

Introduction to Magnetic Neutron Diffraction and Magnetic Structures

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Outline:

1. Magnetic Structures and neutron scattering
2. Symmetry and Magnetic Structures
3. Magnetic Structure determination

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- 1. Magnetic Structures and neutron scattering**
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Magnetic dipole moment in classical electromagnetism



In terms of orbital angular momentum for an electron

$$\boldsymbol{\mu}_L = -\left(\frac{e}{2m_e}\right)\mathbf{L}$$

$$\boldsymbol{\mu}_S = -\left(\frac{e}{m_e}\right)\mathbf{S}$$

$$\mathbf{J} = \mathbf{L} + \mathbf{S}$$

Dirac postulated in 1928 that the electron should have an *intrinsic* angular momentum: the “spin”

$$\boldsymbol{\mu}_J = -g\left(\frac{e}{2m_e}\right)\mathbf{J}$$

Magnetic moment

Angular momenta are measured in units of $\hbar = \frac{h}{2\pi}$

$$\boldsymbol{\mu} = -g\mu_B\mathbf{J} \quad \text{with} \quad \mu_B = \frac{e\hbar}{2m_e} \quad \text{Bohr Magnetron}$$

The gyromagnetic ratio is defined as the ratio of the magnetic dipole moment to the total angular momentum

$$\gamma = -g\left(\frac{e}{2m_e}\right) \rightarrow -g\mu_B = \gamma\hbar$$

So we have: $\boldsymbol{\mu} = -g\mu_B\mathbf{J} = \gamma\hbar\mathbf{J}$

Magnetic properties of the neutron

According to quantum mechanics the classical angular momentum is replaced by an operator σ

$$\mu = \gamma \hbar \sigma$$

The neutrons have a spin-only angular momentum operator with eigenvalues $\pm \frac{1}{2} \hbar$. The components of the operator σ for a spin- $\frac{1}{2}$ particle are the Pauli spin matrices:

$$\sigma_x = \frac{1}{2} \hbar \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_y = \frac{1}{2} \hbar \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_z = \frac{1}{2} \hbar \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Magnetic properties of the neutron

Gyromagnetic ratios of common spin-1/2 particles

Electron: 1.76×10^5 MHz/T

Proton: 267 MHz/T

Neutron: 183 MHz/T

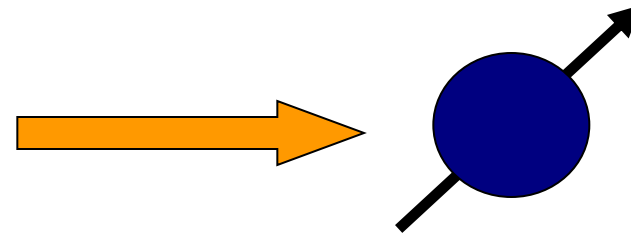
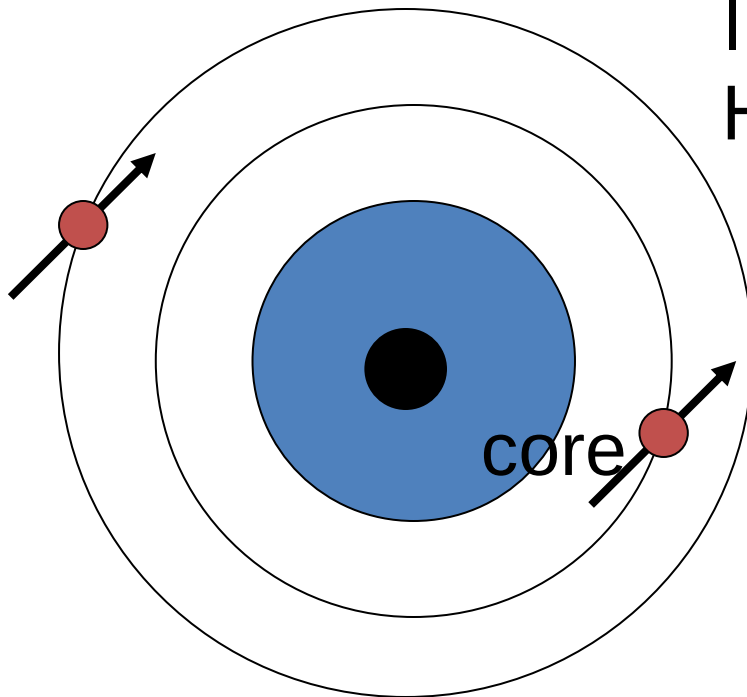
The neutron moment is around 960 times smaller than the electron moment.

Nuclear magnetons: $\mu_N = \frac{e\hbar}{2m_p}$ proton $\mu_p = 2.793\mu_N$ neutron $\mu_n = 1.913\mu_N$

For neutrons: $\boldsymbol{\mu}_n = -\gamma_n \mu_N \boldsymbol{\sigma}$ with $\gamma_n = 1.913$

Atoms/ions with unpaired electrons

Intra-atomic electron correlation
Hund's rule: maximum S/J



Ni^{2+}

$$\mathbf{m} = -g_J \mu_B \mathbf{J} \quad (\text{rare earths})$$

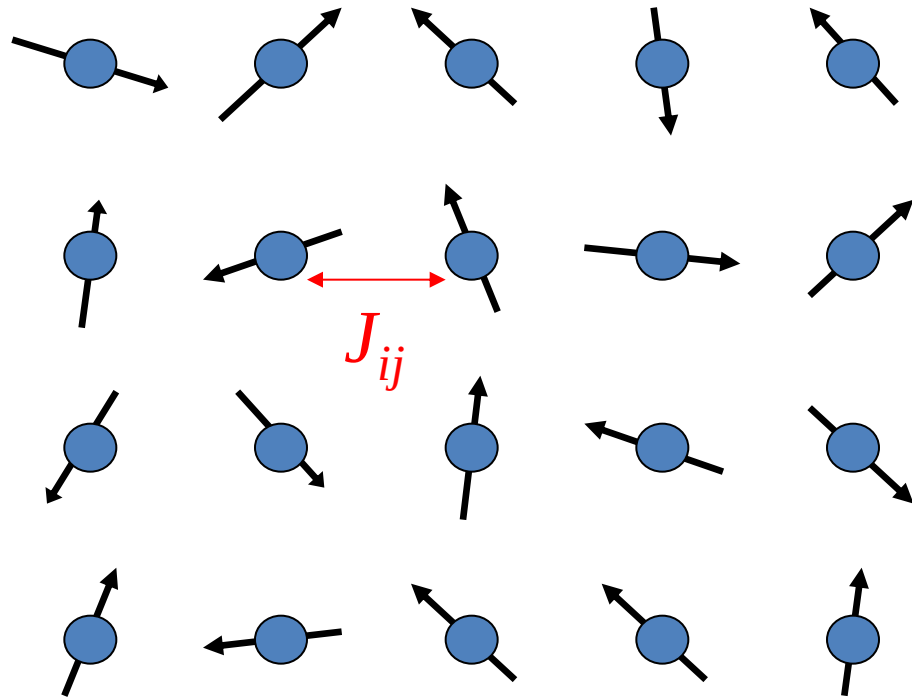
$$\mathbf{m} = -g_S \mu_B \mathbf{S} \quad (\text{transition metals})$$

What is a magnetic structure?

Paramagnetic state:
Snapshot of magnetic moment configuration

$$E_{ij} = -J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j$$

$$\langle \mathbf{S}_i \rangle = 0$$



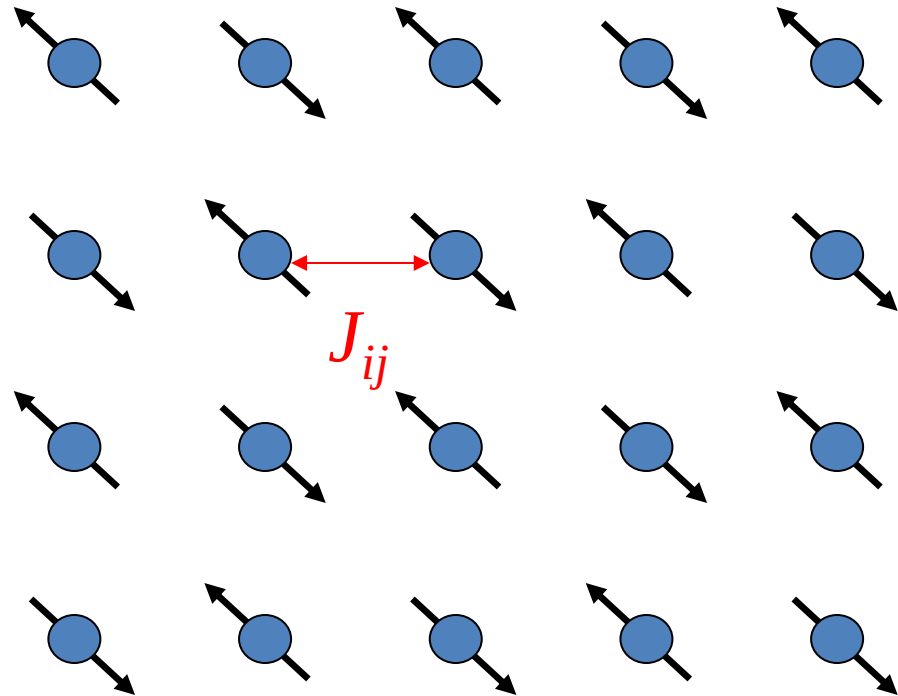
What is a magnetic structure?

Ordered state: Anti-ferromagnetic

Small fluctuations (spin waves) of the static configuration

$$E_{ij} = -J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j$$

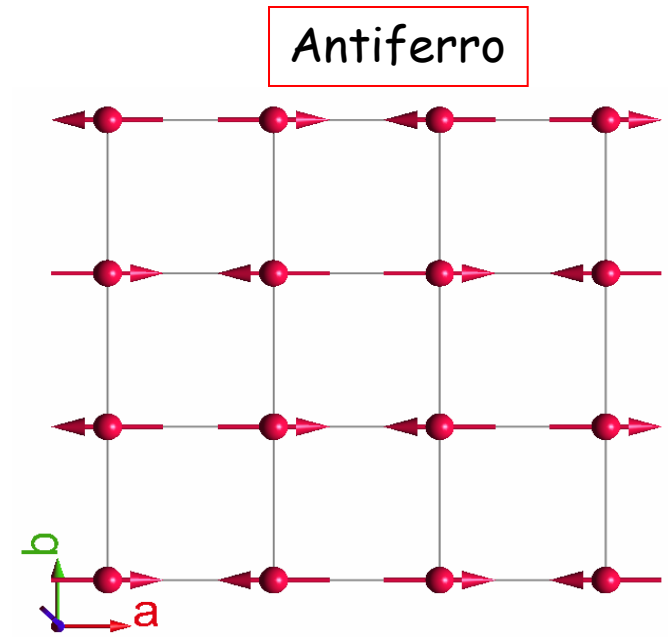
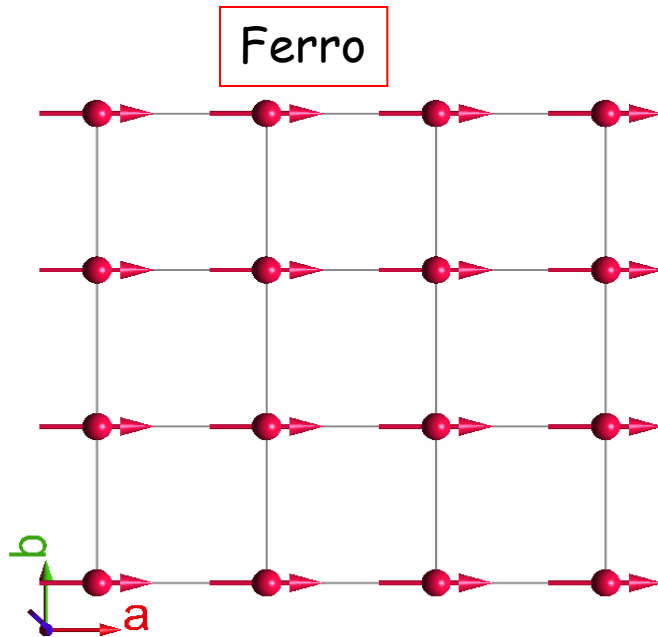
$$\langle \mathbf{S}_i \rangle \neq 0$$



Magnetic structure:

Quasi-static configuration of magnetic moments

Types of magnetic structures



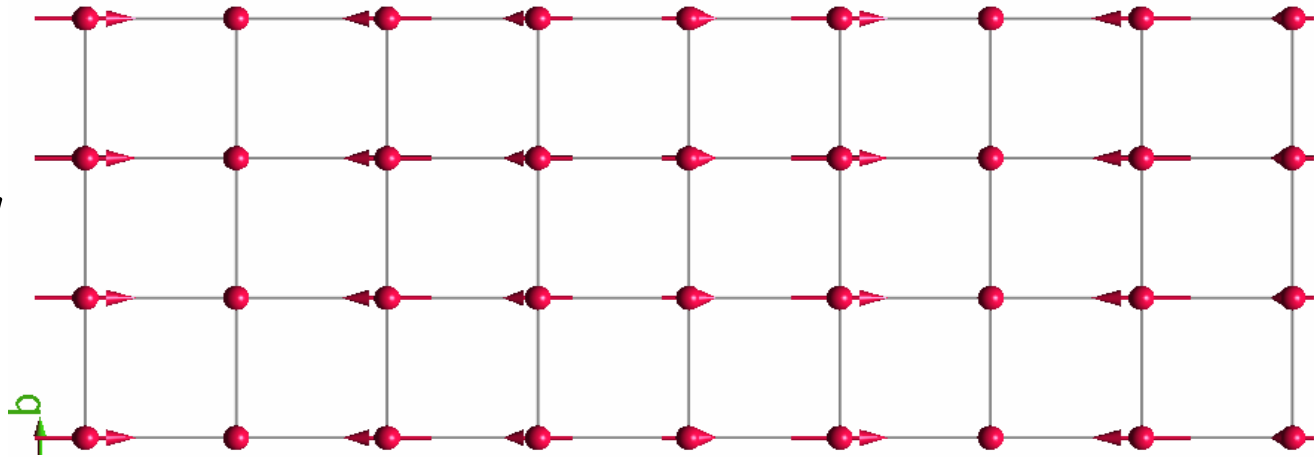
Very often magnetic structures are complex due to :

- competing exchange interactions (i.e. RKKY)
- geometrical frustration
- competition between exchange and single ion anisotropy
-

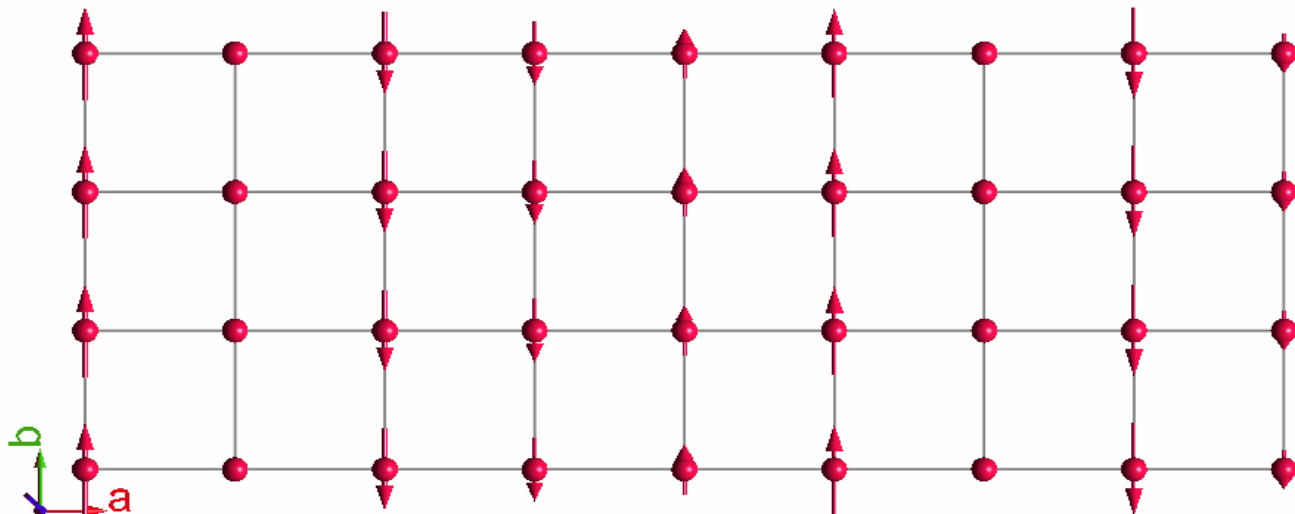
Types of magnetic structures

Amplitude-modulated or Spin-Density Waves

"Longitudinal"

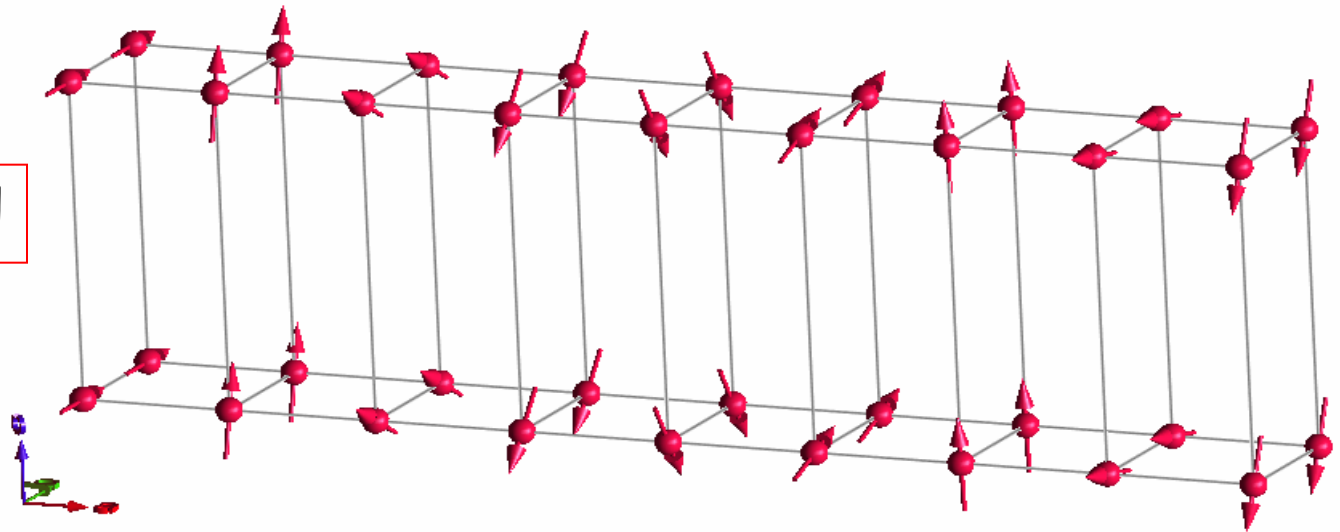


"Transverse"

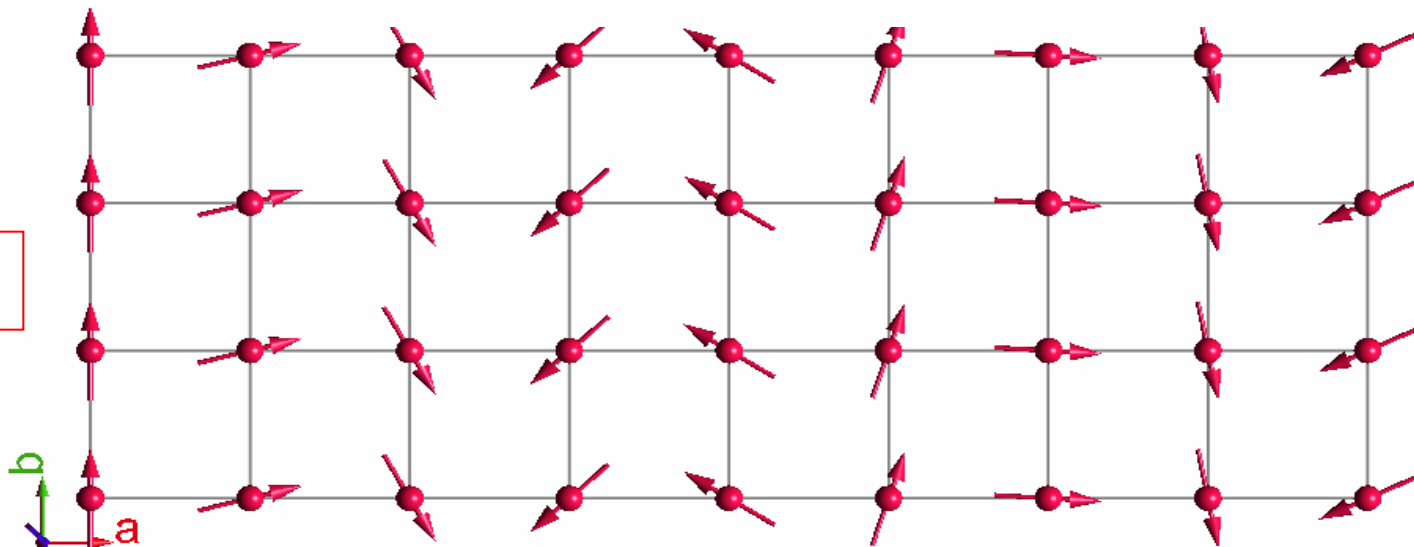


Types of magnetic structures

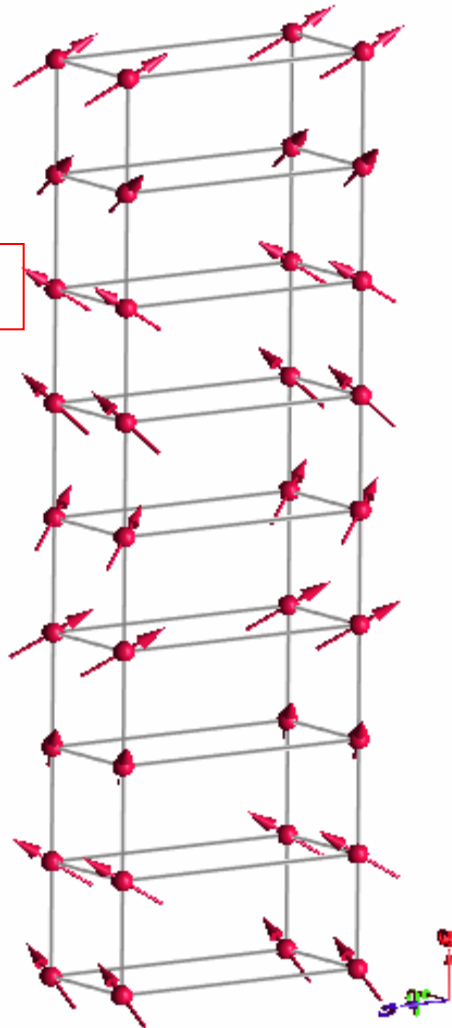
Spiral



Cycloid



Types of magnetic structures



The (magnetic) structure of crystalline solids possess always a series of geometrical transformations that leave invariant the atomic (spin) arrangement.

