 0 0.2145) as **k** = (0 0 0.25) is not a symmetry point. While one is commensurate and the other not, they both lead to spin density waves.

## 5.2 Transverse Sine Wave- a Spin Density Wave

In this case, the basis vector is perpendicular to the propagation vector:

- Open transverse SDW.fst

## 5.3 Longitudinal Sine Wave- a Spin Density Wave

In this case, the basis vector is parallel to the propagation vector:

- Open longitudinal SDW.fst

## 5.4 Non-collinear incommensurate structures

### 5.4.1 Ψ is complex, k is incommensurate, and the real and imaginary components are transverse and equal in magnitude

As the **k** vector is incommensurate contributions are required from the vector **k** and from -**k**. Therefore, we begin again from Equation 10:

$$\mathbf{m}_j = 2\mathrm{Re}(\mathbf{\Psi}_j^{\mathbf{k}})\cos(2\pi\mathbf{k}\cdot\mathbf{t}) + 2\mathrm{Im}(\mathbf{\Psi}_j^{\mathbf{k}})\sin(2\pi\mathbf{k}\cdot\mathbf{t}) \qquad (12)$$

The resultant structure is made up of a component that is modulated according to a cosine function and a component transverse to it that follows a sine function, *i.e.* two transverse components with a phase difference of $\pi/2$. This forma a helix.

If the sine and cosine components are of the same length they may be projected onto a circle, the resulting structure is said to be a 'circular helix', *i.e.* one in which the magnitude of the moment is constant, but its orientation changes.

### 5.4.2 Ψ is complex, k is incommensurate, and the real and imaginary components are transverse and not equal in magnitude

As the real and imaginary components are of different size, the equation

$$\mathbf{m}_j = 2\mathrm{Re}(\mathbf{\Psi}_j^{\mathbf{k}})\cos(2\pi\mathbf{k}\cdot\mathbf{t}) + 2\mathrm{Im}(\mathbf{\Psi}_j^{\mathbf{k}})\sin(2\pi\mathbf{k}\cdot\mathbf{t}) \quad (13)$$

describes an incommensurate structure that projects onto an ellipse rather than a circle. The resulting structure is referred to as an 'elliptical helix'

## 5.5 Helical structures: circular helices and elliptical helices

The following files show how the non-collinear real and imaginary components add together to form a helix:

- Open helix separated components.fst
- Open helix.fst

## 5.6 Cycloidal structures

In the previous examples of circular and elliptical helices, the basis vectors (and moment components) lie in a plane that is perpendicular to the propagation vector **k**. If the basis vectors have components that are parallel to **k**, this component will change in magnitude and sign as the structure propagates. The result is a magnetic structure where the moments appear to twist, this is called a cycloid.

So, a cycloidal structure is one where the moments turn in the direction of the propagation vector.

- cycloid.fst

The following file shows the separate components

- Open cycloid separated components.fst

These components may toggled to contribute together by changing the line:
MATOM Fe FE .0000 .5000 .0000 SCALE 2.0
to
MATOM Fe FE .0000 .5000 .0000 SCALE 2.0 GROUP

*Cycloids have become very important in recent research because their symmetry is such that they can allow a coupling to occur between the moments and the electric dipoles. This can cause the magnetic ordering and electronic dipole ordering to be linked, leading to a new type of multiferroic behaviour.*

# References


[1] J. Rossat-Mignod in: 'Methods in Experimental Physics', ed. K. Sköld and D.L. Price (Academic Press, 1987). J. Rossat-Mignod in 'Systematics and the Propeties of the Lanthanides', Ed. S.P. Sinha, D. Reidel Publishing (1983).
*This is a classic text going into magnetic symmetry and types of magnetic order. I thoroughly recommend it and make all my students read it!*

[2] J. Schweizer, in: 'Hercules- Neutron and Synchrotron Radiation for Condensed Matter Research', Springer Verlag, Berlin (1994).
*Another good text bringing the ideas of magnetic structures and representational theory together.*

[3] A.S. Wills, *Physica B* **276-278**, 680 (2000). A new protocol for the determination of magnetic structures using Simulated Annealing and Representational Analysis- SARA*h* - Program available from www.ccp14.ac.uk.
*SARAh was built to allow the refinement of magnetic structures in terms of the weighted sum of basis vectors. Looking back, it was the first program to work this way and it was transformative. It inspired ideas that have been taken forward in FullProf, TOPAS and hopefully in GSAS-II.*

[4] A.S. Wills, *Zeitschrift fr Kristallographie Supplement* **30**, 39 (2009).
*This paper has some new ideas of how you can use the Brillouin zone to help determine the value of the propagation vector* **k** *from powder data. The routines in SARAh are the first to use algebraic searches through the points, lines and planes of the Brillouin zone and to couple these ideas with Monte Carlo direct space refinement.*

[5] A.S. Wills, *Zeitschrift fr Kristallographie Supplement* **26**, 53 (2007), Validation of magnetic structures.
*This paper has the goal of giving a simple description of what information is required to describe a magnetic structure.*