Francesco Ricci School, Neutron Scattering from Magnetic Systems

Neutron Polarimetry: I Theory of Polarised Neutron Scattering

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Outline: Theory of Polarised Neutron Scattering

Notation

θ_B	Bragg angle
γ_N	Gyromagnetic ratio of the neutron
Ω_L	Larmor precession frequency
m_N	Neutron mass
E_f	Fermi energy
T_C	Curie Temperature
T_N	Néel Temperature
$\mathbf{M}$	Magnetic moment vector
$\mathbf{M}(\mathbf{r})$	Magnetisation at $\mathbf{r}$
$\mathbf{M}(\mathbf{k})$	Magnetic structure factor at $\mathbf{k}$.
$\mathbf{M}_\perp(\mathbf{k})$	Magnetic interaction vector at $\mathbf{k}$.
$\mathbf{M}_\perp$	Magnetic interaction vector (shorthand form)
$\mathbf{M}^*_\perp(\mathbf{k})$	Complex conjugate of $\mathbf{M}_\perp(\mathbf{k})$
$\mathbf{M}^*_\perp$	Complex conjugate of $\mathbf{M}_\perp(\mathbf{k})$ (shorthand form)
$M_{\perp i}$	ith component of magnetic interaction vector
$N(\mathbf{k})$	Nuclear structure factor at $\mathbf{k}$.
N	Nuclear structure factor (shorthand form)
N^*	Complex conjugate of nuclear structure factor

Notation (cont.)

$\mathbf{P}$	Incident polarisation
P	modulus of $\mathbf{P}$
P_i	ith component of incident polarisation
$\mathbf{P}'$	Scattered polarisation
P'_i	ith component of scattered polarisation
$\mathbf{P}''$	Polarisation created by scattering
P''_i	ith component of polarisation created by scattering
$\mathscr{P}$	Polarisation tensor
$\mathscr{P}_{ij}$	ijth element of the polarisaton tensor
P_{ij}	Polarisation matrix (the experimental result)
P_{ij}	ijth element of the polarisaton tensor
$\mathbf{k}$	Crystallographic scattering vector $\mathbf{k} = \mathbf{k_f} - \mathbf{k_i}$
k	$\lvert\mathbf{k}\rvert$
$\mathbf{r}$	A vector in real space
$\mathbf{a}$ $\mathbf{b}$ $\mathbf{c}$	Unit cell vectors
$\mathbf{g}$	A reciprocal lattice vector
$\boldsymbol{l}$	A lattice vector
τ	Magnetic propagation vector
$\hat{\mathbf{u}}$	A unit vector parallel to $\mathbf{u}$

Introduction

- In the following we will consider how the theory of neutron scattering can be amplified to take account of neutron polarisation.
- For simplicity the discussion will concentrate on elastic Bragg scattering although most of the formulae are equally applicable to inelastic scattering if the appropriate cross-sections are substituted and energy conservation terms are taken into account.
- We first consider what is meant by Neutron Polarisation

Polarisation of a single neutron

The spin wave-function of any single neutron can be written

$$\psi_S = a\psi^+ + b\psi^- \quad \text{where} \quad aa^* + bb^* = 1$$

ψ^+ and ψ^- are eigenfunctions of spin with eigenvalues $\pm\frac{1}{2}$ respectively.

Using the Pauli spin matrices

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_y = \begin{pmatrix} 0 & -\imath \\ \imath & 0 \end{pmatrix} \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

The matrix for the component of spin in a direction with spherical polar coordinates θ ϕ is

$$\mathbf{S}_{\theta,\phi} = \frac{1}{2}\begin{pmatrix} \cos\theta & \sin\theta(\cos\phi - \imath\sin\phi) \\ \sin\theta(\cos\phi + \imath\sin\phi) & -\cos\theta \end{pmatrix}$$

Operating with $\mathbf{S}_{\theta,\phi}$ on ψ_S gives
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$$\mathbf{S}_{\theta,\phi}\psi_S = (\tfrac{1}{2}\cos\theta + \sin\theta\cos\phi + \imath\sin\theta\sin\phi)\psi^+ + \sin\theta(\cos\phi - \imath\sin\theta\sin\phi - \tfrac{1}{2}\cos\theta)\psi^-$$