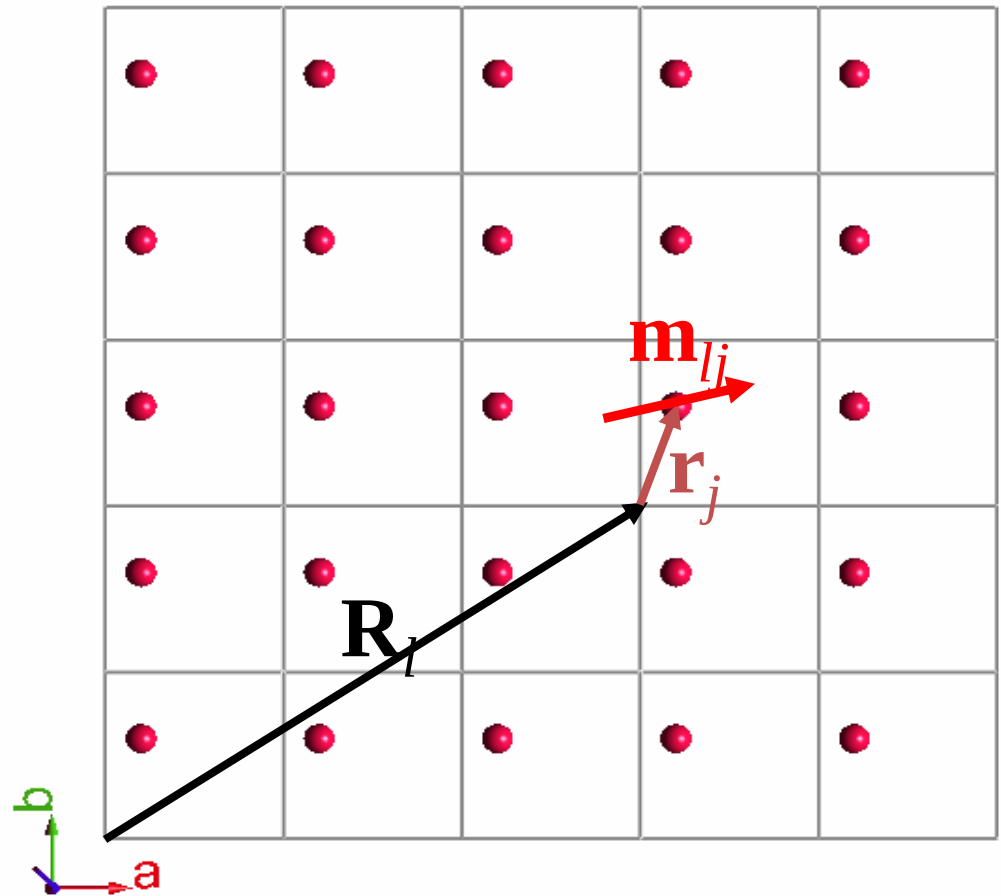
These transformations constitute a **symmetry group** in the mathematical sense: point groups, space groups, Shubnikov groups, superspace groups, ...

The Shubnikov groups describe commensurate magnetic structures

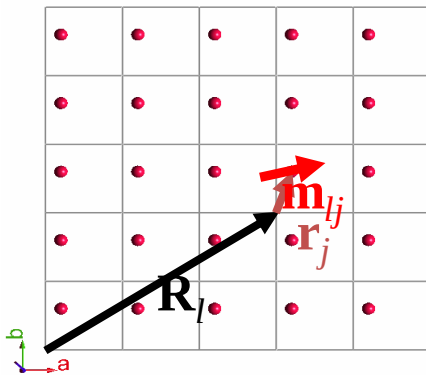
The position of atom j in unit-cell l is given by:

$$\mathbf{R}_{lj} = \mathbf{R}_l + \mathbf{r}_j$$

where $\mathbf{R}_l$ is a pure lattice translation



Whatever kind of magnetic structure in a crystal can be described mathematically by using a Fourier series



$$\mathbf{m}_{lj} = \sum_{\{\mathbf{k}\}} \mathbf{S}_{\mathbf{k}j} \exp\{-2\pi i \mathbf{k} \mathbf{R}_l\}$$

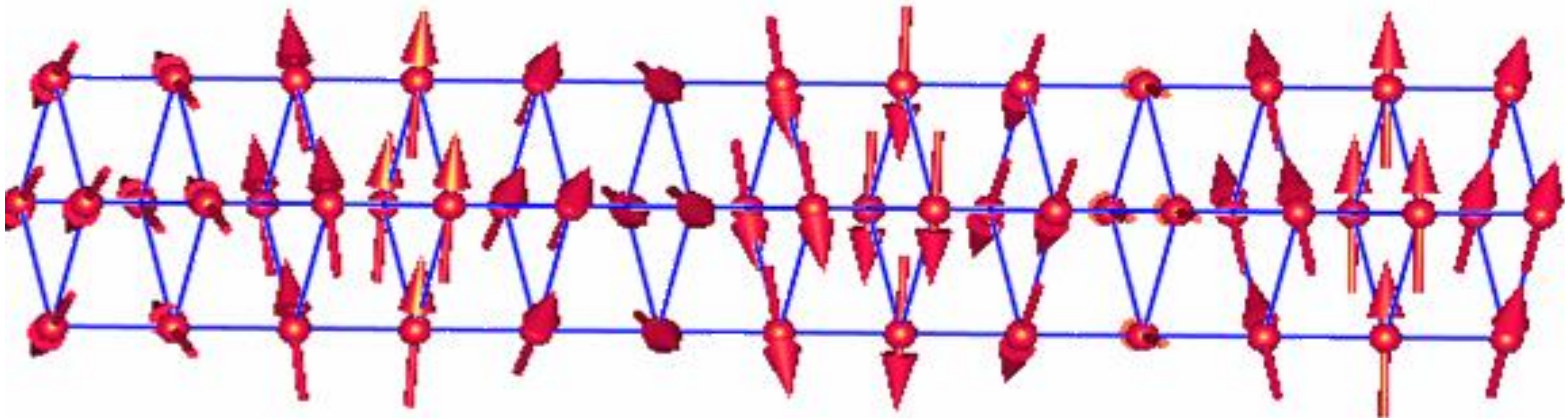
$$\mathbf{R}_{lj} = \mathbf{R}_l + \mathbf{r}_j = l_1 \mathbf{a} + l_2 \mathbf{b} + l_3 \mathbf{c} + x_j \mathbf{a} + y_j \mathbf{b} + z_j \mathbf{c}$$

Necessary condition for real $\mathbf{m}_{lj}$

$$\mathbf{S}_{-\mathbf{k}j} = \mathbf{S}_{\mathbf{k}j}^*$$

A magnetic structure is fully described by:

- i) Wave-vector(s) or propagation vector(s) $\{\mathbf{k}\}$.
- ii) Fourier components $S_{\mathbf{k}j}$ for each magnetic atom j and wave-vector $\mathbf{k}$, $S_{\mathbf{k}j}$ is a complex vector (6 components) !!!



$$\mathbf{m}_{ljs} = \sum_{\{\mathbf{k}\}} \mathbf{S}_{\mathbf{k}js} \exp\{-2\pi i \mathbf{k} \mathbf{R}_l\}$$

l : index of a direct lattice point (origin of an arbitrary unit cell)

j : index for a Wyckoff site (orbit)

s : index of a sublattice of the j site

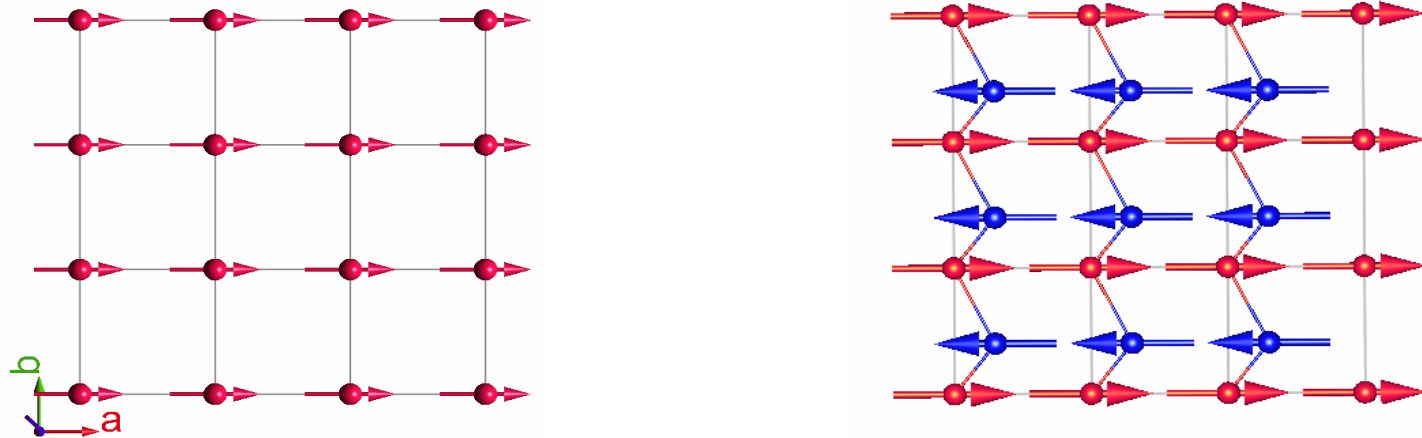
Necessary condition for real moments $\mathbf{m}_{ljs} \Rightarrow \mathbf{S}_{-\mathbf{k}js} = \mathbf{S}_{\mathbf{k}js}^*$

General expression of the Fourier coefficients (complex vectors) for an arbitrary site (drop of js indices) when $\mathbf{k}$ and $-\mathbf{k}$ are not equivalent:

$$\mathbf{S}_{\mathbf{k}} = \frac{1}{2} (\mathbf{R}_{\mathbf{k}} + i \mathbf{I}_{\mathbf{k}}) \exp\{-2\pi i \phi_{\mathbf{k}}\}$$

Only six parameters are independent. The writing above is convenient when relations between the vectors $\mathbf{R}$ and $\mathbf{I}$ are established (e.g. when $|\mathbf{R}| = |\mathbf{I}|$, or $\mathbf{R} \cdot \mathbf{I} = 0$)

Single propagation vector: $\mathbf{k}=(0,0,0)$

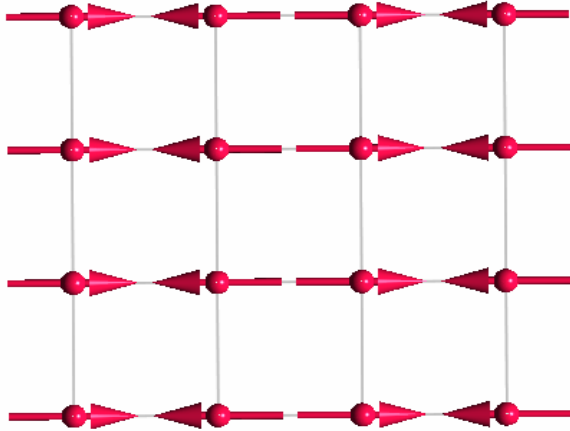


The propagation vector $\mathbf{k}=(0,0,0)$ is at the centre of the Brillouin Zone.

$$\mathbf{m}_{lj} = \sum_{\{\mathbf{k}\}} \mathbf{S}_{\mathbf{k}j} \exp\{ -2\pi i \mathbf{k} \mathbf{R}_l \} = \mathbf{S}_{\mathbf{k}j} = \mathbf{R}_{\mathbf{k}}$$

- The magnetic structure may be described within the crystallographic unit cell
- Magnetic symmetry: conventional crystallography plus spin reversal operator: crystallographic magnetic groups

Single propagation vector: $\mathbf{k} = \frac{1}{2}\mathbf{H}$



The propagation vector is a special point of the Brillouin Zone surface and $\mathbf{k} = \frac{1}{2}\mathbf{H}$, where $\mathbf{H}$ is a reciprocal lattice vector.

$$\mathbf{m}_{lj} = \sum_{\{\mathbf{k}\}} \mathbf{S}_{\mathbf{k}j} \exp\{-2\pi i \mathbf{k} \mathbf{R}_l\} = \mathbf{S}_{\mathbf{k}j} \exp\{-\pi i \mathbf{H} \mathbf{R}_l\}$$

$$\mathbf{m}_{lj} = \mathbf{S}_{\mathbf{k}j} (-1)^{n(l)}$$

REAL Fourier coefficients $\equiv$ magnetic moments

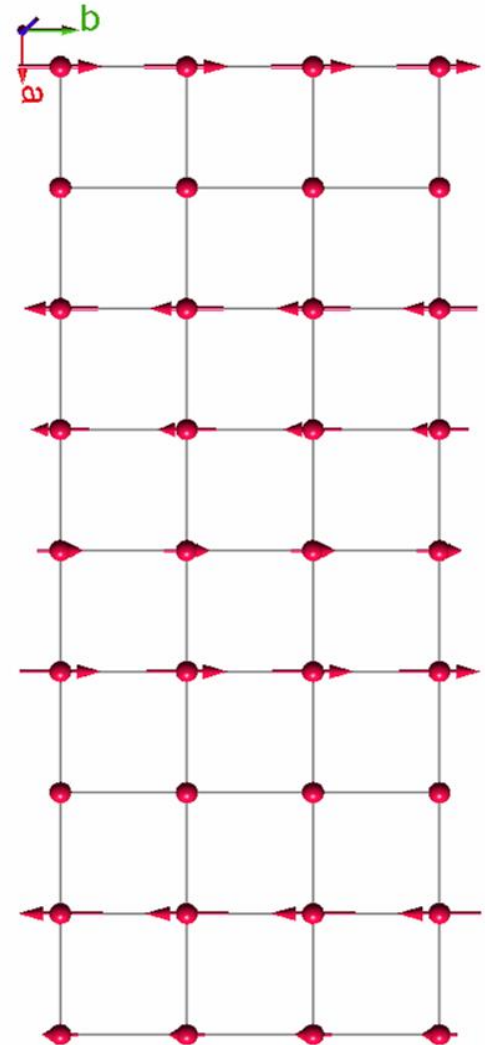
The magnetic symmetry may also be described using crystallographic magnetic space groups

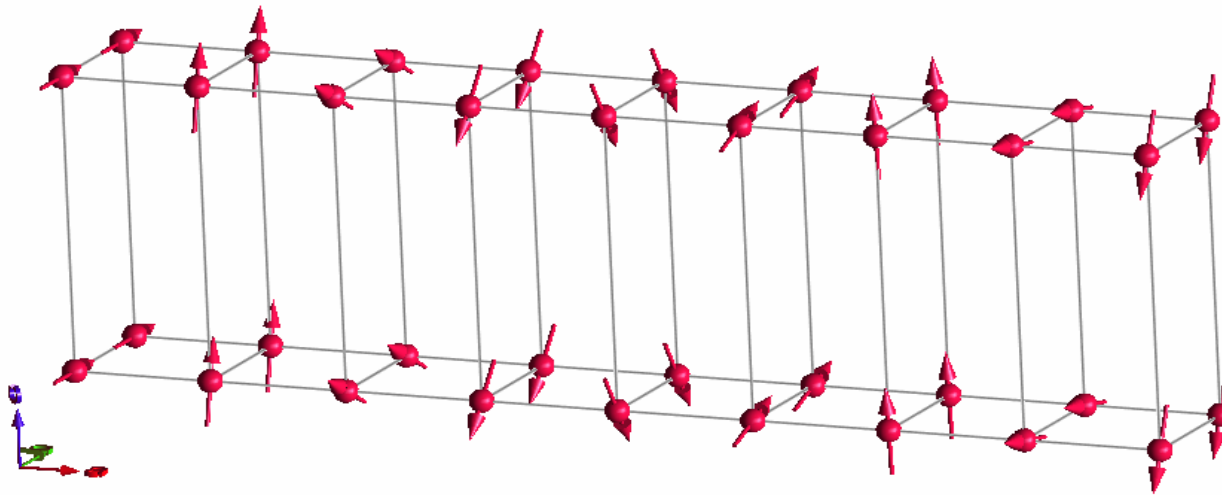
- $\mathbf{k}$ interior of the Brillouin zone (IBZ)
(pair $\mathbf{k}$, $-\mathbf{k}$)
- Real $S_{\mathbf{k}}$, or imaginary component in the
same direction as the real one

$$\mathbf{m}_{lj} = S_{\mathbf{k}j} \exp(-2\pi i \mathbf{k} \mathbf{R}_l) + S_{-\mathbf{k}j} \exp(2\pi i \mathbf{k} \mathbf{R}_l)$$

$$S_{\mathbf{k}j} = \frac{1}{2} m_j \mathbf{u}_j \exp(-2\pi i \phi_{\mathbf{k}j})$$

$$\mathbf{m}_{lj} = m_j \mathbf{u}_j \cos 2\pi(\mathbf{k} \mathbf{R}_l + \phi_{\mathbf{k}j})$$



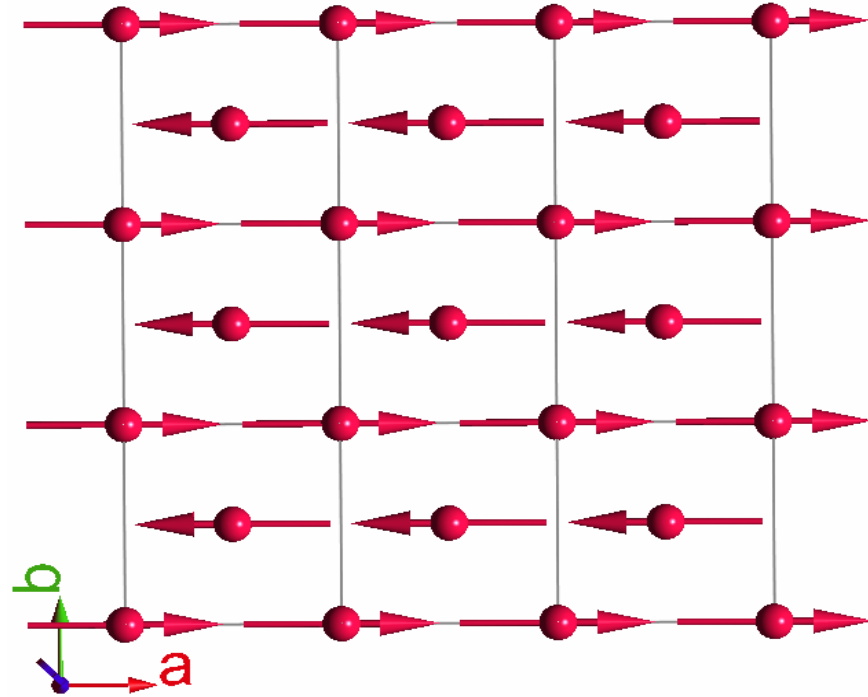


- $\mathbf{k}$ interior of the Brillouin zone
- Real component of $\mathbf{S}_{\mathbf{k}}$ perpendicular to the imaginary component

$$\mathbf{S}_{\mathbf{k}j} = \frac{1}{2} [m_{uj} \mathbf{u}_j + im_{vj} \mathbf{v}_j] \exp(-2\pi i \phi_{\mathbf{k}j})$$

$$\mathbf{m}_{lj} = m_{uj} \mathbf{u}_j \cos 2\pi(\mathbf{kR}_l + \phi_{\mathbf{k}j}) + m_{vj} \mathbf{v}_j \sin 2\pi(\mathbf{kR}_l + \phi_{\mathbf{k}j})$$

Note on centred cells



$$\mathbf{m}_{lj} = \sum_{\{\mathbf{k}\}} \mathbf{S}_{\mathbf{k}j} \exp\{-2\pi i \mathbf{k} \mathbf{R}_l\}$$

The $\mathbf{k}$ vectors are referred to the reciprocal basis of the conventional direct cell and for centred cells may have values $> 1/2$

$\mathbf{k}=(1,0,0)$ or $(0,1,0)$?

$$\mathbf{R}_{lj} = \mathbf{R}_l + \mathbf{r}_j = l_1 \mathbf{a} + l_2 \mathbf{b} + l_3 \mathbf{c} + x_j \mathbf{a} + y_j \mathbf{b} + z_j \mathbf{c}$$

The translation vectors have fractional components when using centred cells. The index j runs on the atoms contained in a PRIMITIVE cell

$$\mathbf{m}_{ljs} = \sum_{\{\mathbf{k}\}} \mathbf{S}_{\mathbf{k}js} \exp\{-2\pi i \mathbf{k} \mathbf{R}_l\}$$

The program **FullProf Studio** performs the above sum and represents graphically the magnetic structure.

This program can help to learn about this formalism because the user can write manually the Fourier coefficients and see what is the corresponding magnetic structure immediately.

Web site: <http://www.ill.eu/sites/fullprof>

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1. Magnetic Structures and **neutron scattering**
2. Symmetry and Magnetic Structures
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Differential neutron cross-section:

$$\left(\frac{d^2\sigma}{d\Omega dE'} \right)_{s\lambda \rightarrow s'\lambda'} = \frac{k'}{k} \left(\frac{m_n}{2\pi\hbar^2} \right)^2 \left| \langle \mathbf{k}' s' \lambda' | V_m | \mathbf{k} s \lambda \rangle \right|^2 \delta(E_\lambda - E_{\lambda'} + \hbar\omega)$$

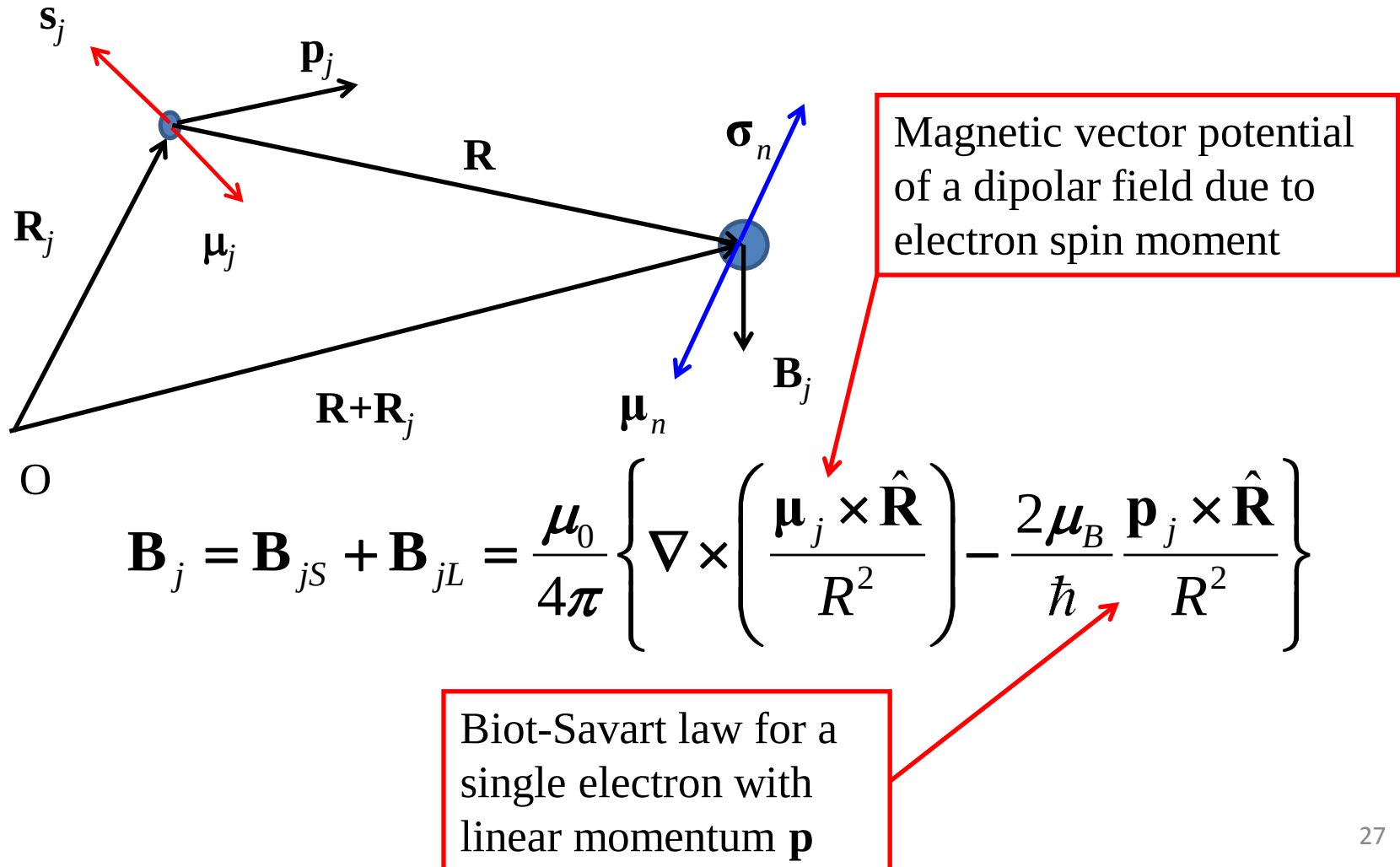
This expression describes all processes in which:

- The state of the scatterer changes from λ to λ'
- The wave vector of the neutron changes from $\mathbf{k}$ to $\mathbf{k}'$ where $\mathbf{k}'$ lies within the solid angle $d\Omega$
- The spin state of the neutron changes from s to s'

$V_m = \boldsymbol{\mu}_n \cdot \mathbf{B}$ is the potential felt by the neutron due to the magnetic field created by moving electrons. It has an orbital and spin part.

Magnetic scattering: magnetic fields

Magnetic field due to spin and orbital moments of an electron:



Evaluating the spatial part of the transition matrix element for electron j :

$$\langle \mathbf{k}' | V_m^j | \mathbf{k} \rangle \propto \exp(i\mathbf{Q}\mathbf{R}_j) \left\{ \hat{\mathbf{Q}} \times (\mathbf{s}_j \times \hat{\mathbf{Q}}) + \frac{i}{\hbar Q} (\mathbf{p}_j \times \hat{\mathbf{Q}}) \right\}$$

Where $\hbar\mathbf{Q} = \hbar(\mathbf{k} - \mathbf{k}')$ is the momentum transfer

Summing for all unpaired electrons we obtain:

$$\sum_j \langle \mathbf{k}' | V_m^j | \mathbf{k} \rangle \propto \hat{\mathbf{Q}} \times (\mathbf{M}(\mathbf{Q}) \times \hat{\mathbf{Q}}) = \mathbf{M}(\mathbf{Q}) - (\mathbf{M}(\mathbf{Q}) \cdot \hat{\mathbf{Q}}) \hat{\mathbf{Q}} = \mathbf{M}_\perp(\mathbf{Q})$$

$\mathbf{M}_\perp(\mathbf{Q})$ is the perpendicular component of the Fourier transform of the magnetisation in the scattering object to the scattering vector. It includes the orbital and spin contributions.

$\mathbf{M}_\perp(\mathbf{Q})$ is the perpendicular component of the Fourier transform of the magnetisation in the sample to the scattering vector.

Magnetic structure factor

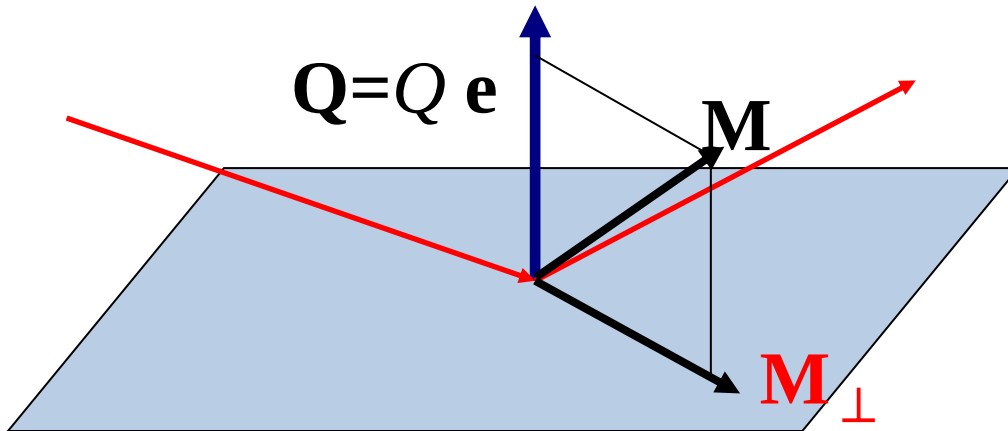
$$\mathbf{M}(\mathbf{Q}) = \int \mathbf{M}(\mathbf{r}) \exp(i\mathbf{Q} \cdot \mathbf{r}) d^3\mathbf{r}$$

Magnetic interaction vector

$$\mathbf{M}_\perp = \mathbf{e} \times \mathbf{M} \times \mathbf{e} = \mathbf{M} - \mathbf{e}(\mathbf{e} \cdot \mathbf{M})$$

Elastic scattering:

$$\left(\frac{d\sigma}{d\Omega} \right) = (\gamma r_0)^2 \mathbf{M}_\perp^* \mathbf{M}_\perp$$



Neutrons only see the components of the magnetisation that are perpendicular to the scattering vector

Scattering by a collection of magnetic atoms

We will consider in the following only elastic scattering.

We suppose the magnetic matter made of atoms with unpaired electrons that remain close to the nuclei.

Vector position of electron e : $\mathbf{R}_e = \mathbf{R}_{lj} + \mathbf{r}_{je}$

The Fourier transform of the magnetization can be written in discrete form as

$$\mathbf{M}(\mathbf{Q}) = \sum_e \mathbf{s}_e \exp(i\mathbf{Q} \cdot \mathbf{R}_e) = \sum_{lj} \exp(i\mathbf{Q} \cdot \mathbf{R}_{lj}) \sum_{e_j} \exp(i\mathbf{Q} \cdot \mathbf{r}_{je}) \mathbf{s}_{je}$$

$$\mathbf{F}_j(\mathbf{Q}) = \sum_e \mathbf{s}_{je} \exp(i\mathbf{Q} \cdot \mathbf{r}_{je}) = \int \boldsymbol{\rho}_j(\mathbf{r}) \exp(i\mathbf{Q} \cdot \mathbf{r}) d^3\mathbf{r}$$

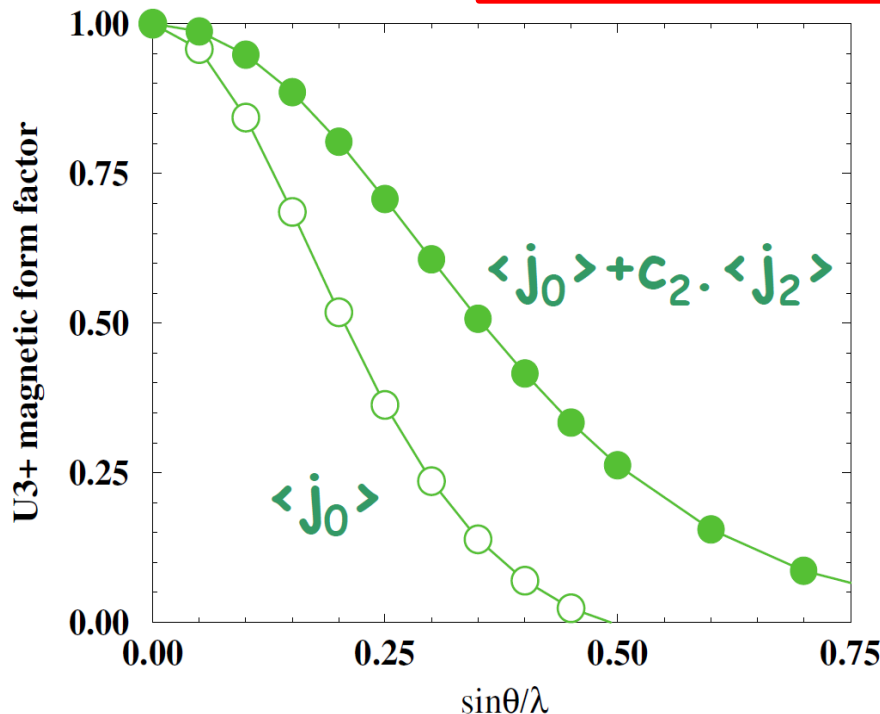
$$\mathbf{F}_j(\mathbf{Q}) = \mathbf{m}_j \int \rho_j(\mathbf{r}) \exp(i\mathbf{Q} \cdot \mathbf{r}) d^3\mathbf{r} = \mathbf{m}_j f_j(\mathbf{Q})$$

$$\mathbf{M}(\mathbf{Q}) = \sum_{lj} \mathbf{m}_{lj} f_{lj}(\mathbf{Q}) \exp(i\mathbf{Q} \cdot \mathbf{R}_{lj})$$

Scattering by a collection of magnetic atoms

$$\mathbf{F}_j(\mathbf{Q}) = \sum_e \mathbf{s}_{je} \exp(i\mathbf{Q} \cdot \mathbf{r}_{je}) = \int \boldsymbol{\rho}_j(\mathbf{r}) \exp(i\mathbf{Q} \cdot \mathbf{r}) d^3\mathbf{r}$$

$$\mathbf{F}_j(\mathbf{Q}) = \mathbf{m}_j \int \boldsymbol{\rho}_j(\mathbf{r}) \exp(i\mathbf{Q} \cdot \mathbf{r}) d^3\mathbf{r} = \mathbf{m}_j f_j(Q)$$



If we use the common variable $s = \sin\theta/\lambda$, then the expression of the form factor is the following:

$$f(s) = \sum_{l=0,2,4,6} W_l \langle j_l(s) \rangle$$

$$\langle j_l(s) \rangle = \int_0^\infty U^2(r) j_l(4\pi sr) 4\pi r^2 dr$$

$$\langle j_l(s) \rangle = s^2 \left(A_l \exp\{-a_l s^2\} + B_l \exp\{-b_l s^2\} + C_l \exp\{-c_l s^2\} + D_l \right) \quad \text{for } l = 2, 4, 6$$

$$\langle j_0(s) \rangle = A_0 \exp\{-a_0 s^2\} + B_0 \exp\{-b_0 s^2\} + C_0 \exp\{-c_0 s^2\} + D_0$$

Elastic Magnetic Scattering by a crystal (1)



The Fourier transform of the magnetization of atomic discrete objects can be written in terms of atomic magnetic moments and a form factor for taking into account the spread of the density around the atoms

$$\mathbf{M}(\mathbf{Q}) = \sum_{lj} \mathbf{m}_{lj} f_{lj}(Q) \exp(i\mathbf{Q} \cdot \mathbf{R}_{lj})$$

For a crystal with a commensurate magnetic structure the content of all unit cell is identical, so the expression above becomes factorised as:

$$\mathbf{M}(\mathbf{Q}) = \sum_j \mathbf{m}_j f_j(Q) \exp(i\mathbf{Q} \cdot \mathbf{r}_j) \sum_l \exp(i\mathbf{Q} \cdot \mathbf{R}_l) \propto \sum_j \mathbf{m}_j f_j(Q) \exp(2\pi i \mathbf{H} \cdot \mathbf{r}_j)$$

The lattice sum is only different from zero when $\mathbf{Q} = 2\pi\mathbf{H}$, where $\mathbf{H}$ is a reciprocal lattice vector of the magnetic lattice. The vector $\mathbf{M}$ is then proportional to the magnetic structure factor of the magnetic cell

Elastic Magnetic Scattering by a crystal (2)

For a general magnetic structure that can be described as a Fourier series:

$$\mathbf{m}_{lj} = \sum_{\{\mathbf{k}\}} \mathbf{S}_{\mathbf{k}j} \exp\{-2\pi i \mathbf{k} \mathbf{R}_l\}$$

$$\mathbf{M}(\mathbf{h}) = \sum_{lj} \sum_{\mathbf{k}} \mathbf{S}_{\mathbf{k}j} \exp(-2\pi i \mathbf{k} \mathbf{R}_l) f_{lj}(h) \exp(2\pi i \mathbf{h} \cdot \mathbf{R}_{lj})$$

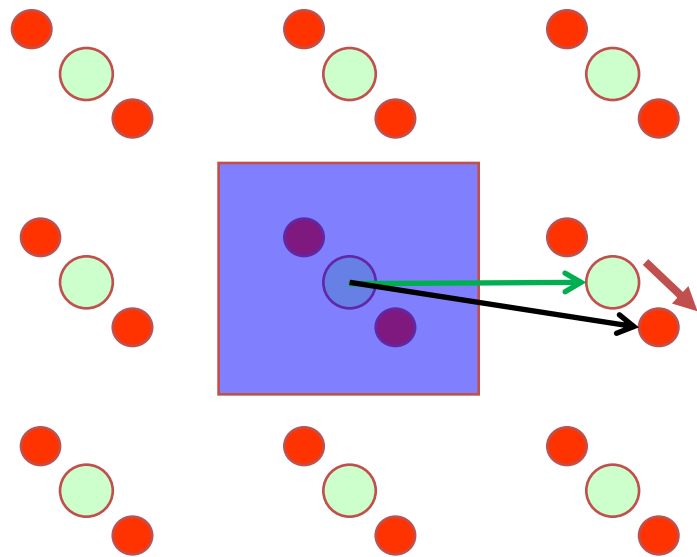
$$\mathbf{M}(\mathbf{h}) = \sum_j f_j(h) \exp(2\pi i \mathbf{h} \cdot \mathbf{r}_j) \sum_{\mathbf{k}} \mathbf{S}_{\mathbf{k}j} \sum_l \exp(2\pi i (\mathbf{h} - \mathbf{k}) \cdot \mathbf{R}_l)$$

$$\mathbf{M}(\mathbf{h}) \propto \sum_j \mathbf{S}_{\mathbf{k}j} f_j(Q) \exp(2\pi i (\mathbf{H} + \mathbf{k}) \cdot \mathbf{r}_j)$$

The lattice sum is only different from zero when $\mathbf{h} - \mathbf{k}$ is a reciprocal lattice vector $\mathbf{H}$ of the crystallographic lattice. The vector $\mathbf{M}$ is then proportional to the **magnetic structure factor of the unit cell** that now contains the Fourier coefficients $\mathbf{S}_{\mathbf{k}j}$ instead of the magnetic moments $\mathbf{m}_j$.

Diff. Patterns of magnetic structures

Portion of reciprocal space



● Magnetic reflections

● Nuclear reflections

$$\mathbf{h} = \mathbf{H} + \mathbf{k}$$

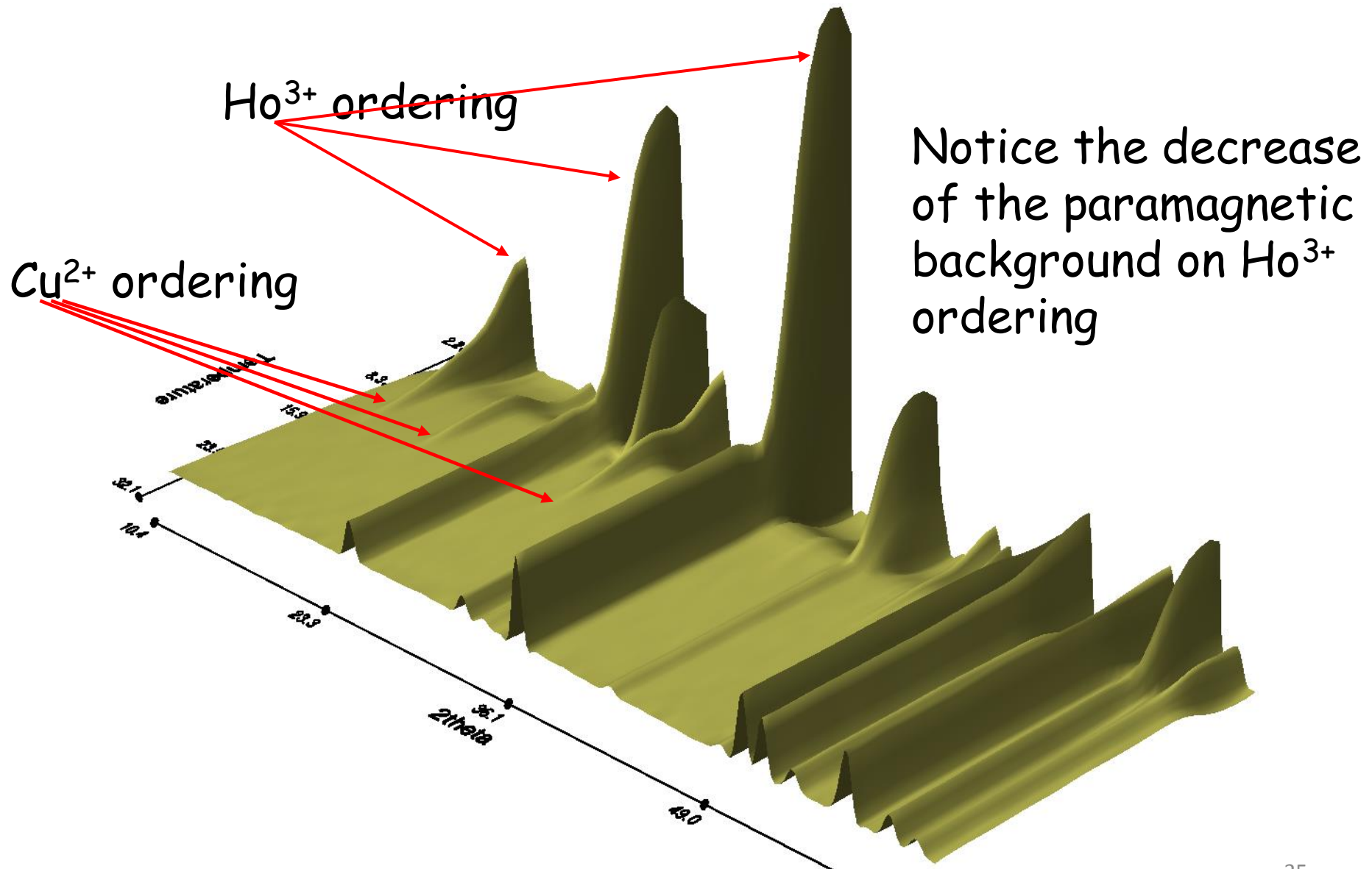
Magnetic reflections: indexed by a set of propagation vectors $\{\mathbf{k}\}$

$\mathbf{h}$ is the scattering vector indexing a magnetic reflection

$\mathbf{H}$ is a reciprocal vector of the crystallographic structure

$\mathbf{k}$ is one of the propagation vectors of the magnetic structure
($\mathbf{k}$ is reduced to the Brillouin zone)

Diffraction patterns of magnetic structures



Elastic Magnetic Scattering by a crystal (3)



From now on we will call $\mathbf{M}(\mathbf{h})$ the magnetic structure factor

$$\mathbf{M}(\mathbf{h}) = \sum_j \mathbf{S}_{kj} f_j(Q) \exp(2\pi i(\mathbf{H} + \mathbf{k}) \cdot \mathbf{r}_j)$$

And its perpendicular component to $\mathbf{h}$, $\mathbf{M}_\perp(\mathbf{h})$, is the magnetic interaction vector of the crystallographic unit cell. The elastic cross section (intensity of a Bragg reflection) is then:

$$\left(\frac{d\sigma}{d\Omega} \right) = (\gamma r_0)^2 \mathbf{M}_\perp^* \mathbf{M}_\perp$$

Where $\mathbf{M}_\perp(\mathbf{h})$ is calculated for a finite number of magnetic atoms inside the crystallographic unit cell. Notice that the magnetic moments do not appear directly in the expression of $\mathbf{M}(\mathbf{h})$.

Outline:

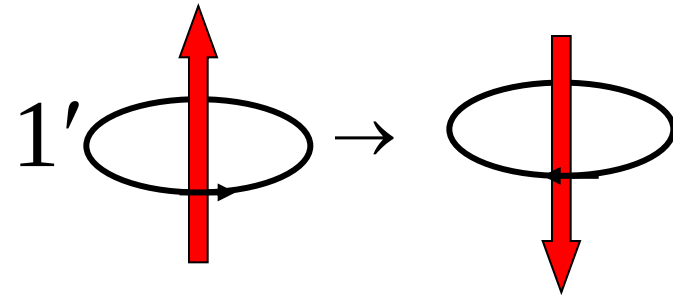
1. Magnetic Structures and neutron scattering
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Magnetic moments as axial vectors

The magnetic moment (shortly called "spin") of an atom can be considered as an "axial vector". It may be associated to a "current loop". The behaviour of elementary current loops under symmetry operators can be deduced from the behaviour of the "velocity" vector that is a "polar" vector.

Time reversal = spin reversal

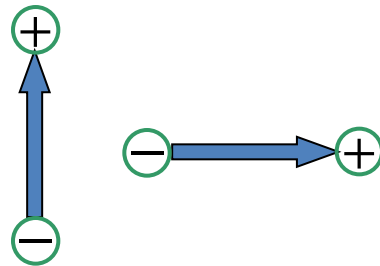
(change the sense of the current)



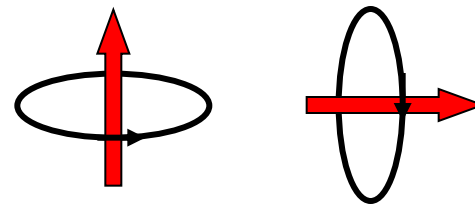
A **new operator** can be introduced and noted as **1'**, it **flips the magnetic moment**. This operator is called "spin reversal" operator or classical "time reversal" operator

Magnetic moments as axial vectors

Electrical dipole



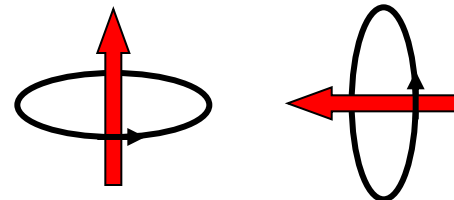
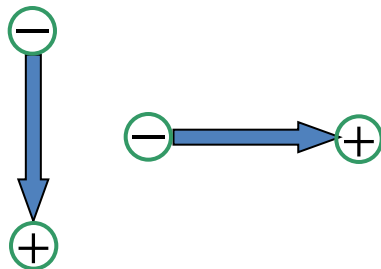
Magnetic dipole



Polar vector

Mirror plane

Axial vector



$$\mathbf{m}_j' = g \mathbf{m}_j = \det(h) \delta h \mathbf{m}_j$$

Magnetic space groups (Shubnikov groups)

The position of an arbitrary atom in the crystal can be deduced from the information given above. And using the following formula:

Atom positions in a crystal:

$$\mathbf{R}_{ljs} = \mathbf{R}_l + \mathbf{r}_{js} = \mathbf{R}_l + \{h | \mathbf{t}_h\}_s \mathbf{r}_j = l_1 \mathbf{a} + l_2 \mathbf{b} + l_3 \mathbf{c} + \{h | \mathbf{t}_h\}_s (x_j \mathbf{a} + y_j \mathbf{b} + z_j \mathbf{c})$$

$$\mathbf{R}_{ljs} = (\mathbf{a} \quad \mathbf{b} \quad \mathbf{c}) \begin{pmatrix} l_1 \\ l_2 \\ l_3 \end{pmatrix} + (\mathbf{a} \quad \mathbf{b} \quad \mathbf{c}) \begin{pmatrix} h_{11}^s & h_{12}^s & h_{13}^s \\ h_{21}^s & h_{22}^s & h_{23}^s \\ h_{31}^s & h_{32}^s & h_{33}^s \end{pmatrix} \begin{pmatrix} x_j \\ y_j \\ z_j \end{pmatrix} + (\mathbf{a} \quad \mathbf{b} \quad \mathbf{c}) \begin{pmatrix} t_1^s \\ t_2^s \\ t_3^s \end{pmatrix}$$

$$\mathbf{R}_{ljs} = (\mathbf{a} \quad \mathbf{b} \quad \mathbf{c}) \left\{ \begin{pmatrix} l_1 + t_1^s \\ l_2 + t_2^s \\ l_3 + t_3^s \end{pmatrix} + \begin{pmatrix} h_{11}^s & h_{12}^s & h_{13}^s \\ h_{21}^s & h_{22}^s & h_{23}^s \\ h_{31}^s & h_{32}^s & h_{33}^s \end{pmatrix} \begin{pmatrix} x_j \\ y_j \\ z_j \end{pmatrix} \right\}$$

l : index of a direct lattice point (origin of an arbitrary unit cell)

j : index for a Wyckoff site (orbit)

s : index of a sublattice of the j site

For a primitive basis the indices l_i are integers. For a centred cell they can also be rational numbers. In general, the fractional coordinates giving the atom positions in the asymmetric unit are real numbers.

Example from ITC: Space groups

International Tables of Crystallography (Volume A).