ψ_S is an eigen function of $\mathbf{S}_{\theta,\phi}$ with spin eigenvalue $\frac{1}{2}$ when

$$\tan\frac{\theta}{2} = \frac{|a|^2}{|b|^2} \quad \text{and} \quad \tan\phi = \frac{\Im(ab^*)}{\Re(ab^*)}$$

A single neutron is always perfectly polarised in some direction

A Neutron Beam

- Experimentally we are always dealing with beams containing many neutrons each of which may be polarised in a different direction.
- We determine the numbers of neutrons scattered with spins parallel and anti-parallel to some chosen polarisation direction.
- This is equivalent, in quantum mechanical terms, to determining the mean value of the neutron spin parallel to this direction.
- Evaluation of the mean values of properties of systems, such as neutron beams, which consist of an incoherent superposition of particles in different pure states is conveniently done using the density matrix formalism.
- A very clear account of this formalism is given by:
  U. Fano,(1957) Rev. Mod. Phys **19** 74.

The quantum mechanical density matrix

- Consider a pure state described in terms of the eigenvectors u_n of a complete set of operators by the wave-function $\psi = \sum_n c_n u_n$.
- The mean value of the property given by an operator Q represented by the matrix Q_{nm} is

$$\langle Q \rangle = \sum_{n,m} Q_{mn} c_m^* c_n$$

- A mixed state can be described by a superposition of pure states ψ^i with statistical weights p^i.
- The mean value of Q for the mixed state is

$$\langle Q \rangle = \sum_{n,m} Q_{mn} \sum_i p^i {c^i}_m{}^* {c^i}_n$$

- The density matrix is defined as

$$\rho_{n,m} = \sum_i p^i {c^i}_m{}^* {c^i}_n$$

$$\text{and} \quad \langle Q \rangle = \sum_{n,m} Q_{nm} \rho_{nm} = \sum_m (Q\rho)_{mm} = \mathrm{Tr}(Q\rho)$$

The Polarisation density matrix

- The polarisation of a neutron beam parallel to a unit vector $\hat{\mathbf{u}}$ with components u_x, u_y, u_z is defined by

$$P_{\mathbf{u}} = \frac{N^{+\mathbf{u}} - N^{-\mathbf{u}}}{N^{+\mathbf{u}} + N^{-\mathbf{u}}} = 2\langle S_{\mathbf{u}} \rangle \quad \text{so that} \quad -1 < P_{\mathbf{u}} < 1$$

where $N^{+\mathbf{u}}$ and $N^{-\mathbf{u}}$ are the numbers of neutrons in the beam with spins parallel and antiparallel to $\mathbf{u}$.

- We define a polarisation density matrix ρ such that

$$P_{\mathbf{u}} = 2\langle S_u \rangle = \mathrm{Tr}(\rho \sigma_u)$$

$$\text{with} \quad \sigma_u = \begin{pmatrix} u_z & u_x - \imath u_y \\ u_x + \imath u_y & -u_z \end{pmatrix} \quad \text{and} \quad \mathrm{Tr}(\rho) = 1$$

The Polarisation density matrix

Notation
Polarised Neutron Scattering
Neutron Polarisation
A single neutron
The polarisation density matrix
The Scattering Cross-section for Polarised Neutrons
The Blume Maleev Equations

- Like any Hermitian matrix ρ can be expressed as a linear combination of the unit matrix $\mathbf{I}$ and the three Pauli spin matrices $\sigma_x, \sigma_y, \sigma_z$. Let

$$\begin{aligned} \rho &= A(\mathbf{I} + p_x\sigma_x + p_y\sigma_y + p_z\sigma_z) = A \begin{pmatrix} 1+p_z & p_x - \imath p_y \\ p_x + \imath p_y & 1-p_z \end{pmatrix} \\ A &= \tfrac{1}{2} \text{ for } \mathrm{Tr}(\rho) = 1 \end{aligned}$$