Example: group number 46, $Ima2$

Can be interpreted as a
"representation" of the
symmetry operations

Site symmetry and positions of space group $Ima2$

		$(0, 0, 0)^+$	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})^+$	
8 c	1	(1) x, y, z	(2) $-x, -y, z$	(3) $x+\frac{1}{2}, -y, z$ (4) $-x+\frac{1}{2}, y, z$
4 b	m ..	$\frac{1}{4}, y, z$	$\frac{1}{4}, -y, z$	
4 a	.. 2	$0, 0, z$	$\frac{1}{2}, 0, z$	

T- coset representatives

Symmetry operations

For $(0, 0, 0)^+$ set

(1) 1 (2) 2 $0, 0, z$ (3) a $x, 0, z$ (4) m $\frac{1}{4}, y, z$

For $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})^+$ set

(1) $t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ (2) 2 $(0, 0, \frac{1}{2})$ $\frac{1}{4}, \frac{1}{4}, z$ (3) c $x, \frac{1}{4}, z$ (4) n $(0, \frac{1}{2}, \frac{1}{2})$ $0, y, z$

Maximal non-isomorphic subgroups of $Ima2$

I [2] $I 1 1 2$ (C 2) (1; 2)+

[2] $I 1 a 1$ (C c) (1; 3)+

[2] $I m 1 1$ (C m) (1; 4)+

IIa [2] $P m a 2$ 1; 2; 3; 4

[2] $P n c 2$ 1; 2; (3; 4) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$

[2] $P n a 2_1$ 1; 3; (2; 4) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$

[2] $P m c 2_1$ 1; 4; (2; 3) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$

IIb none

The group $R = \{1, 1'\}$ is called **the time/spin reversal group**. **Magnetic point and space groups** can be obtained as **outer direct product of point and space groups with R** . The operators of a magnetic group are called **"primed"** if they result from the combination of the crystallographic operator with the element $1'$ of R . Those combined with 1 are called **"unprimed"**.

A general operator $g = \{h | \mathbf{t}_h + \mathbf{n}\}$ acting on an atom $\mathbf{r}_j$ in the cell at the origin (zero-cell) having a magnetic moment $\mathbf{m}_j$ is transformed as follows:

$$\mathbf{r}_j' = g \mathbf{r}_j = \{h | \mathbf{t}_h + \mathbf{n}\} \mathbf{r}_j = h \mathbf{r}_j + \mathbf{t}_h + \mathbf{n} = \mathbf{r}_i + \mathbf{a}_{gj}$$

$$\mathbf{m}_j' = g \mathbf{m}_j = \det(h) \delta h \mathbf{m}_j$$

The **"signature"** is $\delta = 1$ for unprimed elements
and $\delta = -1$ for primed elements

Magnetic space groups

Whatever crystallographic magnetic group, $\mathbf{M}$, can be obtained as a subgroup of the outer direct product of $\mathbf{R}$ by the crystallographic group $\mathbf{G}$:
 $\mathbf{M} \subset \mathbf{G} \otimes \mathbf{R}$.

The group $\mathbf{G}$ is always a magnetic group ("colourless")
Paramagnetic ("grey") groups are of the form: $\mathbf{P} = \mathbf{G} + \mathbf{G}1'$.

Nontrivial groups ("black-white" groups)

Constructive lemma: *the magnetic groups derived from the crystallographic group $\mathbf{G}$ can be constructed considering the index 2 subgroups $\mathbf{H}$ of $\mathbf{G}$ as constituting the "unprimed" elements and the rest of operators, $\mathbf{G} - \mathbf{H}$, those that are multiplied by the time reversal operator.*

The magnetic group is then related to the subgroup $\mathbf{H} \subset \mathbf{G}$ (of index 2) by the expression: $\mathbf{M} = \mathbf{H} + (\mathbf{G} - \mathbf{H}) 1'$.

This is valid for all kind of groups: point groups, translation groups and space groups. This is a consequence of "primed" $\times$ "primed" = "unprimed"

Example: construction of magnetic point groups

ITA: maximal subgroups and minimal super-groups of point groups

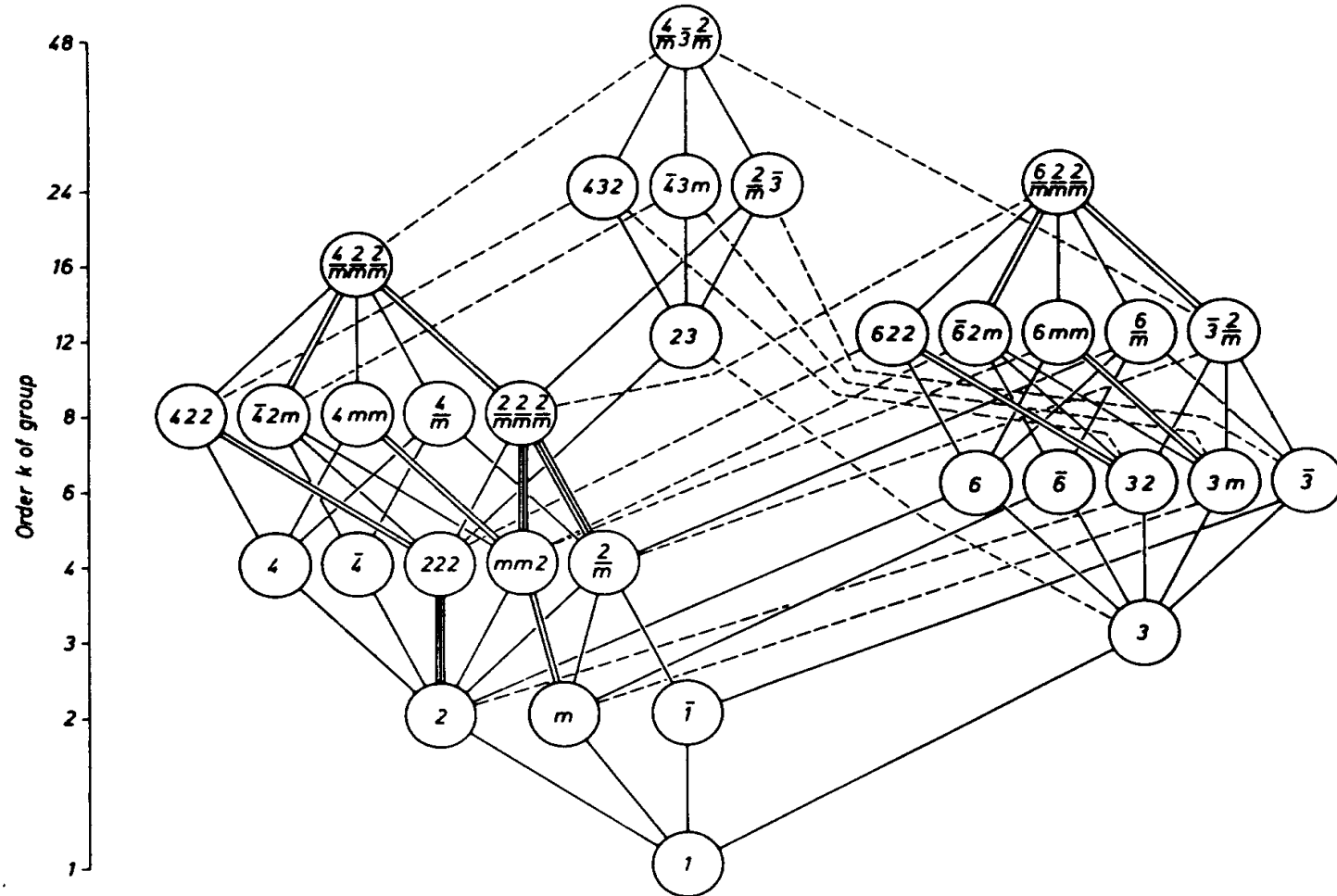


Fig. 10.3.2. Maximal subgroups and minimal supergroups of the three-dimensional crystallographic point groups. Solid lines indicate maximal normal subgroups; double or triple solid lines mean that there are two or three maximal normal subgroups with the same symbol. Dashed lines refer to sets of maximal conjugate subgroups. The group orders are given on the left. Full Hermann-Mauguin symbols are used.

Example: construction of magnetic point groups

It is easy to apply the constructive lemma to the crystallographic point groups and deduce that we have **32** trivial magnetic point groups (identical to the 32 crystallographic point groups), **32** paramagnetic groups, and **<3+3>+ (5)+(13+5)+ [5]+ [13+8]+3=58** black-white point groups.

This is obtained by counting the number of lines connecting groups with subgroups of index 2 in the previous figure.

The symbols <>, (), [] surrounding the figures refers to cubic, hexagonal-trigonal and tetragonal-orthorhombic groups; the absence of parenthesis for the last figure refers to monoclinic-triclinic point groups.

Example: magnetic point groups from 4/m

Consider the point group $\mathbf{G}=4/m$ of order 8. Its subgroups of index 2 are $\mathbf{H}_1=4$, $\mathbf{H}_2=2/m$ and $\mathbf{H}_3=2/m$. There are then four magnetic point groups derived from $\mathbf{G}$, they have the following elements:

$$\mathbf{G} = 4/m = \{1, 4_z^+, 2_z, 4_z^-, \bar{1}, m_z, \overline{4_z^+}, \overline{4_z^-}\}$$

$$\mathbf{H}_1 = 4 = \{1, 4_z^+, 2_z, 4_z^-\}$$

$$\mathbf{H}_2 = \bar{4} = \{1, \overline{4_z^+}, 2_z, \overline{4_z^-}\}$$

$$\mathbf{H}_3 = 2/m = \{1, 2_z, \bar{1}, m_z\}$$

$$\mathbf{M}_0 = \mathbf{G} = 4/m$$

$$\mathbf{M}_1 = \mathbf{H}_1 + (\mathbf{G} - \mathbf{H}_1)1' = \{1, 4_z^+, 2_z, 4_z^-, \bar{1}', m_z', \overline{4_z^+}', \overline{4_z^-}'\} = 4/m'$$

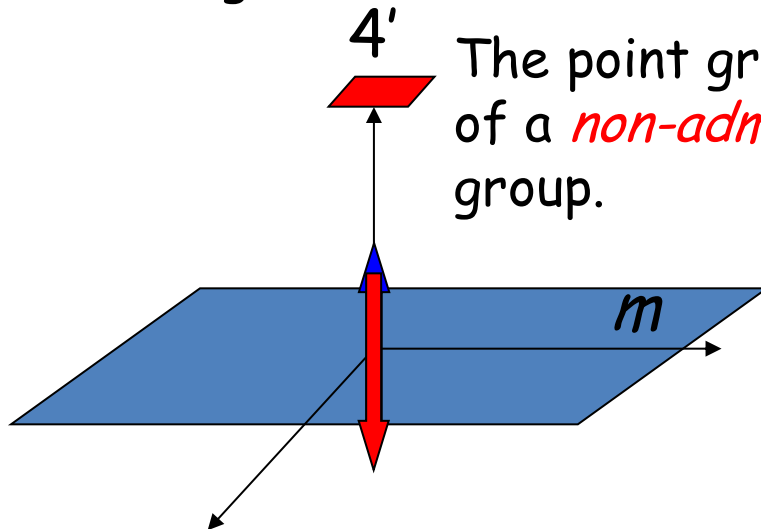
$$\mathbf{M}_2 = \mathbf{H}_2 + (\mathbf{G} - \mathbf{H}_2)1' = \{1, 4_z^+', 2_z, 4_z^-, \bar{1}', m_z', \overline{4_z^+}', \overline{4_z^-}'\} = 4'/m'$$

$$\mathbf{M}_3 = \mathbf{H}_3 + (\mathbf{G} - \mathbf{H}_3)1' = \{1, 4_z^+', 2_z, 4_z^-, \bar{1}, m_z, \overline{4_z^+}', \overline{4_z^-}'\} = 4'/m$$

In magnetically ordered systems, the magnetic point group of a magnetic atom cannot be one of the paramagnetic groups. Moreover many of the **colourless** and **black-white** magnetic point groups cannot be realized in ordered system.

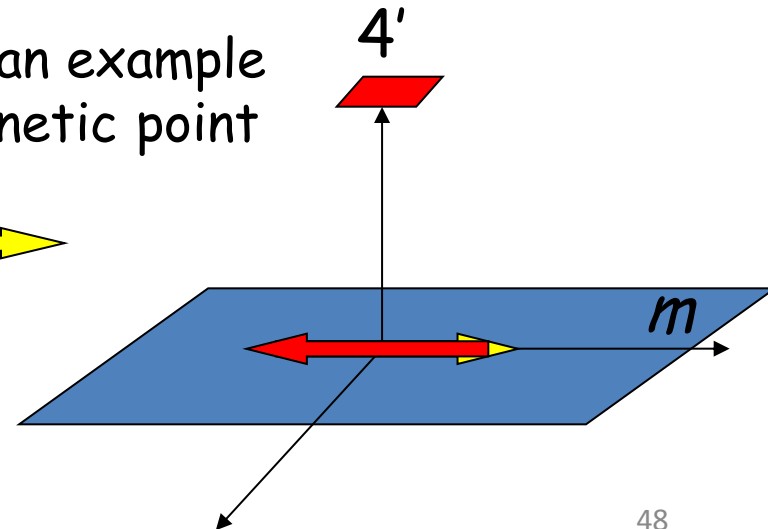
Let us consider the magnetic point group $\mathbf{M}3=4'/m$.

Action of $4'$ when the spin is along its axis



The point group $4'/m$ is an example of a **non-admissible** magnetic point group.

Action of m when the spin is within it



Admissible magnetic point groups

1			
2'	2'/m'	m'm2'	
m'			
m			
m'm'm			
2'2'2			
2	2/m	m'm'2	
4		4/m	42'2'
4m'm'		2m'	4/mm'm'
3		32'	3m' m'
6		6/m	62'2'
6m'm'		m'2'	6/mm'm'

Admissible spin direction

Any direction	[1]
Perpendicular to the 2-fold axis	[3]
Any direction within the plane	[1]
Perpendicular to the plane	[1]
Perpendicular to the unprimed plane	[1]
Along the unprimed axis	[1]
Along the 2-fold axis	[3]
Along the four-fold axis	[3]
Along the four-fold axis	[3]
Along the three-fold axis	[4]
Along the six-fold axis	[3]
Along the six-fold axis	[3]

27 admissible magnetic point groups!

For primitive Bravais lattices integer linear combinations of the three vectors $\{\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3\}$ generate the whole lattice:

$$\mathbf{T}_P = \{\mathbf{t} \mid \mathbf{t} = l_1 \mathbf{a}_1 + l_2 \mathbf{a}_2 + l_3 \mathbf{a}_3, l_i \in \mathbb{Z}\}$$

If we consider centred lattices the whole group is generated not only by the integer linear combinations of the basis vector representing the conventional cell but by adding centring vectors $\mathbf{t}_{cn}$ ($n=1 \dots m$):

$$\mathbf{T}_C = \{\mathbf{t} \mid \mathbf{t} = l_1 \mathbf{a}_1 + l_2 \mathbf{a}_2 + l_3 \mathbf{a}_3 + n_1 \mathbf{t}_{c1} + n_2 \mathbf{t}_{c2} + \dots n_{cm} \mathbf{t}_{cm}; l_i \in \mathbb{Z}, n_i \in \{0,1\}\}$$

The centring vectors have rational components when referred to the conventional basis: $\mathbf{t}_{ci} = q_{1i} \mathbf{a}_1 + q_{2i} \mathbf{a}_2 + q_{3i} \mathbf{a}_3$ ($q_i \in \mathbb{Q}$)

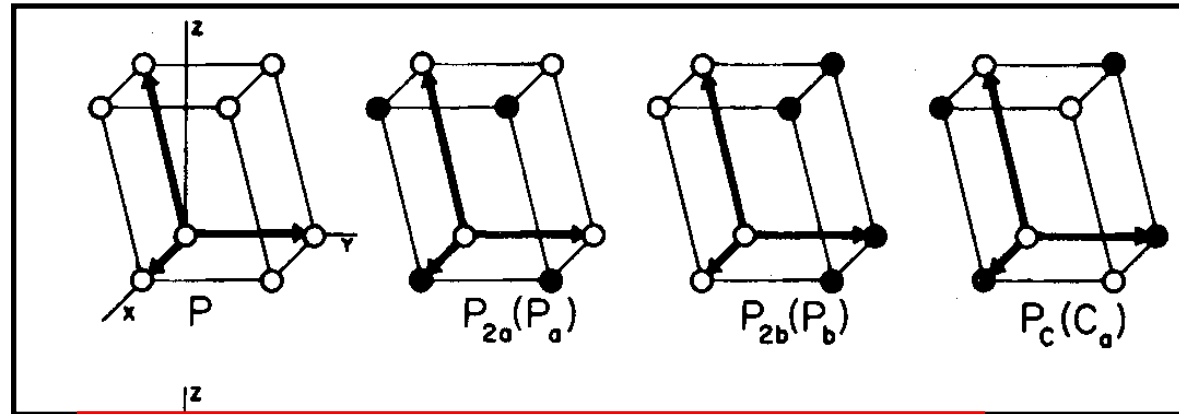
A subgroup, of index 2, of the translation group can be obtained just by suppressing half the translations, for instance if we take $l_1 = 2n$ we obtain a lattice $\mathbf{L}$ that is described with a unit cell with $\mathbf{a}_1' = 2\mathbf{a}_1$.

This lattice generates a subgroup of index 2 of $\mathbf{T}$ ($\mathbf{L} \subset \mathbf{T}$, $[\mathbf{i}] = n(\mathbf{T})/n(\mathbf{L}) = 2$), the lost translations ($\mathbf{T} - \mathbf{L}$) can be associated with time reversal for constructing the magnetic lattice: $\mathbf{M}_L = \mathbf{L} + (\mathbf{T} - \mathbf{L})1'$.

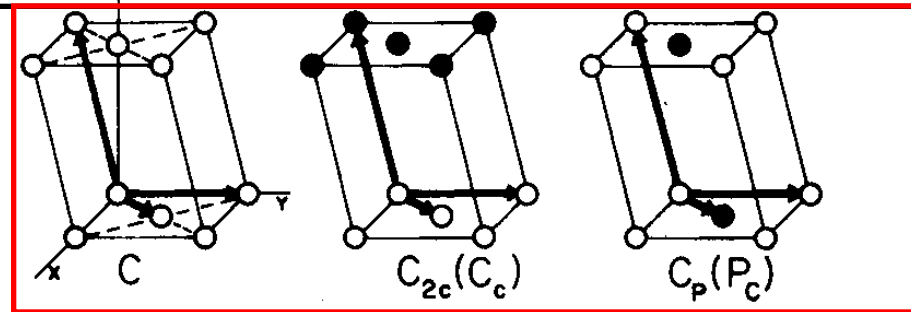
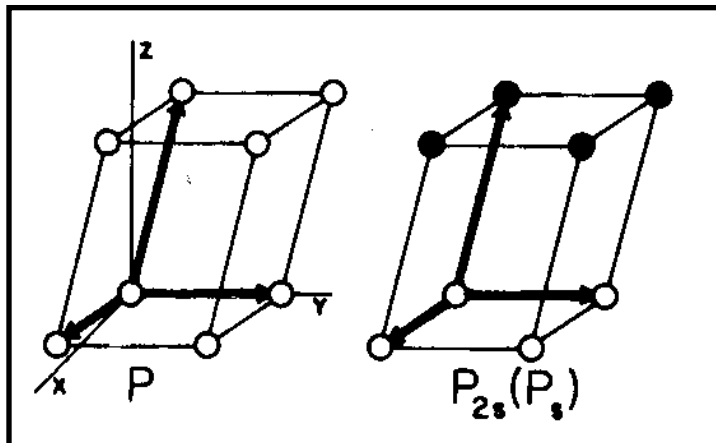
Magnetic Lattices

Open circles: Translations

Black circles: Anti-translations (primed)

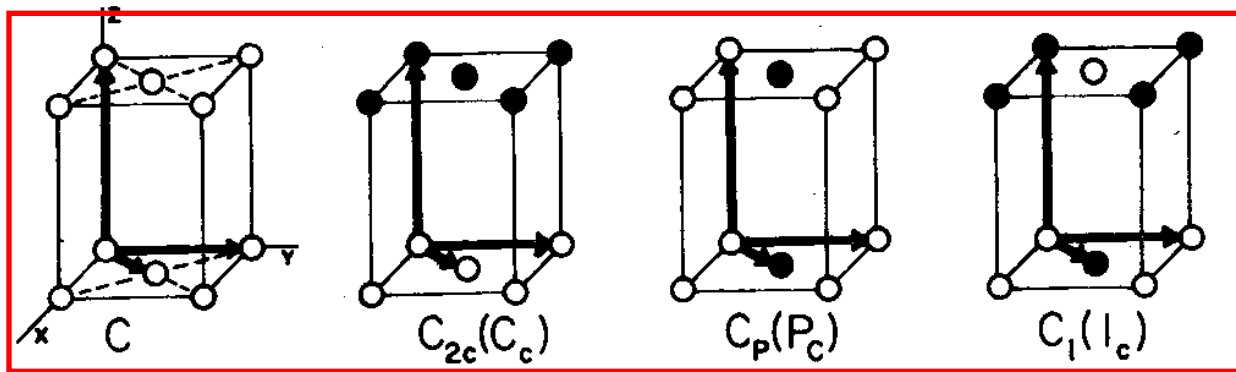
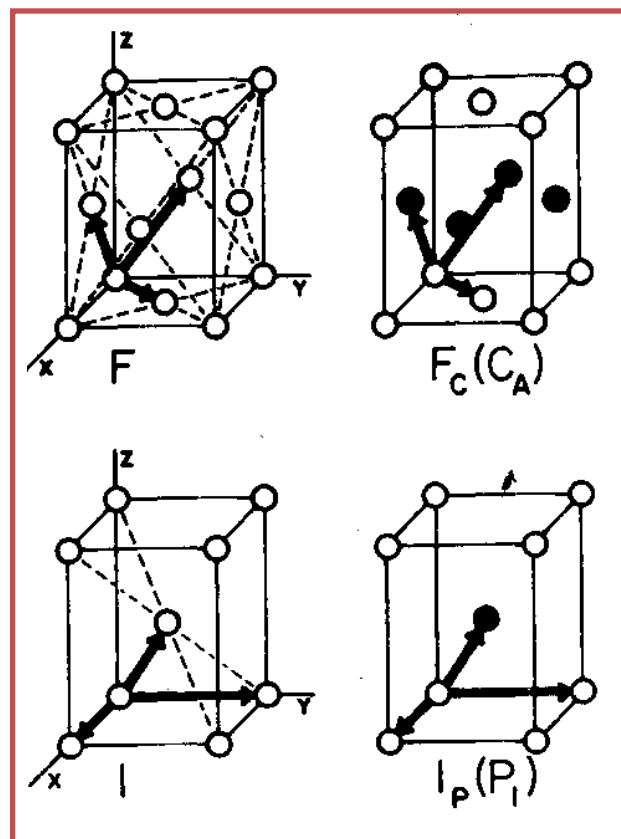
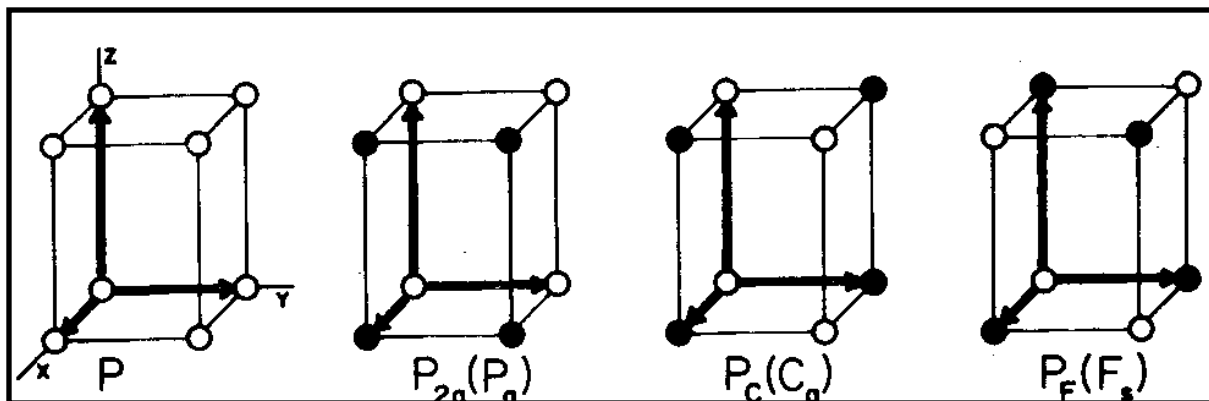


Magnetic Lattices of the Triclinic System

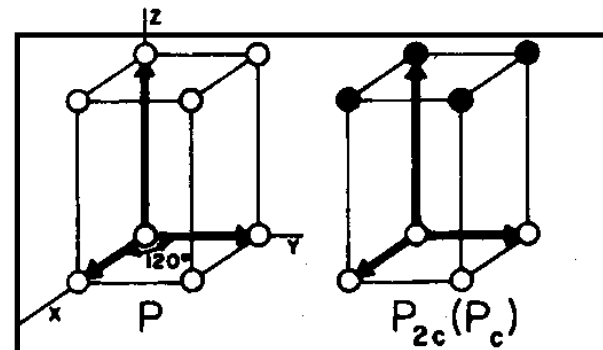
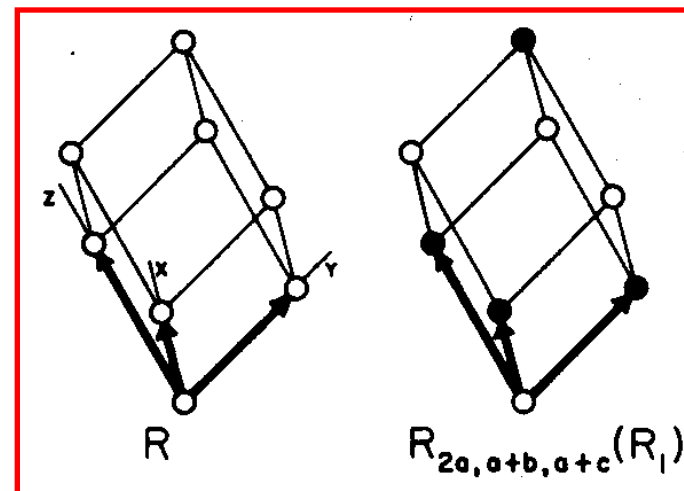
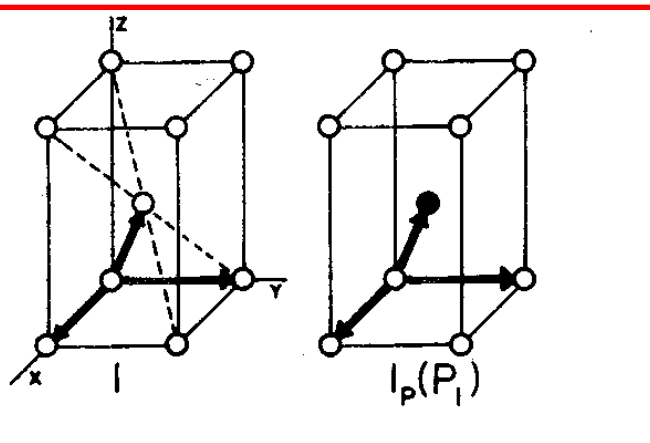
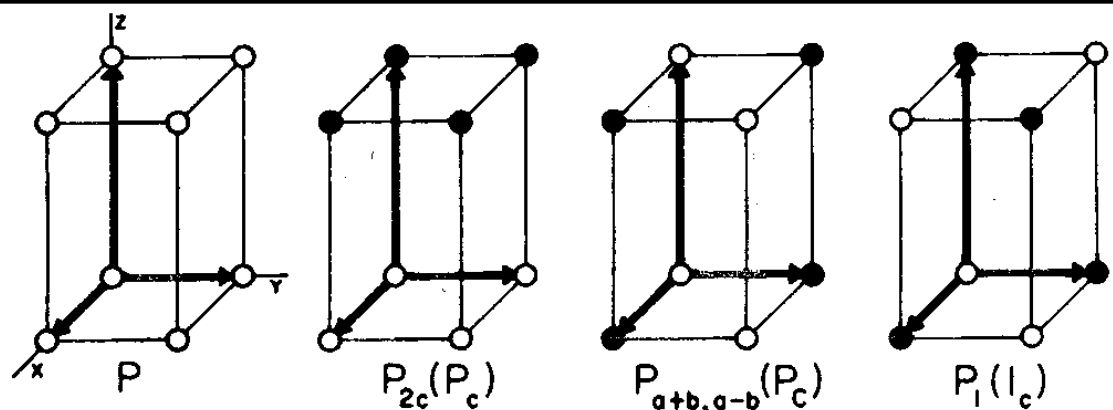


Magnetic Lattices of the Monoclinic System

Magnetic Lattices of the Orthorhombic System

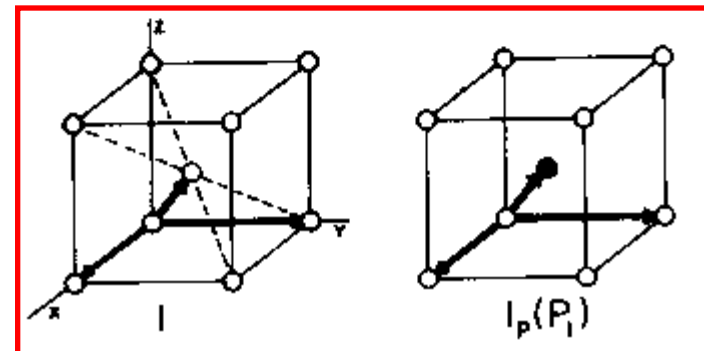
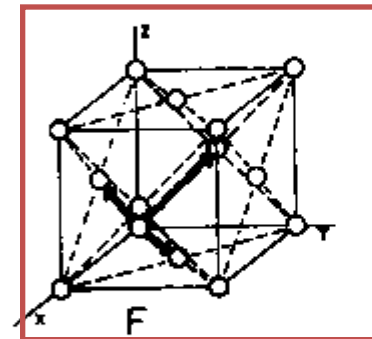
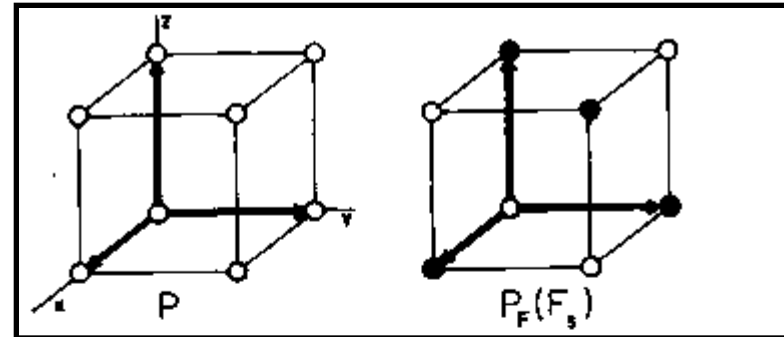


Magnetic Lattices of the Tetragonal System



Magnetic Lattices of the Hexagonal and Trigonal Systems

Magnetic Lattices of the Cubic System



Shubnikov Groups: Magnetic Space Groups

The same procedure points groups and Bravais lattices can be applied to space groups. One obtains a total of **1651** types of Shubnikov groups.

T1: 230 are of the form $M_0 = G$ ("monochrome", "colourless" groups),

T2: 230 of the form $P = G + G1'$ ("paramagnetic" or "grey" groups)

1191 of the form $M = H + (G - H)1'$ ("black-white", BW, groups).

T3: Among the BW group there are **674** in which the subgroup $H \subset G$ is an **equi-translation** group: **H** has the same translation group as **G** (first kind, BW1).

T4: The rest of black-white groups, **517**, are **equi-class** group (second kind, BW2). In this last family the translation subgroup contains "anti-translations" (pure translations associated with the spin reversal operator).

There are two notations to denote the magnetic space groups: the Opechowsky-Guccione (**OG**) and the Belov-Neronova-Smirnova (**BNS**) notations. They differ in the notation for the magnetic lattices and for the **BW2** groups. In the **BNS** notations the primed elements do not appear in the symbol of the group, they can be deduced from the magnetic lattice type.

In the **BW1** groups (**type 3**) the subgroup of translations is the same as that of the space group of which they derive, so **the spin reversal operator is not associated with translations**: the magnetic unit cell is the same as the crystallographic cell.

In the **BW2** groups (**type 4**) there are **some translations associated with spin reversal**, so that the "**magnetic primitive cell**" is **bigger** than the crystal primitive cell.

Shubnikov Groups: Example using ITA

The magnetic space groups can be constructed using the International Tables of Crystallography (Volume A).

Example: group number 46, $Ima2$

Site symmetry and positions of space group $Ima2$

		$(0, 0, 0)^+$	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})^+$		
8 c	1	(1) x, y, z	(2) $-x, -y, z$	(3) $x+\frac{1}{2}, -y, z$	(4) $-x+\frac{1}{2}, y, z$
4 b	$m \dots$	$\frac{1}{4}, y, z$	$\frac{1}{4}, -y, z$		
4 a	$\dots 2$	$0, 0, z$	$\frac{1}{2}, 0, z$		

Symmetry operations

For $(0, 0, 0)^+$ set

(1) 1	(2) $2\ 0,0,z$	(3) $a\ x,0,z$	(4) $m\ \frac{1}{4}, y,z$
-------	----------------	----------------	---------------------------

For $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})^+$ set

(1) $t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	(2) $2(0,0, \frac{1}{2})\ \frac{1}{4}, \frac{1}{4}, z$	(3) $c\ x, \frac{1}{4}, z$	(4) $n(0, \frac{1}{2}, \frac{1}{2})\ 0, y, z$
--	--	----------------------------	---

Maximal non-isomorphic subgroups of $Ima2$

I	[2] $I\ 1\ 1\ 2\ (C\ 2)\ (1; 2)^+$
	[2] $I\ 1\ a\ 1\ (C\ c)\ (1; 3)^+$
	[2] $I\ m\ 1\ 1\ (C\ m)\ (1; 4)^+$

IIa	[2] $P\ m\ a\ 2$	1; 2; 3; 4
	[2] $P\ n\ c\ 2$	1; 2; (3; 4) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
	[2] $P\ n\ a\ 2_1$	1; 3; (2; 4) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
	[2] $P\ m\ c\ 2_1$	1; 4; (2; 3) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$

IIb none

Shubnikov Groups: Example using ITA

The groups **I** correspond to the *translationengleiche* of *t*-subgroups and the groups **II** to the *klassengleiche* or *k*-subgroups that are also subdivided in order to distinguish those having the same conventional cell (**IIa**) from those having a multiple cell (**IIb**). The division I and II correspond to the **BW1** and **BW2** respectively.

Applying the formula $\mathbf{M} = \mathbf{H} + (\mathbf{G} - \mathbf{H}) \mathbf{1}'$ we obtain:

Colourless trivial magnetic group: $\mathbf{M}_0 = I m a 2 = \{1, 2_z, a_y, m_x\} \mathbf{T}$

For simplicity we remove the translation group and use only the coset representatives.

$$\begin{aligned} \mathbf{I} \quad \mathbf{M}_1 &= I 1 1 2 + (I m a 2 - I 1 1 2) \mathbf{1}' = \{1, 2_z\} + \{a_y, m_x\} \mathbf{1}' = I m' a' 2 \\ \mathbf{M}_2 &= I 1 a 1 + (I m a 2 - I 1 a 1) \mathbf{1}' = \{1, a_y\} + \{2_z, m_x\} \mathbf{1}' = I m' a 2' \\ \mathbf{M}_3 &= I m 1 1 + (I m a 2 - I m 1 1) \mathbf{1}' = \{1, m_x\} + \{2_z, a_y\} \mathbf{1}' = I m a' 2' \end{aligned}$$

For the **BW2** groups, the translation subgroup is that formed by integer linear combinations of conventional cell parameters. The centring translations $\mathbf{t}_c = (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ become anti-translations, so the magnetic lattice contains the following set of translations and anti-translations

$$\begin{aligned} \mathbf{L} &= \{\mathbf{t} \mid \mathbf{t} = l_1 \mathbf{a}_1 + l_2 \mathbf{a}_2 + l_3 \mathbf{a}_3; \quad l_i \in \mathbb{Z}\} \\ \mathbf{L}' &= (\mathbf{T} - \mathbf{L}) \mathbf{1}' = \{\mathbf{t}' \mid \mathbf{t}' = l_1 \mathbf{a}_1 + l_2 \mathbf{a}_2 + l_3 \mathbf{a}_3 + \mathbf{t}_c; \quad l_i \in \mathbb{Z}\} \end{aligned}$$

Shubnikov Groups: Example using ITA

IIa We write below the **BW2** groups using the data of the ITA and show the **BNS** and the **OG** notation. It is clearly seen that the **BNS** notation correspond directly to the subgroups written in ITA by putting the lattice symbol P_I for stating that an original body centred lattice becomes primitive and the centring translations become anti-translations. None of the generators appearing in the symbol is primed. This is a characteristic of the BNS notation for all **BW2** groups.

On the contrary the **OG** conserves the original HM symbol changing the lattice type to I_p and using primed generators when they appear. From the information given in the decomposition of the magnetic group in terms of translations and anti-translations one can derive easily the **BNS** (makes reference to the coset representatives with respect to L) or the **OG** notation (makes reference to the coset representatives with respect to L').

ITA	Notations:	BNS	OG
[2] $P m a 2$	$\mathbf{M}_4 = \{1, 2_z, a_y, m_x\}L + \{1, 2_{1z}, c_y, n_x\}L' = P_I m a 2$		$I_p m a 2$
[2] $P n c 2$	$\mathbf{M}_5 = \{1, 2_z, c_y, n_x\}L + \{1, 2_{1z}, a_y, m_x\}L' = P_I n c 2$		$I_p m' a' 2$
[2] $P n a 2_1$	$\mathbf{M}_6 = \{1, a_y, 2_{1z}, n_x\}L + \{1, 2_z, c_y, m_x\}L' = P_I n a 2_1$		$I_p m' a 2'$
[2] $P m c 2_1$	$\mathbf{M}_7 = \{1, m_x, 2_{1z}, c_y\}L + \{1, 2_z, a_y, n_x\}L' = P_I m c 2_1$		$I_p m a' 2'$

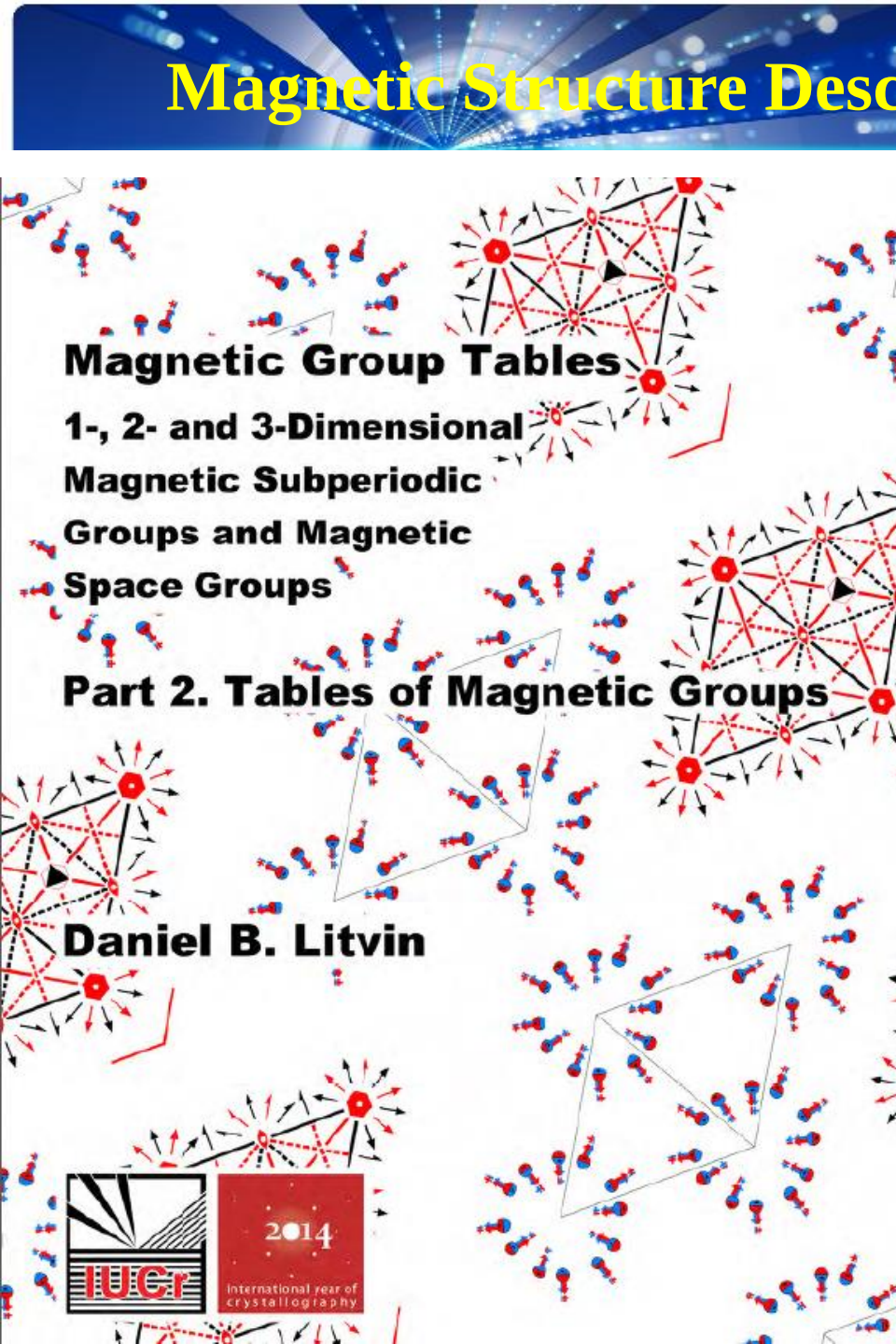
Magnetic Structure Description and Determination

2001: Daniel B. Litvin provides for the first time the full description of all Shubnikov (Magnetic Space) Groups. Acta Cryst. **A57**, 729-730

<http://www.bk.psu.edu/faculty/litvin/home.html>



Magnetic Structure Description and Determination



Magnetic Group Tables

1-, 2- and 3-Dimensional
Magnetic Subperiodic
Groups and Magnetic
Space Groups

Part 2. Tables of Magnetic Groups

Daniel B. Litvin



We are concerned here with the tables of Magnetic Groups, but many other papers from D.B. Litvin can be downloaded from its personal page at

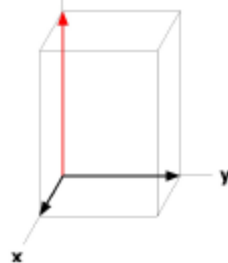
<http://www.bk.psu.edu/faculty/litvin/>

The first part is a comprehensive introduction to the tables and the second part contain each individual Magnetic Space Group item with Wyckoff positions and diagrams

Magnetic Structure Description and Determination

Group Ordering Number (BNS): 548, BNS: 62.450, OG: 59.9.486

OG: $P_{2c}m'mm$
BNS: $P_n nma$



$P_{2c}m'mn$

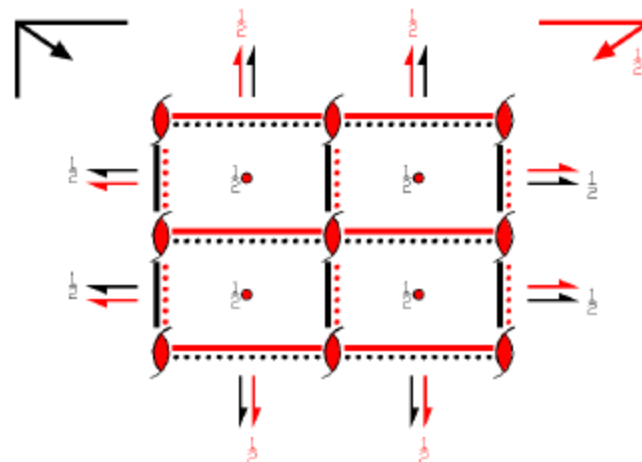
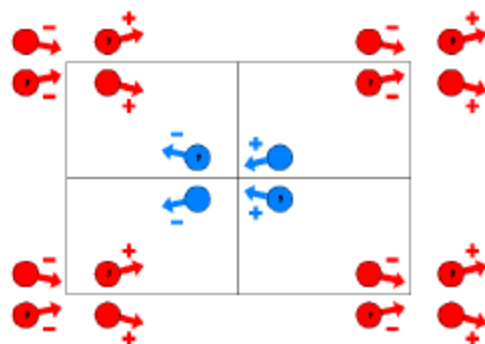
59.9.486

$mmm1'$

$P_{2c}2_1/m'2_1'/m2'/n$

Orthorhombic

OG-BNS transformation: $(1/2, 1/2, 1/2; c, -b, 2a)$



Origin at $m'm2'/n$ at $1/4, 1/4, 0$ from $\bar{1}'$

Asymmetric unit $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

Symmetry Operations

For $(0,0,0) + \text{set}$

(1) 1
(1|0,0,0)

(2) $2'$ $0,0,z$
(2_z |0,0,0)'

(3) $2'$ $(0,1/2,0)$ $1/4,y,0$
(2_y | $1/2,1/2,0$)'

(4) 2 $(1/2,0,0)$ $x,1/4,0$
(2_x | $1/2,1/2,0$)

(5) $\bar{1}'$ $1/4,1/4,0$
($\bar{1}$ | $1/2,1/2,0$)'

(6) n $(1/2,1/2,0)$ $x,y,0$
(m_z | $1/2,1/2,0$)

(7) m $x,0,z$
(m_y |0,0,0)

(8) m' $0,y,z$
(m_x |0,0,0)'

For $(0,0,1)' + \text{set}$

(1) t' $(0,0,1)$
(1|0,0,1)'

(2) 2 $(0,0,1)$ $0,0,z$
(2_z |0,0,1)

(3) 2 $(0,1/2,0)$ $1/4,y,1/2$
(2_y | $1/2,1/2,1$)

(4) $2'$ $(1/2,0,0)$ $x,1/4,1/2$
(2_x | $1/2,1/2,1$)'

(5) $\bar{1}$ $1/4,1/4,1/2$
($\bar{1}$ | $1/2,1/2,1$)

(6) n' $(1/2,1/2,0)$ $x,y,1/2$
(m_z | $1/2,1/2,1$)'

(7) c' $(0,0,1)$ $x,0,z$
(m_y |0,0,1)'

(8) c $(0,0,1)$ $0,y,z$
(m_x |0,0,1)

Only recently the magnetic space groups have been made available in a computer database

Magnetic Space Groups

Compiled by Harold T. Stokes and Branton J. Campbell
Brigham Young University, Provo, Utah, USA
June 2010

These data are based on data from:

Daniel Litvin, **Magnetic Space Group Types**,
Acta Cryst. **A57** (2001) 729-730.

<http://www.bk.psu.edu/faculty/litvin/Download.html>

Symmetry of Special Projections

Along $[0,0,1]$ $c2mm1'$
 $a^* = a$ $b^* = b$
Origin at $0,0,z$

Along $[1,0,0]$ $p2mg$
 $a^* = b$ $b^* = c$
Origin at $x,1/4,0$

Along $[0,1,0]$ $p2mg1'$
 $a^* = -a$ $b^* = c$
Origin at $1/4,y,0$

ISOTROPY Software Suite

Harold T. Stokes, Dorian M. Hatch, and Branton J. Campbell, Department of Physics and Astronomy, Brigham Young University, Provo, Utah 84606, USA, stokesh@byu.edu

Description: The ISOTROPY software suite is a collection of software which applies group theoretical methods to the analysis of phase transitions in crystalline solids.

How to cite: ISOTROPY Software Suite, iso.byu.edu.

References and Resources

Isotropy subgroups and distortions

- **ISODISTORT**: Explore and visualize distortions of crystalline structures. Possible distortions include atomic displacements, atomic ordering, strain, and magnetic moments.
- **ISOSUBGROUP**: Coming soon!
- **ISOTROPY**: Interactive program using command lines to explore isotropy subgroups and their associated distortions.
- **SMODES**: Find the displacement modes in a crystal which brings the dynamical matrix to block-diagonal form, with the smallest possible blocks.
- **FROZSL**: Calculate phonon frequencies and displacement modes using the method of frozen phonons.

Space groups and irreducible representations

- **ISOCIF**: Create or modify CIF files.
- **FINDSYM**: Identify the space group of a crystal, given the positions of the atoms in a unit cell.
- **New! ISO-IR**: Tables of Irreducible Representations. The 2011 version of IR matrices.
- **ISO-MAG**: Tables of magnetic space groups, both in human-readable and computer-readable forms.

Superspace Groups

- **ISO(3+d)D**: (3+d)-Dimensional Superspace Groups for $d=1,2,3$
- **ISO(3+1)D**: Isotropy Subgroups for Incommensurately Modulated Distortions in Crystalline Solids: A Complete List for One-Dimensional Modulations
- **FINDSSG**: Identify the superspace group symmetry given a list of symmetry operators.
- **TRANSFORMSSG**: Transform a superspace group to a new setting.

Phase Transitions

- **COPL**: Find a complete list of order parameters for a phase transition, given the space-group symmetries of the parent and subgroup phases.
- **INVARIANTS**: Generate invariant polynomials of the components of order parameters.
- **COMSUBS**: Find common subgroups of two structures in a reconstructive phase transition

Linux

- **ISOTROPY Software Suite for Linux**: includes ISOTROPY, FINDSYM, SMODES, COMSUBS.



FCT/ZTF

bilbao crystallographic server



[The crystallographic site at the Condensed Matter Physics Dept. of the University of the Basque Country]

[Space Groups] [Layer Groups] [Rod Groups] [Frieze Groups] [Wyckoff Sets]



2014: International Year of Crystallography

NEW!

Satellite workshop of the 2014 IUCr Congress:

Role of Magnetic Symmetry in the Description
and Determination of Magnetic Structures.
Hamilton, Canada
14-16 August 2014

Space Groups Retrieval Tools

GENPOS	Generators and General Positions of Space Groups
WYCKPOS	Wyckoff Positions of Space Groups
HKLCD	Reflection conditions of Space Groups
MAXSUB	Maximal Subgroups of Space Groups
SERIES	Series of Maximal Isomorphic Subgroups of Space Groups
WYCKSETS	Equivalent Sets of Wyckoff Positions
NORMALIZER	Normalizers of Space Groups
KVEC	The k-vector types and Brillouin zones of Space Groups
SYMMETRY OPERATIONS	Geometric interpretation of matrix column representations of symmetry operations

Magnetic Symmetry and Applications

MGENPOS	General Positions of Magnetic Space Groups
MWYCKPOS	Wyckoff Positions of Magnetic Space Groups
MAGNEXT	Extinction Rules of Magnetic Space Groups
MAXMAGN 	Maximal magnetic space groups for a given space group and a propagation vector

Sections

[Retrieval Tools](#)

[Magnetic Symmetry and Applications](#)

[Group-Subgroup](#)

The program **Mag_Info** has been included, as a console application, for obtaining information about magnetic space groups. In the near future this program will be extended with a GUI and a wizard to create PCR files for magnetic structures using Shubnikov groups in whatever setting.

The program reads the database 'magnetic_data.txt' compiled by Harold T. Stokes and Branton J. Campbell (Brigham Young University, Provo, Utah, USA) based on data from: Daniel Litvin, "Magnetic Space Group Types", Acta Cryst **A57** (2001) 729.
<http://www.bk.psu.edu/faculty/litvin/Download.html>

Shubnikov Groups: Computing tools

Administrator: Intel Composer XE 2011 IA-32 Visual Studio 2010 - Mag_Info

----- MAGNETIC SPACE GROUPS INFORMATION -----

Program to get information about magnetic groups

The program uses following database:

Magnetic Space Groups

Compiled by Harold T. Stokes and Branton J. Campbell

Brigham Young University, Provo, Utah, USA

June 2010

These data are based on data from:

Daniel Litvin, "Magnetic Space Group Types," Acta Crystallographica (2001)

A57 729-730. (<http://www.bk.psu.edu/faculty/litvin/Download.html>)

C. J. Bradley and A. P. Cracknell, "The Mathematical Theory of Symmetry in Solids" (Clarendon Press, Oxford, 1972).

Program written by JRC, ILL, November 2012

Main Menu

[0] Exit

[1] Get Full Information from the Litvin final number

[2] Get Full Information from the OG symbol

[3] Get Full Information from the OG full number label

[4] Get Full Information from the BNS symbol

[5] Get Full Information from the BNS full number label

[6] List of Shubnikov groups from the family of a Space Group (OG)

[7] List of Shubnikov groups from the family of a Space Group (BNS)

OPTION:

Opechowski-Guccione Description

Number of OG operators: 32

# 1:	$\langle 1 0,0,0 \rangle$	# 2:	$\langle 2yz 0,0,0 \rangle$	# 3:	$\langle 2-xz 0,0,0 \rangle$	# 4:	$\langle 4y 0,0,0 \rangle$
# 5:	$\langle 4x-1 0,0,0 \rangle$	# 6:	$\langle 2-yz 0,0,0 \rangle$	# 7:	$\langle 2xz 0,0,0 \rangle$	# 8:	$\langle 4x 0,0,0 \rangle$
# 9:	$\langle -1 0,0,0 \rangle$	# 10:	$\langle myz 0,0,0 \rangle$	# 11:	$\langle m-xz 0,0,0 \rangle$	# 12:	$\langle -4y 0,0,0 \rangle$
# 13:	$\langle -4x-1 0,0,0 \rangle$	# 14:	$\langle m-yz 0,0,0 \rangle$	# 15:	$\langle mxz 0,0,0 \rangle$	# 16:	$\langle -4x 0,0,0 \rangle$
# 17:	$\langle 1 1,0,0 \rangle'$	# 18:	$\langle 2yz 1,0,0 \rangle'$	# 19:	$\langle 2-xz 1,0,0 \rangle'$	# 20:	$\langle 4y 1,0,0 \rangle'$
# 21:	$\langle 4x-1 1,0,0 \rangle'$	# 22:	$\langle 2-yz 1,0,0 \rangle'$	# 23:	$\langle 2xz 1,0,0 \rangle'$	# 24:	$\langle 4x 1,0,0 \rangle'$
# 25:	$\langle -1 1,0,0 \rangle'$	# 26:	$\langle myz 1,0,0 \rangle'$	# 27:	$\langle m-xz 1,0,0 \rangle'$	# 28:	$\langle -4y 1,0,0 \rangle'$
# 29:	$\langle -4x-1 1,0,0 \rangle'$	# 30:	$\langle m-yz 1,0,0 \rangle'$	# 31:	$\langle mxz 1,0,0 \rangle'$	# 32:	$\langle -4x 1,0,0 \rangle'$

Number of OG lattice translations: 3

# 1:	$\langle 1,-1,0 \rangle$	# 2:	$\langle 1,1,0 \rangle$	# 3:	$\langle 0,0,1 \rangle$
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Number of OG Wyckoff positions: 21

Wyckoff site # 1: 32 32u

# 1:	$\langle x,y,z;u,v,w \rangle$	# 2:	$\langle -y,x,z;-v,u,w \rangle$	# 3:	$\langle y,-x,z;v,-u,w \rangle$
# 4:	$\langle x,-y,-z;u,-v,-w \rangle$	# 5:	$\langle -x,y,-z;-u,v,-w \rangle$	# 6:	$\langle -x,-y,z;-u,-v,w \rangle$
# 7:	$\langle y,x,-z;v,u,-w \rangle$	# 8:	$\langle -y,-x,-z;-v,-u,-w \rangle$	# 9:	$\langle -x,-y,-z;u,v,w \rangle$
# 10:	$\langle y,-x,-z;-v,u,-w \rangle$	# 11:	$\langle -y,x,-z;v,-u,-w \rangle$	# 12:	$\langle -x,y,z;u,-v,-w \rangle$
# 13:	$\langle x,-y,z;-u,v,-w \rangle$	# 14:	$\langle x,y,-z;-u,-v,w \rangle$	# 15:	$\langle -y,-x,z;v,u,-w \rangle$
# 16:	$\langle y,x,z;-v,-u,-w \rangle$	# 17:	$\langle x+1,y,z;-u,-v,-w \rangle$	# 18:	$\langle -y+1,x,z;v,-u,-w \rangle$
# 19:	$\langle y+1,-x,z;-v,u,-w \rangle$	# 20:	$\langle x+1,-y,-z;-u,v,w \rangle$	# 21:	$\langle -x+1,y,-z;u,-v,w \rangle$
# 22:	$\langle -x+1,-y,z;u,v,-w \rangle$	# 23:	$\langle y+1,x,-z;-v,-u,w \rangle$	# 24:	$\langle -y+1,-x,-z;v,u,w \rangle$
# 25:	$\langle -x+1,-y,-z;-u,-v,-w \rangle$	# 26:	$\langle y+1,-x,-z;v,-u,-w \rangle$	# 27:	$\langle -y+1,x,-z;-v,u,-w \rangle$
# 28:	$\langle -x+1,y,z;-u,v,w \rangle$	# 29:	$\langle x+1,-y,z;u,-v,w \rangle$	# 30:	$\langle x+1,y,-z;u,v,-w \rangle$
# 31:	$\langle -y+1,-x,z;-v,-u,-w \rangle$	# 32:	$\langle y+1,x,z;v,u,w \rangle$		

Wyckoff site # 2: 16 16t

# 1:	$\langle x,x+1/2,z;u,u,w \rangle$	# 2:	$\langle -x-1/2,x,z;-u,u,w \rangle$	# 3:	$\langle x+1/2,-x,z;u,-u,w \rangle$
# 4:	$\langle x-1/2,-x,-z;u,-u,-w \rangle$	# 5:	$\langle -x+1/2,x,-z;-u,u,-w \rangle$	# 6:	$\langle -x,-x-1/2,z;-u,-u,w \rangle$
# 7:	$\langle x,x-1/2,-z;u,u,-w \rangle$	# 8:	$\langle -x,-x+1/2,-z;-u,-u,-w \rangle$	# 9:	$\langle -x,-x-1/2,-z;u,u,w \rangle$
# 10:	$\langle x+1/2,-x,-z;-u,u,w \rangle$	# 11:	$\langle -x-1/2,x,-z;u,-u,w \rangle$	# 12:	$\langle -x+1/2,x,z;u,-u,-w \rangle$
# 13:	$\langle x-1/2,-x,z;-u,u,-w \rangle$	# 14:	$\langle x,x+1/2,-z;-u,-u,w \rangle$	# 15:	$\langle -x,-x+1/2,z;u,u,-w \rangle$
# 16:	$\langle x,x-1/2,z;-u,-u,-w \rangle$				

Wyckoff site # 3: 16 16s

# 1:	$\langle x,x,z;u,-u,0 \rangle$	# 2:	$\langle -x,x,z;u,u,0 \rangle$	# 3:	$\langle x,-x,z;-u,-u,0 \rangle$
# 4:	$\langle x,-x,-z;u,u,0 \rangle$	# 5:	$\langle -x,x,-z;-u,-u,0 \rangle$	# 6:	$\langle -x,-x,z;-u,u,0 \rangle$
# 7:	$\langle x,x,-z;-u,u,0 \rangle$	# 8:	$\langle -x,-x,-z;u,-u,0 \rangle$	# 9:	$\langle x+1,x,z;-u,u,0 \rangle$
# 10:	$\langle -x+1,x,z;-u,-u,0 \rangle$	# 11:	$\langle x+1,-x,0 \rangle$	# 12:	$\langle x+1,-x,-z;-u,-u,0 \rangle$
# 13:	$\langle -x+1,x,-z;u,u,0 \rangle$	# 14:	$\langle -x+1,-x,z;u,-u,0 \rangle$	# 15:	$\langle x+1,x,-z;u,-u,0 \rangle$
# 16:	$\langle -x+1,-x,-z;-u,u,0 \rangle$				

Wyckoff site # 4: 16 16r

# 1:	$\langle 0,y,z;u,0,0 \rangle$	# 2:	$\langle -y,0,z;0,u,0 \rangle$	# 3:	$\langle y,0,z;0,-u,0 \rangle$
# 4:	$\langle 0,-y,-z;u,0,0 \rangle$	# 5:	$\langle 0,y,-z;-u,0,0 \rangle$	# 6:	$\langle 0,-y,z;-u,0,0 \rangle$
# 7:	$\langle y,0,-z;0,u,0 \rangle$	# 8:	$\langle -y,0,-z;0,-u,0 \rangle$	# 9:	$\langle 1,y,z;-u,0,0 \rangle$
# 10:	$\langle -y+1,0,z;0,-u,0 \rangle$	# 11:	$\langle y+1,0,z;0,u,0 \rangle$	# 12:	$\langle 1,-y,-z;-u,0,0 \rangle$
# 13:	$\langle 1,y,-z;u,0,0 \rangle$	# 14:	$\langle 1,-y,z;u,0,0 \rangle$	# 15:	$\langle y+1,0,-z;0,-u,0 \rangle$
# 16:	$\langle -y+1,0,-z;0,u,0 \rangle$				

Wyckoff site # 5: 16 16q

# 1:	$\langle x,y,1/2;0,0,w \rangle$	# 2:	$\langle -y,x,1/2;0,0,w \rangle$	# 3:	$\langle y,-x,1/2;0,0,w \rangle$
# 4:	$\langle x,-y,-1/2;0,0,-w \rangle$	# 5:	$\langle -x,y,-1/2;0,0,-w \rangle$	# 6:	$\langle -x,-y,1/2;0,0,w \rangle$
# 7:	$\langle y,x,-1/2;0,0,-w \rangle$	# 8:	$\langle -y,-x,-1/2;0,0,-w \rangle$	# 9:	$\langle x+1,y,1/2;0,0,-w \rangle$
# 10:	$\langle -y+1,x,1/2;0,0,-w \rangle$	# 11:	$\langle y+1,-x,1/2;0,0,-w \rangle$	# 12:	$\langle x+1,-y,-1/2;0,0,w \rangle$
# 13:	$\langle -x+1,y,-1/2;0,0,w \rangle$	# 14:	$\langle -x+1,-y,1/2;0,0,-w \rangle$	# 15:	$\langle y+1,x,-1/2;0,0,w \rangle$
# 16:	$\langle -y+1,-x,-1/2;0,0,w \rangle$				

Wyckoff site # 6: 16 16p

# 1:	$\langle x,y,0;0,0,w \rangle$	# 2:	$\langle -y,x,0;0,0,w \rangle$	# 3:	$\langle y,-x,0;0,0,w \rangle$
# 4:	$\langle x,-y,0;0,0,-w \rangle$	# 5:	$\langle -x,y,0;0,0,-w \rangle$	# 6:	$\langle -x,-y,0;0,0,w \rangle$
# 7:	$\langle y,x,0;0,0,-w \rangle$	# 8:	$\langle -y,-x,0;0,0,-w \rangle$	# 9:	$\langle x+1,y,0;0,0,-w \rangle$
# 10:	$\langle -y+1,x,0;0,0,-w \rangle$	# 11:	$\langle y+1,-x,0;0,0,-w \rangle$	# 12:	$\langle x+1,-y,0;0,0,w \rangle$
# 13:	$\langle -x+1,y,0;0,0,w \rangle$	# 14:	$\langle -x+1,-y,0;0,0,-w \rangle$	# 15:	$\langle y+1,x,0;0,0,w \rangle$
# 16:	$\langle -y+1,-x,0;0,0,w \rangle$				

Group representations (representation analysis)



Bertaut is the principal developer of the representation analysis applied to magnetic structures

Representation analysis of magnetic structures

E.F. Bertaut, Acta Cryst. (1968). A24, 217-231



Yurii Alexandrovich Izyumov (1933-2010)
and collaborators, mainly V.E. Naish and
R.P. Ozerov.

They published a series of 5 articles in
**Journal of Magnetism and Magnetic
Materials** on representation analysis and
magnetic structure description and
determination, **giving explicit and general
formulae for deducing the basis functions
of irreps.**

**Symmetry Analysis in Neutron Diffraction Studies of Magnetic
Structures, JMMM 1979-1980**

Summary of Group representation theory

A **representation of a group** is a set of matrices satisfying the same operation rules as the group elements

$$\Gamma = \{\Gamma(g) \mid g \in G\}, \quad \Gamma(g_1 g_2) = \Gamma(g_1) \Gamma(g_2)$$

Under the ordinary matrix product the given set constitutes an isomorphic group (preserves the multiplication table).

A **similarity transformation applied to all matrices provides an equivalent representation** (the matrix U is generally unitary: $U^{-1} = U^\dagger$).

$$\Gamma(g) = U \Gamma(g) U^{-1} \{ \text{with } g \in G \}$$

A particular group has an infinite number of representations of arbitrary dimensions. The most important representations are called "Irreducible Representations" (Irreps). An **arbitrary representation may be reduced to "block-diagonal form" by an appropriate similarity transformation**. Those representations that cannot be reduced are the Irreps.

Summary of Group representation theory

Given the representation $\Gamma = \{\Gamma(e), \Gamma(a), \Gamma(b), \dots\}$ of the group $G = \{e, a, b, \dots\}$, if we are able to find a similarity transformation U converting all matrices to the same block-diagonal form, we obtain an equivalent representation that can be decomposed as follows:

$$\Gamma(g) = U \Gamma(g) U^{-1} \quad \{\text{with } g \in G\} \Rightarrow \Gamma = U \Gamma U^{-1}$$

$$\Gamma(g) = \begin{pmatrix} A_{11} & A_{12} & 0 & 0 & 0 & 0 & 0 \\ A_{21} & A_{22} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & B_{11} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & B_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{11} & C_{12} & C_{13} \\ 0 & 0 & 0 & 0 & C_{21} & C_{22} & C_{23} \\ 0 & 0 & 0 & 0 & C_{31} & C_{32} & C_{33} \end{pmatrix} = A(g) \oplus 2B(g) \oplus C(g)$$

Irreducible representations

$$\Gamma^1 = \{A(e), A(a), A(b), \dots\}$$

$$\Gamma^2 = \{B(e), B(a), B(b), \dots\}$$

$$\Gamma^3 = \{C(e), C(a), C(b), \dots\}$$

In general:

$$\Gamma = \sum_{\oplus \nu} n_{\nu} \Gamma^{\nu} = n_1 \Gamma^1 \oplus n_2 \Gamma^2 \dots \oplus n_m \Gamma^m$$

Master formulae of group representation theory

We shall note the different irreducible representations with the index ν and a symbol Γ that may be used also for matrices. The dimension of the representation Γ_ν is l_ν . The characters of a representation (traces of the matrices) will be represented as $\chi^\nu(g)$

The great orthogonality theorem:

$$\sum_{g \in G} \Gamma_{ij}^\nu(g) \Gamma_{lm}^{*\mu}(g) = \frac{n(G)}{l_\nu} \delta_{il} \delta_{jm} \delta_{\mu\nu}$$

Particularized for the characters:

$$\sum_{g \in G} \chi^\nu(g) \chi^{*\mu}(g) = n(G) \delta_{\mu\nu}$$

Decomposition of a representation in Irreps:

$$\Gamma = \sum_{\oplus \nu} n_\nu \Gamma_\nu, \quad n_\nu = \frac{1}{n(G)} \sum_{g \in G} \chi(g) \chi^{*\nu}(g)$$

The elements of the symmetry groups act on position vectors. For each particular problem we can select a set of physically relevant variables φ_i $\{i=1, 2, \dots, p\}$ spanning a working functional space $\mathbf{W}$. These functions constitute a basis of the $\mathbf{W}$ space.

The action of the operator associated to a symmetry operator when applied to a function of position vectors is defined by the expression:

$$O(g)\varphi(\mathbf{r}) = \varphi(g^{-1}\mathbf{r}) \equiv \varphi'(\mathbf{r})$$

When using the functions $\varphi_i(\mathbf{r})$, the action of the operator $O(g)$ gives rise to a linear combination, defining a representation of the group G :

$$O(g)\varphi_j(\mathbf{r}) = \varphi'(\mathbf{r}) = \sum_i \Gamma_{ij}(g)\varphi_i(\mathbf{r})$$

If we take another basis ψ related to the initial one by a unitary transformation we may get the matrices of the Γ representation in block-diagonal form.

$$\psi_j(\mathbf{r}) = \sum_i U_{ij}(g) \varphi_i(\mathbf{r})$$

The system of p ψ -functions splits in subsystems defining irreducible subspaces of the working space $\mathbf{W}$. If we take one of these subspaces (labelled ν), the action of the operator $O(g)$ on the basis functions is:

$$O(g)\psi_j(\mathbf{r}) = \sum_{i=1}^{l_\nu} \Gamma_{ij}^\nu(g) \psi_i(\mathbf{r})$$

Here the functions are restricted to those of the subspace ν

Projection operators

There is a way for obtaining the basis functions of the Irreps for the particular physical problem by applying the following projection operator formula:

$$\psi_i^\nu = P^\nu \varphi = \frac{1}{n(G)} \sum_{g \in G} \Gamma_{i[j]}^{*\nu}(g) O(g) \varphi \quad (i = 1, \dots, l_\nu)$$

The result of the above operation is zero or a basis function of the corresponding Irrep. The index $[j]$ is fixed, taking different values provide new basis functions or zero.

Representations of the translation group

The translation group is Abelian so the Irreps are all *one-dimensional*.

Considering the properties of the translation operators and the Born-Von Karman periodic boundary conditions the representation matrix (a single number equal to its character) is given by the expression:

$$O(\mathbf{t}) = O(l_1 \mathbf{a}_1 + l_2 \mathbf{a}_2 + l_3 \mathbf{a}_3) = O(\mathbf{a}_1)^{l_1} O(\mathbf{a}_2)^{l_2} O(\mathbf{a}_3)^{l_3}$$

$$O(\mathbf{a}_j)^{N_j+1} = O(\mathbf{a}_j)$$

$$O(\mathbf{t}) \rightarrow \exp \left\{ 2\pi i \left(\frac{p_1 l_1}{N_1} + \frac{p_2 l_2}{N_2} + \frac{p_3 l_3}{N_3} \right) \right\}, \quad 0 \leq p_i \in \mathbb{Z} \leq N_i - 1$$

There are $N = N_1 \times N_2 \times N_3$ representations labelled by the reciprocal space vector:

$$\mathbf{k} = \left(\frac{p_1}{N_1}, \frac{p_2}{N_2}, \frac{p_3}{N_3} \right) = \frac{p_1}{N_1} \mathbf{b}_1 + \frac{p_2}{N_2} \mathbf{b}_2 + \frac{p_3}{N_3} \mathbf{b}_3$$

Representations of the translation group (2)

The matrix of the representation $\mathbf{k}$ corresponding to the translation $\mathbf{t}$ is then:

$$\Gamma^{\mathbf{k}}(\mathbf{t}) = \exp \left\{ 2\pi i \left(\frac{p_1 l_1}{N_1} + \frac{p_2 l_2}{N_2} + \frac{p_3 l_3}{N_3} \right) \right\} = \exp \{ 2\pi i \mathbf{k} \mathbf{t} \}$$

Where the $\mathbf{k}$ vectors in reciprocal space are restricted to the first Brillouin Zone. It is clear that adding a reciprocal lattice vector $\mathbf{H}$ to $\mathbf{k}$, does not change the matrix, so the vectors $\mathbf{k}' = \mathbf{H} + \mathbf{k}$ and $\mathbf{k}$ are equivalent.

The basis functions of the group of translations must satisfy the equation:

$$O(\mathbf{t})\psi^{\mathbf{k}}(\mathbf{r}) = \Gamma^{\mathbf{k}}(\mathbf{t})\psi^{\mathbf{k}}(\mathbf{r}) = \exp \{ 2\pi i \mathbf{k} \mathbf{t} \} \psi^{\mathbf{k}}(\mathbf{r})$$

The most general form for the functions $\psi^{\mathbf{k}}(\mathbf{r})$ are the Bloch functions:

$$\psi^{\mathbf{k}}(\mathbf{r}) = u_{\mathbf{k}}(\mathbf{r}) \exp \{ -2\pi i \mathbf{k} \mathbf{r} \}, \text{ with } u_{\mathbf{k}}(\mathbf{r} \pm \mathbf{t}) = u_{\mathbf{k}}(\mathbf{r})$$

This is easily verified by applying the rules or the action of operators on functions

$$\begin{aligned} O(\mathbf{t})\psi^{\mathbf{k}}(\mathbf{r}) &= \psi^{\mathbf{k}}(\mathbf{r} - \mathbf{t}) = u_{\mathbf{k}}(\mathbf{r} - \mathbf{t}) \exp \{ -2\pi i \mathbf{k}(\mathbf{r} - \mathbf{t}) \} = \\ &= \exp \{ 2\pi i \mathbf{k} \mathbf{t} \} u_{\mathbf{k}}(\mathbf{r}) \exp \{ -2\pi i \mathbf{k} \mathbf{r} \} = \exp \{ 2\pi i \mathbf{k} \mathbf{t} \} \psi^{\mathbf{k}}(\mathbf{r}) \end{aligned}$$

The k-vector Types of Group 10 [$P2/m$]

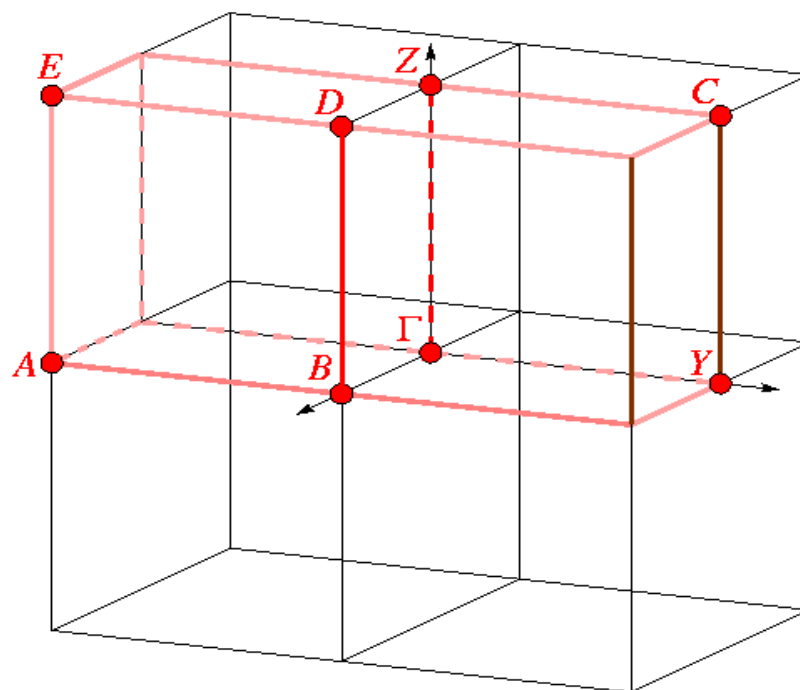
Brillouin zone

(Diagram for arithmetic crystal class $2/m\bar{P}$)

$P112/m$ ($P2/m$)- C_{2h}^1 (10), $P112_1/m$ ($P2_1/m$)- C_{2h}^2 (11), $P112/a$ ($P2/c$)- C_{2h}^4 (13), $P112_1/a$ ($P2_1/c$)- C_{2h}^5 (14)

Reciprocal-space group ($P112/m$)*, No. 10

The table with the k vectors.



The k-vector Types of Group 71 [*Immm*]

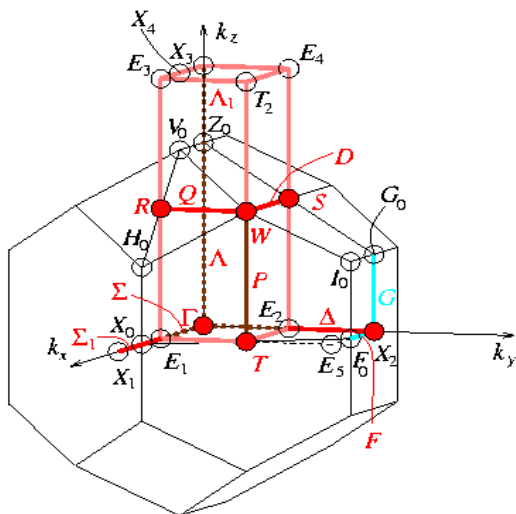
Brillouin zone

(Diagram for arithmetic crystal class *mmm*)

($b > a > c$ or $b > c > a$) $Immm-D_{2h}^{25}$ (71) to $Imma-D_{2h}^{28}$ (74)

Reciprocal-space group ($Fmmm$)*, No.69 : $b^* < a^* < c^*$ or $b^* < c^* < a^*$

The table with the k vectors.



The k-vector Types of Group 71 [*Immm*]

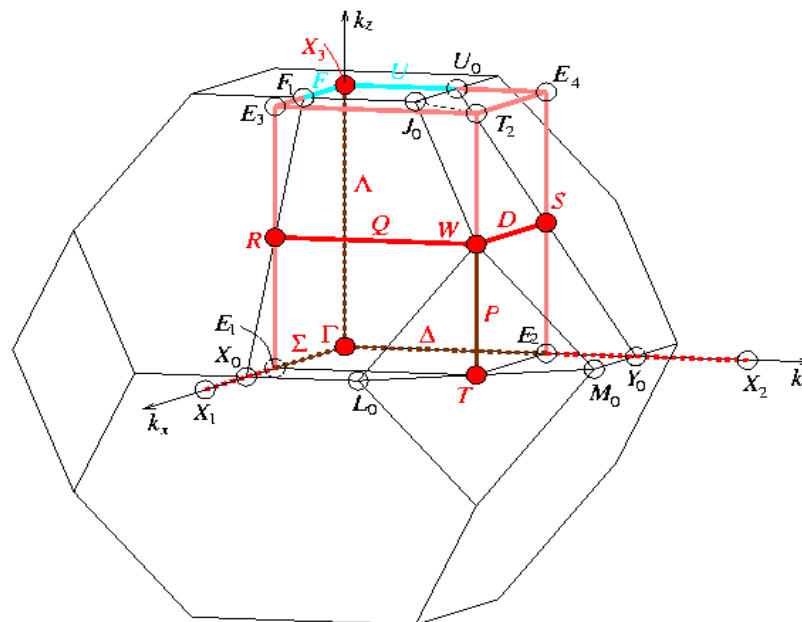
Brillouin zone

(Diagram for arithmetic crystal class *mmm*)

($c > b > a$ or $c > a > b$) $Immm-D_{2h}^{25}$ (71) to $Imma-D_{2h}^{28}$ (74)

Reciprocal-space group ($Fmmm$)*, No.69 : $c^* < b^* < a^*$ or $c^* < a^* < b^*$

The table with the k vectors.



Representations of space groups: basis functions

For constructing the representations of the space groups it is important to start with the basis functions. Let us see [how the Bloch functions behave under the action of a general element of the space group \$g=\{h|\mathbf{t}_h\}\$](#)

$$O(g)\psi^{\mathbf{k}}(\mathbf{r}) = \{h|\mathbf{t}_h\}\psi^{\mathbf{k}}(\mathbf{r}) = \psi'(\mathbf{r})$$

To determine the form of the functions $\psi'(\mathbf{r})$ one can see that [they should also be Bloch functions with a different \$\mathbf{k}\$ -label](#)

$$\begin{aligned} O(\mathbf{t})\psi'(\mathbf{r}) &= \{1|\mathbf{t}\}\psi'(\mathbf{r}) = \{1|\mathbf{t}\}\{h|\mathbf{t}_h\}\psi^{\mathbf{k}}(\mathbf{r}) = \{h|\mathbf{t}_h\}\{1|h^{-1}\mathbf{t}\}\psi^{\mathbf{k}}(\mathbf{r}) = \\ &= \{h|\mathbf{t}_h\}\exp\{2\pi i \mathbf{k} h^{-1}\mathbf{t}\}\psi^{\mathbf{k}}(\mathbf{r}) = \exp\{2\pi i \mathbf{k} h^{-1}\mathbf{t}\}\{h|\mathbf{t}_h\}\psi^{\mathbf{k}}(\mathbf{r}) = \\ &= \exp\{2\pi i h\mathbf{k}\mathbf{t}\}\psi'(\mathbf{r}) \end{aligned}$$

So that: $O(g)\psi^{\mathbf{k}}(\mathbf{r}) = \{h|\mathbf{t}_h\}\psi^{\mathbf{k}}(\mathbf{r}) = \psi^{h\mathbf{k}}(\mathbf{r})$

The Bloch functions also serve as basis functions but the representations are no longer one-dimensional because the Bloch functions whose wave vectors are related by the rotational part of $g \in \mathbf{G}$ belong to a same subspace.

The star of the vector $\mathbf{k}$: little group

The set of non-equivalent $\mathbf{k}$ vectors obtained by applying the rotational part of the symmetry operators of the space group constitute the so called “**star of $\mathbf{k}$** ”

$$\{\mathbf{k}\} = \{\mathbf{k}_1, h_1\mathbf{k}_1, h_2\mathbf{k}_1, h_3\mathbf{k}_1, \dots\} = \{\mathbf{k}_1, \mathbf{k}_2, \dots, \mathbf{k}_{l_k}\}$$

The $\mathbf{k}_i$ vectors are called the **arms of the star**. The number l_k is less or equal to the order of the point group $n(\mathbf{G}_0)$

The set of elements $g \in \mathbf{G}$ leaving the $\mathbf{k}$ vector invariant, or equal to an equivalent vector, form the group $\mathbf{G}_\mathbf{k}$. Called the **group of the wave vector** (or **propagation vector group**) or the “**little group**”. It is always a subgroup of $\mathbf{G}$. **The whole space/point group (little co-group) can be decomposed in cosets of the propagation vector group:**

$$\mathbf{G} = \mathbf{G}_\mathbf{k} + g_2\mathbf{G}_\mathbf{k} + \dots = \sum_{L=1}^{l_k} g_L \mathbf{G}_\mathbf{k} \quad \mathbf{k}_L = g_L \mathbf{k}$$

$$\mathbf{G}_0 = \mathbf{G}_{0\mathbf{k}} + h_2\mathbf{G}_{0\mathbf{k}} + \dots = \sum_{L=1}^{l_k} h_L \mathbf{G}_{0\mathbf{k}} \quad \mathbf{k}_L = h_L \mathbf{k}$$

The representations of G_k and G

We need to know the Irreps of G_k $\Gamma^{k\nu}$ only for the coset representatives (with respect to the translation group) of G_k

$$G_k = 1T + g_2T + g_3T + \dots + g_nT$$

For a general element of G_k we have:

$$\Gamma^{k\nu}(g) = \Gamma^{k\nu}(\{h | \mathbf{t}_h + \mathbf{t}\}) = \Gamma^{k\nu}(\{1 | \mathbf{t}\} \{h | \mathbf{t}_h\}) = \Gamma^{k\nu}(\{1 | \mathbf{t}\}) \Gamma^{k\nu}(\{h | \mathbf{t}_h\})$$

$$\Gamma^{k\nu}(\{h | \mathbf{t}_h + \mathbf{t}\}) = e^{2\pi i \mathbf{k} \cdot \mathbf{t}} \Gamma^{k\nu}(\{h | \mathbf{t}_h\})$$

The matrices $\Gamma^{k\nu}$ can be easily calculated from the projective (or *loaded*) representations that are tabulated in the Kovalev book

$$\Gamma^{k\nu}(g) = \Gamma^{k\nu}(\{h | \mathbf{t}_h\}) = \Gamma_{proj}^{\nu}(h) e^{2\pi i \mathbf{k} \cdot \mathbf{t}_h}$$

Alternatively they can be calculated using special algorithms (Zak's method)

The representations of $\mathbf{G}_k$ and $\mathbf{G}$

Let us note the irreducible representations of $\mathbf{G}_k$ as Γ^{kv} of dimensionality l_v .

The basis functions should be of the form: $\psi_i^{kv}(\mathbf{r}) = u_{ki}^v(\mathbf{r}) \exp(-2\pi i \mathbf{k} \cdot \mathbf{r})$ ($i=1, \dots, l_v$)

Under the action of the elements of $\mathbf{G}_k$ the functions transform into each other with the same $\mathbf{k}$ -vector.

Using the elements of $\mathbf{G}$ not belonging to $\mathbf{G}_k$ one generates other sets of basis functions: $\psi_i^{k_1v}(\mathbf{r}); \psi_i^{k_2v}(\mathbf{r}); \dots \psi_i^{k_{l_k}v}(\mathbf{r})$ that constitute the basis functions of the representations of the total space group.

These representations are labelled by the star of the $\mathbf{k}$ vector as: $\Gamma^{\{\mathbf{k}\}v}$ and are of dimensionality $l_v \times l_k$. Each irreducible “small representation” induces an irreducible representation of the total space group. The induction formula is:

$$\Gamma_{Li, Mj}^{\{\mathbf{k}\}v}(g) = \Gamma_{ij}^{kv}(g_L^{-1} g g_M) \delta_{g_L^{-1} g g_M \in \mathbf{G}_k}$$

The last symbol is 1 if the subscript condition is true, otherwise is zero

Outline:

1. Magnetic Structures and neutron scattering
2. Symmetry and Magnetic Structures
- 3. Magnetic Structure determination**

Intensity (non-polarised neutrons)

$$I_{\mathbf{h}} = N_{\mathbf{h}} N_{\mathbf{h}}^* + \mathbf{M}_{\perp \mathbf{h}} \cdot \mathbf{M}_{\perp \mathbf{h}}^*$$

Magnetic interaction vector

$$\mathbf{M}_{\perp \mathbf{h}} = \mathbf{e} \times \mathbf{M}(\mathbf{h}) \times \mathbf{e} = \mathbf{M}(\mathbf{h}) - \mathbf{e} (\mathbf{e} \cdot \mathbf{M}(\mathbf{h}))$$

$$\mathbf{h} = \mathbf{H} + \mathbf{k} \quad \Leftarrow \text{Scattering vector} \quad \mathbf{e} = \frac{\mathbf{h}}{h}$$

Magnetic structure factor: Shubnikov groups

The use of Shubnikov groups implies the use of the **magnetic unit cell** for indexing the Bragg reflections

$$\mathbf{M}_{\perp} = \mathbf{e} \times \mathbf{M} \times \mathbf{e} = \mathbf{M} - \mathbf{e} (\mathbf{e} \cdot \mathbf{M}) \quad I \propto \mathbf{M}_{\perp}^* \mathbf{M}_{\perp}$$

Magnetic structure factor:
$$\mathbf{M}(\mathbf{H}) = p \sum_{m=1}^{N_{mag}} \mathbf{m}_m f_m(H) \exp(2\pi i \mathbf{H} \cdot \mathbf{r}_m)$$

n independent magnetic sites labelled with the index j

The index s labels the representative symmetry operators of the Shubnikov group: $\mathbf{m}_{js} = \det(h_s) \delta_s h_s \mathbf{m}_j$ is the magnetic moment of the atom sited at the sublattice s of site j .

$$\mathbf{M}(\mathbf{H}) = p \sum_{j=1}^n O_j f_j(H) T_j \sum_s \det(h_s) \delta_s h_s \mathbf{m}_j \exp\{2\pi i [(\mathbf{H} \{h | \mathbf{t}\}_s \mathbf{r}_j)]\}$$

The maximum number of parameters n_p is, in general, equal to $3n$ magnetic moment components. Special positions make $n_p < 3n$.

Magnetic Structure Factor: k-vectors

$$\mathbf{M}(\mathbf{h}) = p \sum_{j=1}^n O_j f_j(\mathbf{h}) T_j \sum_s \mathbf{S}_{\mathbf{k}js} \exp\{2\pi i[(\mathbf{H} + \mathbf{k})\{S|\mathbf{t}\}_s \mathbf{r}_j]\}$$

j : index running for all magnetic atom sites in the magnetic asymmetric unit ($j=1, \dots, n$)

s : index running for all atoms of the orbit corresponding to the magnetic site j ($s=1, \dots, p_j$). Total number of atoms: $N = \sum p_j$

$\{S|\mathbf{t}\}_s$ Symmetry operators of the propagation vector group or a subgroup

If no symmetry constraints are applied to $\mathbf{S}_{\mathbf{k}}$, the maximum number of parameters for a general incommensurate structure is $6N$ (In practice $6N-1$, because a global phase factor is irrelevant)

According to the Landau theory of phase transitions, **it is expected that the configuration of the magnetic moments can be described in terms of the basis functions of the Irreps of the propagation vector group G_k** . The Irreps of G_k are tabulated or can be calculated independently of the problem

But, knowing the classical Hamiltonian of the spin system, the ground state (magnetic structure at $T = 0$ K) should minimize the energy

$$H = \sum_{jl\alpha, im\beta} J_{jl,im}^{\alpha\beta} S_{jl\alpha} S_{im\beta} + \dots O(S^n)$$

The symmetry of the Hamiltonian may be higher than the space group symmetry (e.g. isotropic exchange interactions)

Group Theory and representation analysis

A **reducible representation** of the propagation vector group can be constructed by selecting the atoms of a Wyckoff position and applying the symmetry operators to both positions and axial vectors. This gives rise to the so called **Magnetic Representation** of dimension: $3n_a$ (being n_a the number of atoms in the primitive cell)

This representation can be decomposed in Irreps and the number of times a particular Irreps, Γ^ν , is included can be easily calculated

$$\Gamma_{Mag} = \Gamma_{Perm} \otimes \Gamma_{Axial} = \sum_{\oplus \nu} n_\nu \Gamma^\nu$$

The basis functions, for each Irrep and each sublattice of a Wyckoff site, can be calculated by using the **projection operator formula**. The basis functions are **constant vectors** of the form (1,0,0), (0.5, 1,0) ... with components **referred to the crystallographic unitary frame**: {a/a, b/b, c/c} attached to each sublattice.

The working space for symmetry analysis of magnetic structures: magnetic representation

One can generate a reducible representation of $\mathbf{G}_k$ by considering the complex working space spanned by all the components of $\mathbf{S}_{kjs}$.

Each vector has three complex components.

As the atoms belonging to different sites do not mix under symmetry operators, we can treat separately the different sites. The index j is then fixed and the index s varies from 1 to p_j . Being p_j the number of sublattices generated by the site j .

Case $\alpha=y$ and s

The working complex space for site j has dimension $n_j=3 \times p_j$ is then spanned by unit vectors $\{\mathbf{e}_{\alpha s}^{kj}\}$ ($\alpha = 1, 2, 3$ —or x, y, z and $s = 1 \dots p_j$), represented as column vectors (with a single index n) with zeroes everywhere except for $n=\alpha+3(s-1)$. The n_j vectors refers to the zero-cell.

$$\mathbf{e}_{ys}^{kj} = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ 0 \\ 1 \\ 0 \\ \vdots \\ \vdots \\ \vdots \\ 0 \\ 0 \end{pmatrix} \begin{pmatrix} x, 1 \\ y, 1 \\ \vdots \\ z, s-1 \\ x, s \\ y, s \\ z, s \\ \vdots \\ \vdots \\ \vdots \\ y, p_j \\ z, p_j \end{pmatrix}$$

The working space for symmetry analysis of magnetic structures: magnetic representation

One can extend the basis vectors to the whole crystal by using the Bloch propagation then forming column vectors of $n_j \times N$ dimensions:

$$\boldsymbol{\varphi}_{\alpha s}^{\mathbf{k}j} = \sum_{\oplus l} \boldsymbol{\varepsilon}_{\alpha s}^{\mathbf{k}j} \exp(-2\pi i \mathbf{k} \mathbf{R}_l)$$

If one applies the symmetry operators of $\mathbf{G}_{\mathbf{k}}$ to the vectors $\{\boldsymbol{\varepsilon}_{\alpha s}^{\mathbf{k}j}\}$, taking into account that they are axial vectors, we obtain another vector (after correcting for the Bloch phase factor if the operator moves the atom outside the reference zero-cell) of the same basis. The matrices $\Gamma_{\alpha s, \beta q}^{\mathbf{k}j}(g)$ of dimension $n_j \times n_j = 3p_j \times 3p_j$ corresponding to the different operators constitute what is called the “Magnetic Representation” for the site j and propagation vector $\mathbf{k}$.

The magnetic representation

The vectors $\{\mathbf{\epsilon}_{\alpha s}^j\}$ are formed by direct sums (juxtaposition) of normal 3D vectors $\mathbf{u}_{\alpha s}^j$. Applying a symmetry operator to the vector position and the unit spin associated to the atom js along the α -axis, changes the index js to jq and reorient the spin according to the nature of the operator $g=\{h|\mathbf{t}_h\}$ for axial vectors.

$$g\mathbf{r}_s^j = h\mathbf{r}_s^j + \mathbf{t}_h = \mathbf{r}_q^j + \mathbf{a}_{gs}^j; \quad gs \rightarrow (q, \mathbf{a}_{gs}^j)$$

$$(g\mathbf{u}_{\alpha s}^j)_\beta = \det(h) \sum_n h_{\beta n} (\mathbf{u}_{\alpha s}^j)_n = \det(h) \sum_n h_{\beta n} \delta_{n,\alpha} = \det(h) h_{\beta\alpha}$$

$$O(g)\mathbf{\epsilon}_{\alpha s}^{\mathbf{k}j} = \sum_{\beta q} \Gamma_{\beta q, \alpha s}^{\mathbf{k}j}(g) \mathbf{\epsilon}_{\beta q}^{\mathbf{k}j} = \sum_{\beta q} e^{2\pi i \mathbf{k} \cdot \mathbf{a}_{gs}^j} \det(h) h_{\beta\alpha} \delta_{s,gq}^j \mathbf{\epsilon}_{\beta q}^{\mathbf{k}j}$$

Matrices of the magnetic representation

$$\Gamma_{Mag} \rightarrow \Gamma_{\beta q, \alpha s}^{\mathbf{k}j}(g) = e^{2\pi i \mathbf{k} \cdot \mathbf{a}_{gs}^j} \det(h) h_{\beta\alpha} \delta_{q,gs}^j$$

The magnetic representation as direct product of permutation and axial representations

An inspection to the explicit expression for the magnetic representation for the propagation vector $\mathbf{k}$, the Wyckoff position j , with sublattices indexed by (s, q) , shows that it may be considered as the direct product of the permutation representation, of dimension $p_j \times p_j$ and explicit matrices:

$$\Gamma_{Perm} \rightarrow P_{qs}^{\mathbf{k}j}(g) = e^{2\pi i \mathbf{k} \mathbf{a}_{gs}^j} \delta_{q,gs}^j$$

**Permutation
representation**

by the axial (or in general “vector”) representation, of dimension 3, constituted by the rotational part of the $\mathbf{G}_{\mathbf{k}}$ operators multiplied by -1 when the operator $g = \{h | \mathbf{t}_h\}$ corresponds to an improper rotation.

$$\Gamma_{Axial} \rightarrow V_{\beta\alpha}(g) = \det(h) h_{\beta\alpha}$$

Axial representation

$$\Gamma_{Mag} \rightarrow \Gamma_{\beta q, \alpha s}^{\mathbf{k}j}(g) = e^{2\pi i \mathbf{k} \mathbf{a}_{gs}^j} \det(h) h_{\beta\alpha} \delta_{q,gs}^j$$

**Magnetic
representation**

Basis functions of the Irreps of $\mathbf{G}_k$

The magnetic representation, hereafter called Γ_M irrespective of the indices, can be decomposed in irreducible representations of $\mathbf{G}_k$.

We can calculate a priori the number of possible basis functions of the Irreps of $\mathbf{G}_k$ describing the possible magnetic structures. This number is equal to the number of times the representation Γ^ν is contained in Γ_M times the dimension of Γ^ν . The projection operators provide the explicit expression of the basis vectors of the Irreps of $\mathbf{G}_k$

$$\psi_{\lambda}^{k\nu}(j) = \frac{1}{n(\mathbf{G}_{0k})} \sum_{g \in \mathbf{G}_{0k}} \Gamma_{\lambda[\mu]}^{*\nu}(g) O(g) \boldsymbol{\varepsilon}_{\alpha s}^{kj} \quad (\lambda = 1, \dots, l_\nu)$$

$$\psi_{\lambda}^{k\nu}(j) = \frac{1}{n(\mathbf{G}_{0k})} \sum_{g \in \mathbf{G}_{0k}} \Gamma_{\lambda[\mu]}^{*\nu}(g) \sum_{\beta q} \exp(2\pi i \mathbf{k} \cdot \mathbf{a}_{gs}^j) \det(h) h_{\beta\alpha} \delta_{s,gq}^j \boldsymbol{\varepsilon}_{\beta q}^{kj}$$

It is convenient to use, instead of the basis vectors for the whole set of magnetic atoms in the primitive cell, the so called *atomic components* of the basis vectors, which are normal 3D constant vectors attached to individual atoms:

$$\psi_{\lambda}^{\mathbf{k}\nu}(j) = \sum_{\oplus, s=1, \dots, p_j} \mathbf{S}_{\lambda}^{\mathbf{k}\nu}(js)$$

The explicit expression for the atomic components of the basis functions is:

$$\mathbf{S}_{\lambda}^{\mathbf{k}\nu}(js) \propto \sum_{g \in G_{0\mathbf{k}}} \Gamma_{\lambda[\mu]}^{*\nu}(g) e^{2\pi i \mathbf{k} \mathbf{a}_{gs}^j} \det(h) \delta_{s,g[q]}^j \begin{pmatrix} h_{1\alpha} \\ h_{2\alpha} \\ h_{3\alpha} \end{pmatrix}$$

The fundamental hypothesis of the Symmetry Analysis of magnetic structures is that the Fourier coefficients of a magnetic structure are linear combinations of the basis functions of the irreducible representation of the propagation vector group $\mathbf{G}_k$

$$\mathbf{S}_{\mathbf{k}js} = \sum_{n\lambda} C_{n\lambda}^{\nu} \mathbf{S}_{n\lambda}^{\mathbf{k}\nu}(js)$$



$$\mathbf{M}(\mathbf{h}) = p \sum_{j=1}^n O_j f_j(\mathbf{h}) T_j \sum_{n\lambda} C_{n\lambda}^{\nu} \sum_s \mathbf{S}_{n\lambda}^{\mathbf{k}\nu}(js) \exp\{2\pi i \mathbf{h}_s \mathbf{r}_j\}$$

$$\text{Fourier coeff.} \rightarrow \mathbf{S}_{\mathbf{k}js} = \sum_{n\lambda} C_{n\lambda}^{\nu} \mathbf{S}_{n\lambda}^{\mathbf{k}\nu} (js) \leftarrow \text{Basis vectors}$$

The diagram shows the equation $\mathbf{S}_{\mathbf{k}js} = \sum_{n\lambda} C_{n\lambda}^{\nu} \mathbf{S}_{n\lambda}^{\mathbf{k}\nu} (js)$. A red circle highlights $\mathbf{S}_{\mathbf{k}js}$ with a red arrow pointing to it from the text "Fourier coeff.". A blue circle highlights $\mathbf{S}_{n\lambda}^{\mathbf{k}\nu} (js)$ with a blue arrow pointing to it from the text "Basis vectors". Red arrows also point from the superscripts ν in $C_{n\lambda}^{\nu}$ and $\mathbf{S}_{n\lambda}^{\mathbf{k}\nu}$ to the symbol ν in the text "Indices:" below.

The coefficients $C_{n\lambda}^{\nu}$ are the free parameters of the magnetic structure. Called “mixing coefficients” by Izyumov

Indices:

$\mathbf{k}$: reference to the propagation vector

ν : reference to the irreducible representation Γ^{ν}

n : index running from 1 up to $n_{\nu} \Rightarrow \Gamma_{Mag} = \sum_{\oplus \nu} n_{\nu} \Gamma^{\nu}$

λ : index running from 1 up to $\dim(\Gamma^{\nu})$

Going beyond G_k : more symmetric magnetic structures using the representations of the whole space Group

Up to now we have considered only the Irreps of the little group. In some cases we can add more constraints considering the representations of the whole space group. This is a way of connecting split orbits (j and j') due, for instance to the fact that the operator transforming $\mathbf{k}$ into $-\mathbf{k}$ is lost in G_k .

$$\mathbf{G} = \mathbf{G}_k + g_2 \mathbf{G}_k + \dots g_{l_k} \mathbf{G}_k = \sum_{L=1}^{l_k} g_L \mathbf{G}_k = \sum_{L=1}^{l_k} \{h_L | \mathbf{t}_{h_L}\} \mathbf{G}_k \quad \mathbf{k}_L = h_L \mathbf{k}$$

$$\text{Star of } \mathbf{k}: \{\mathbf{k}\} = \{\mathbf{k}, h_2 \mathbf{k}, h_3 \mathbf{k}, \dots h_{l_k} \mathbf{k}\} = \{\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3, \dots \mathbf{k}_{l_k}\}$$

The little groups $\mathbf{G}_{k_L}$ are conjugate groups to $\mathbf{G}_k$

$$\mathbf{G}_{k_L} = g_L \mathbf{G}_k g_L^{-1} \quad g_L \mathbf{r}_s^j = h_L \mathbf{r}_s^j + \mathbf{t}_{h_L} = \mathbf{r}_q^{j'} + \mathbf{a}_{g_L s}^j$$

$$\Gamma^{\mathbf{k}_L \nu}(g) = \Gamma^{\mathbf{k} \nu}(g_L g g_L^{-1}) \quad \Psi_{\lambda}^{\mathbf{k}_L \nu} = O(g_L) \Psi_{\lambda}^{\mathbf{k} \nu} \quad (\lambda = 1, \dots, l_{\nu})$$

$$\mathbf{S}_{\mathbf{k}js} = \sum_{n\lambda} C_{n\lambda}^{\nu} \mathbf{S}_{n\lambda}^{\mathbf{k}\nu}(js)$$

Applying the formulae we have for applying the operators to the basis vectors we obtain for the atomic components the following relations:

$$g_L \mathbf{r}_s^j = h_L \mathbf{r}_s^j + \mathbf{t}_{h_L} = \mathbf{r}_q^{j'} + \mathbf{a}_{g_L s}^j$$

$$\mathbf{S}_{\lambda}^{\mathbf{k}_L \nu}(j'q) = e^{2\pi i \mathbf{k}_L \cdot \mathbf{a}_{g_L s}^j} \det(R) R(h_L) \mathbf{S}_{\lambda}^{\mathbf{k}\nu}(js)$$

If we consider that our magnetic structure can be described by a representation of the whole space group the Fourier coefficients of atoms that are not connected by a symmetry operator of G_k are related by:

$$\mathbf{S}_{\mathbf{k}_L j'q} = e^{2\pi i \mathbf{k}_L \cdot \mathbf{a}_{g_L s}^j} \det(R_L) R_L \mathbf{S}_{\mathbf{k}js}$$

The maximum number of free coefficients to describe the magnetic structure is proportional to the number m of independent basis vectors

if we consider real coefficients when $\mathbf{k} = \frac{1}{2} \mathbf{H}$

$$n_f = m \times \dim(\Gamma^\vee)$$

if we consider complex coefficients when $\mathbf{k} \in \text{IBZ}$

$$n_f = 2m \times \dim(\Gamma^\vee) - 1$$

The analysis is successful when one of the following conditions apply:

$$n_f = 2m \times \dim(\Gamma^\vee) - 1 < 6p_j \text{ (for } \mathbf{k} \text{ non equivalent to } -\mathbf{k})$$

$$n_f = m \times \dim(\Gamma^\vee) < 3p_j \text{ (for } \mathbf{k} \text{ equivalent to } -\mathbf{k})$$

Where p_j is the number of sublattices (atoms) of site j . The effective number of free parameters is lower in general as soon as one uses the relation between basis vectors of different arms of the star $\{\mathbf{k}\}$ or select special direction in representation space for $\dim(\Gamma^\vee) > 1$.

Alternatively, a more close to traditional crystallographic approaches can be considered in some cases. The Fourier component $\mathbf{k}$ of the magnetic moment of atom j_1 , that transforms to the atom j_s when the symmetry operator $g_s = \{S|t\}_s$ of $G_{\mathbf{k}}$ is applied ($\mathbf{r}_s^j = g_s \mathbf{r}_1^j = S \mathbf{r}_1^j + \mathbf{t}_s$), is transformed as:

$$\mathbf{S}_{\mathbf{k}js} = M_{js} \mathbf{S}_{\mathbf{k}j_1} \exp\{-2\pi i \phi_{\mathbf{k}js}\}$$

$$\mathbf{M}(\mathbf{h}) = p \sum_{j=1}^n O_j f_j(\mathbf{h}) T_j \sum_s \mathbf{S}_{\mathbf{k}js} \exp\{2\pi i [(\mathbf{H} + \mathbf{k})\{S|\mathbf{t}\}_s \mathbf{r}_j - \Phi_{\mathbf{k}j}]\}$$

The matrices M_{js} and phases $\phi_{\mathbf{k}js}$ can be deduced from the relations between the Fourier coefficients and atomic basis functions. The matrices M_{js} correspond, in the case of commensurate magnetic structures, to the rotational parts of the magnetic Shubnikov group acting on magnetic moments.

The irreducible representations of space groups can be obtained consulting tables or using computer programs for calculating them.

The basis functions of the irreducible representations depend on the particular problem to be treated and they have to be calculated by using projection operator formula. A series of programs allow these kind of calculations, that may be quite tedious and prone to errors by hand, to be done.

Concerning magnetic structures three programs are of current use: **BasIreps** (J. Rodríguez-Carvajal), **SARAh** (Andrew Wills) and **MODY** (Wiesława Sikora). One can use also **BCS** (Perez-Mato et al.) or **ISODISTORT** (B.Campbell and H. Stokes)

Programs for symmetry analysis



A series of computing tools for crystallography including magnetic structures are available at Bilbao Crystallographic Server

bilbao crystallographic server

[The crystallographic site at the Condensed Matter Physics Dept. of the University of the Basque Country]

[Space Groups] [Layer Groups] [Rod Groups] [Frieze Groups] [Wyckoff Sets]



2014: International Year of Crystallography

NEW!

Satellite workshop of the 2014 IUCr Congress:

Role of Magnetic Symmetry in the Description
and Determination of Magnetic Structures.
Hamilton, Canada
14-16 August 2014

Space Groups Retrieval Tools

GENPOS	Generators and General Positions of Space Groups
WYCKPOS	Wyckoff Positions of Space Groups
HKLCD	Reflection conditions of Space Groups
MAXSUB	Maximal Subgroups of Space Groups
SERIES	Series of Maximal Isomorphic Subgroups of Space Groups
WYCKSETS	Equivalent Sets of Wyckoff Positions
NORMALIZER	Normalizers of Space Groups
KVEC	The k-vector types and Brillouin zones of Space Groups
SYMMETRY OPERATIONS	Geometric interpretation of matrix column representations of symmetry operations
IDENTIFY GROUP	Identification of a Space Group from a set of generators in an arbitrary setting

Programs for symmetry analysis

Magnetic Symmetry and Applications

MGENPOS	General Positions of Magnetic Space Groups
MWYCKPOS	Wyckoff Positions of Magnetic Space Groups
MAGNEXT	Extinction Rules of Magnetic Space Groups
IDENTIFY MAGNETIC GROUP ⚠	Identification of a Magnetic Space Group from a set of generators in an arbitrary setting
MAXMAGN ⚠	Maximal magnetic space groups for a given a propagation vector and resulting magnetic structural models
k-SUBGROUPSMAG ⚠	Magnetic subgroups consistent with some given propagation vector(s) or a supercell
MAGNDATA ⚠	A collection of magnetic structures with transportable cif-type files

Structure Utilities

CELLTRAN	Transform Unit Cells
STRAIN	Strain Tensor Calculation
WPASSIGN	Assignment of Wyckoff Positions
TRANSTRU	Transform structures.
SETSTRU ⚠	Alternative Settings for a given Crystal Structure
EQUIVSTRU	Equivalent Descriptions for a given Crystal Structure
STRCONVERT	Convert & Edit Structure Data (supports the CIF, mCIF, VESTA, VASP formats -- with magnetic information where available)
VISUALIZE	Visualize structures using Jmol
COMPSTRU ⚠	Comparison of Crystal Structures with the same Symmetry
STRUCTURE RELATIONS ⚠	Evaluation of structure relationships [transformation matrix] between group-subgroup related phases
PSEUDOLATTICE	Pseudosymmetry of a lattice and compatible supergroups

Programs for symmetry analysis

ISOTROPY Software Suite

Harold T. Stokes, Dorian M. Hatch, and Branton J. Campbell, Department of Physics and Astronomy, Brigham Young University, Provo, Utah 84606, USA, stokes@byu.edu

Description: The ISOTROPY software suite is a collection of software which applies group theoretical methods to the analysis of phase transitions in crystalline solids.

How to cite: ISOTROPY Software Suite, iso.byu.edu.

References

A huge amount of work on symmetry has been developed by Harold Stokes, Dorian Hatch and Branton Campbell. Stokes developed ISOTROPY and many algorithms for working with space groups and representations. Together with the programs they have made available databases to be used by external software

- **FINDSYM**: Identify the
- New! **ISO-IR**: Tables of
- **ISO-MAG**: Tables of

Superspace Groups

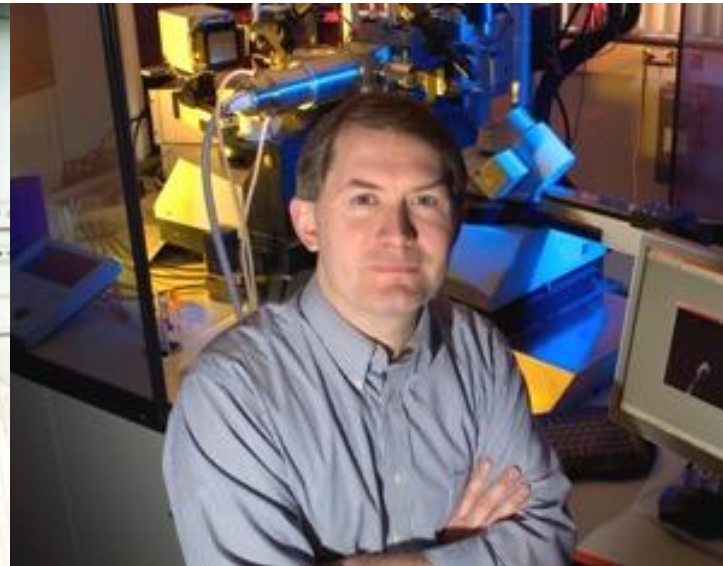
- **ISO(3+d)D**: (3+d)-D
- **ISO(3+1)D**: Isotropy
- **FINDSSG**: Identify the
- **TRANSFORMSSG**:

Phase Transition

- **COPL**: Find a comp
- **INVARIANTS**: Gene
- **COMSUBS**: Find co

Linux

- **ISOTROPY Software**



lations

GUI for BasIreps

BasIreps Gui Interface

File Run Results Help Exit

Code of files: Working Directory:

BasIreps (May-2004, JRC-LLB)
Irreducible representations of Space Groups
Basis functions of polar & axial vector properties

Title:

SpaceGroup (HM/Hall symbols) or generators separated by ",":

K-Vector: Brillouin Zone Label:

☐ Polar Vector ☒ Axial Vector

Number of Atoms: ☐ Explicit Sublattices ☒ Atoms in unit cell

	Symbol	x/a	y/a	z/a
Atom # 1	Tb3+	0.00000	0.00000	0.50000
Atom # 2	Tb4+	0.00000	0.50000	0.25000

Code of files

Title

k-vector

Axial/polar

Number of atoms

Working directory

SG symbol or generators

Brillouin Zone label

Atoms in Unit Cell

Atoms positions

BasIreps provides the basis functions (normal modes) of the irreducible representations of the wave-vector group G_k

$$\mathbf{m}_{ljs} = \sum_{\{\mathbf{k}\}} \mathbf{S}_{\mathbf{k}js} \exp\{-2\pi i \mathbf{k} \mathbf{R}_l\}$$

$$\mathbf{S}_{\mathbf{k}js} = \sum_{n\lambda} C_{n\lambda}^{\nu} \mathbf{S}_{n\lambda}^{\mathbf{k}\nu}(js)$$

Output of ***BasIreps*** $\Rightarrow$ Basis Functions (constant vectors)

$$\mathbf{S}_{n\lambda}^{\mathbf{k}\nu}(js)$$

Output of BasIreps

```
KEDIT - [D:\Docs\Conferences2003\RSEFQ-Madrid\Lamno3.bsr]
File Edit Actions Options Window Help
norm
=> Atomic components of the BASIS FUNCTIONS using PROJECTION OPERATORS:
      Calculation for SITE number: 1
      (Only non-null functions are written)

+++++
=> Basis functions of Representation IRrep( 1) of dimension 1 contained 3 times in GAMMA
+++++

SYMM  x,y,z   -x+1,-y,z+1/2   x-1/2,-y+1/2,-z   -x+1/2,y+1/2,-z+1/2
Atoms:  Mn_1      Mn_2      Mn_3      Mn_4
1:Re (   1   0   0) (  -1   0   0) (   1   0   0) (  -1   0   0)
2:Re (   0   1   0) (   0  -1   0) (   0  -1   0) (   0   1   0)
3:Re (   0   0   1) (   0   0   1) (   0   0  -1) (   0   0  -1)

----- LINEAR COMBINATIONS of Basis Functions: coefficients u,v,w,p,q ....
General expressions of the Fourier coefficients Sk(i) i=1,2,...nat

Fourier coefficient for SYMM x,y,z           Atom: Mn_1 | 0.5000  0.0000  0.0000
              Sk( 1): ( u, v, w )

Fourier coefficient for SYMM -x+1,-y,z+1/2   Atom: Mn_2  0.5000  0.0000  0.5000
              Sk( 2): (-u,-v, w )

Fourier coefficient for SYMM x-1/2,-y+1/2,-z Atom: Mn_3  0.0000  0.5000  0.0000
              Sk( 3): ( u,-v,-w )

Fourier coefficient for SYMM -x+1/2,y+1/2,-z+1/2 Atom: Mn_4  0.0000  0.5000  0.5000
              Sk( 4): (-u, v,-w )

+++++
```

Line=437 Col=69 Alt=3,3:3 Size=526 Files=3 Windows=3 OVR R/W 12:59 AM

Output of BasIreps

```
KEDIT - [D:\Docs\Conferences2003\RSEFQ-Madrid\Lamno3.fp]
File Edit Actions Options Window Help
norm
-->

      X      Y      Z      for site:  1
-> Mn_1   :   0.5000  0.0000  0.0000  : (x,y,z)
-> Mn_2   :   0.5000  0.0000  0.5000  : (-x,-y,z+1/2) + ( 1 , 0 , 0 )
-> Mn_3   :   0.0000  0.5000  0.0000  : (x+1/2,-y+1/2,-z) + (-1 , 0 , 0 )
-> Mn_4   :   0.0000  0.5000  0.5000  : (-x+1/2,y+1/2,-z+1/2) + ( 0 , 0 , 0 )

=> Basis functions of Representation IRrep( 1) of dimension  1 contained 3 times in GAMMA
Representation number      :  1 for Site:  1
Number of basis functions:  3

----- Block-of-lines for PCR start just below this line
P -1                                <--Space group symbol for hkl generation
! Nsym   Cen   Laue Ireps N_Bas
   4       1       1      -1       3
! Real(0)-Imaginary(1) indicator for Ci
  0  0  0
SYMM x,y,z
BASR   1  0  0   0  1  0   0  0  1
BASR   0  0  0   0  0  0   0  0  0
SYMM -x+1,-y,z+1/2
BASR  -1  0  0   0 -1  0   0  0  1
BASR   0  0  0   0  0  0   0  0  0
SYMM x-1/2,-y+1/2,-z
BASR   1  0  0   0 -1  0   0  0 -1
BASR   0  0  0   0  0  0   0  0  0
SYMM -x+1/2,y+1/2,-z+1/2
BASR  -1  0  0   0  1  0   0  0 -1
BASR   0  0  0   0  0  0   0  0  0
```

Format for *FullProf*

$\mathbf{k}=(0,0,0)$, $v=1$, $n=1,2,3$
 $\lambda=1$, $j=1$, $s=1,2,3,4$

$S_{n\lambda}^{k v}(js)$



Steps for magnetic structure determination using powder diffraction

Step

Input

Propagation vector(s)
k_Search

Peak positions of
⇐ magnetic reflections
Cell parameters

Symmetry Analysis
*BasIreps, MODY,
SARAh, BCS, Isotropy*

Propagation vector
⇐ Space Group
Atom positions

Magnetic structure
solution (Sim. Ann.)
FullProf

Integrated intensities
⇐ Atomic components of basis
functions or Shubnikov group
symmetry operators

Input

Magnetic structure
Refinement
FullProf

*Complete structural
⇐ model should be
provided*

Different runs of SAnn jobs may give you an idea of the degeneracy of solutions for your particular problem.

In many cases the number of free parameters is too much high to be refined by LSQ: try to reduce the number of parameters or make soft constraints.

Use spherical components of Fourier coefficients in order to have better control of the amplitude of the magnetic moment

- **FullProf** is now able to produce a magnetic CIF file (extension mCIF) for commensurate magnetic structures described in the magnetic cell. This mCIF file can be directly read by **FP_Studio** and also by the program **VESTA**.

The program converts the user-description of the magnetic structure, using the crystal cell and propagation vector and MSYM operators or basis functions, to the magnetic cell with all the magnetic atoms inside that cell.

This mCIF file may be used to determine the Shubnikov group of the used model thanks to the program ISOCIF that can be executed via the Web at

<http://stokes.byu.edu/iso/isocif.php>

A new option for reading symmetry operators for magnetic structures in **FullProf** has been implemented.

These operators are for commensurate structures and the mix in some sense SYMM and MSYM operators.

The value **Isy=2** is used to inform the program that this kind of operator will be provided. Four forms are recognized by **FullProf**, examples of these operators for are given below:

```
1->  SHUB    x+1/2, -y, z    -u, v, -w
2->  SHUB    x+1/2, -y, z    -mx, my, -mz    +1
3->  SHUB    x+1/2, -y, z    +1
4->  SHUB    x+1/2, -y, z, +1
```

The three operator are identical (the +1 indicated that time reversal is not associated to the operator, a -1 indicates the opposite situation). The keyword SHUB is not strictly needed, it may be replaced by any word or number but it cannot be omitted.

The complete list of symmetry operators corresponding to a particular setting of any magnetic space group may be obtained through the **Bilbao Crystallographic Server** using the programs **MAXMAGN** or **STRCONVERT**.

A console program converting mCIF files (as produced by the **Bilbao Crystallographic Server** or by **ISOCIF**) to PCR files has been included in the new **FullProf Suite**.

The console program is called **mCIF_to_PCR** and will be extended with a GUI in the near future.

Presently the provided PCR file is adequate for a simulation and the user should change by hand the parameters.

New facilities for Magnetic Structures

Structure Data Converter & Editor

Title:

Short Definition:

Source DOI:

Symmetry

Space Group #: (P1)

Lattice Parameters

a: Å b: Å c: Å

α : ° β : ° γ : °

Symmetry Operations [\[Show/Hide\]](#)

Atomic Positions & Displacements

Switch to the treatment of the vectors as: Magnetic Moments

	Label	Element	x	y	z	Occ.	Δ_x	Δ_y	Δ_z
☐	X1	X	0.00000	0.00000	0.00000	1.00000	0.00000	0.00000	0.00000

atoms more.

Longest Arrow size:

[for VESTA format export: Å (Default: $\min(a,b,c)/4$)]
[for Jmol visualize: a proportional coefficient]

Tolerance:

[via [FINDSYM](#) by Stokes & Campbell]

The End!

Some references for Magnetic Neutron Scattering

Theory of Neutron Scattering from Condensed Matter

Volume 2: Polarization Effects and Magnetic Scattering

Stephen W. Lovesay, Clarendon Press (Oxford University Press),
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Yurii A. Izyumov and Ruslan P. Ozerov, Plenum Press (New York),
1970.

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The mathematical theory of symmetry in solids

C.J. Bradley and A.P. Cracknell, Clarendon Press (Oxford University Press, Ely House, London W.1), 1972.

Kronecker Product Tables. Vol. 1.

A.P. Cracknell, B.L. Davies, S.C. Miller, and W.F. Love, (1979).

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Ed. by Harold T. Stokes and Dorian M. Hatch, Gordon and Breach Science Publishers, 1993.

Neutron diffraction of magnetic materials

Y.A. Izyumov, V.E. Naish and R.P. Ozerov

Consultants Bureau, Plenum Publishing Corporation, New York (1991)

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W. Opechowski and R. Guccione. *Magnetic Symmetry*, in Magnetism, Vol. 2A, Ed. G.T. Rado and H. Suhl, Academic Press, 1965.

E. F. Bertaut, Acta Cryst. **A24**, 217 (1968).

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Bilbao Crystallographic Server: <http://www.cryst.ehu.es/>

ISOTROPY Software Suite : <http://stokes.byu.edu/iso/isotropy.php>

FullProf Suite : <http://www.ill.eu/sites/fullprof/>