- then

$$\begin{aligned} P_{\mathbf{u}} &= \tfrac{1}{2}\mathrm{Tr}\left(\begin{pmatrix} u_z & u_x - \imath u_y \\ u_x + \imath u_y & -u_z \end{pmatrix} \begin{pmatrix} 1+p_z & p_x - \imath p_y \\ p_x + \imath p_y & 1-p_z \end{pmatrix} \right) \\ &= (u_z p_z + u_x p_x + u_z p_z) \end{aligned}$$

- A polarisation vector $\mathbf{P}$ with components p_x, p_y, p_z can be identfied whose properties ensure that that

$$P_{\mathbf{u}} = 2\langle S_u \rangle = \hat{\mathbf{u}}(\mathbf{P} \cdot \hat{\mathbf{u}}) \quad \text{and} \quad \rho = \tfrac{1}{2}(\mathbf{I} + \mathbf{P} \cdot \sigma)$$

Useful traces

The following properties of the unit matrix and the Pauli spin matrices are used to help in evaluating the required traces

$$\begin{aligned}
\mathrm{Tr}(I) &= 2 \\
\mathrm{Tr}(\sigma_i) &= 0 \\
\mathrm{Tr}(\sigma_i\sigma_j) &= 2\delta^{ij} \\
\mathrm{Tr}(\sigma_i\sigma_j\sigma_k) &= 2\imath\varepsilon^{ijk} \\
\mathrm{Tr}(\sigma_i\sigma_j\sigma_k\sigma_l) &= 2(\delta^{ij}\delta^{kl} - \delta^{ik}\delta^{jl} + \delta^{il}\delta^{jk})
\end{aligned}$$

i,j,k,l each run over all three components x,y,z and ε^{ijk} is the antisymmetric third rank unit tensor: $\sum_{j,k}\varepsilon^{ijk} = (\mathbf{A}\times\mathbf{B})_i$

The scattering cross-section

Within the Born approximation the intensity I of neutrons scattered with scattering vector $\mathbf{k} = \mathbf{k}_f - \mathbf{k}_i$ is given by

$$I = C\sum_{q,q',i,i'} p_q p_i \left\langle \psi^*_{q'}\phi^*_{i'} \left| V^\dagger_{q,q',i}(\mathbf{k}) V_{q,q',i}(\mathbf{k}) \right| \phi_i\psi_q \right\rangle \delta(\Delta E)$$

- $\psi_q, \psi_{q'}$ and $\phi_i, \phi_{i'}$ represent the initial and final states of the scatterer and the neutron respectively.
- p_q and p_i are the statistical weights of ψ_q and ϕ_i.
- $V(\mathbf{k})$ is the fourier transform of the interaction between the neutron and the scatterer.
- $\delta(\Delta E)$ with $\Delta E = \hbar^2(k_f^2 - k_i^2)/2m_\mathrm{N} + E_{q'} - E_q$ ensures conservation of energy.

The density matrix formalism can be used to do the sum over the initial states of the neutron giving

$$I = C\sum_q p_q \mathrm{Tr}(V^\dagger_{q,q',i}(\mathbf{k}) V_{q,q',i}(\mathbf{k})\rho)\delta(\Delta E)$$

The scattered polarisation

The scattered polarisation is obtained by determining the average of the spin of the scattered neutrons.

$$\mathbf{P}'I = 2C \sum_{q,q',i,i'} p_q p_i \left\langle \psi^*_{q'} \phi^*_{i'} \left| V^\dagger_{q,q',i}(\mathbf{k})\ \mathbf{S}\ V_{q,q',i}(\mathbf{k}) \right| \phi_i \psi_q \right\rangle \delta(\Delta E)$$

which, using the density matrix becomes

$$\mathbf{P}'I = C \sum_q p_q \mathrm{Tr}(V^\dagger_{q,q',i}(\mathbf{k}) \mathbf{S} V_{q,q',i}(\mathbf{k}) \rho) \delta(\Delta E)$$

The traces are to be taken over the neutron spin coordinates only

The magnetic interaction vector

For magnetic scattering the relevant interaction is that between the neutron magnetic moment and the the magnetic induction of the scatterer.

$$V(\mathbf{r}) = 2\mathbf{B}(\mathbf{r}) \cdot \mathbf{S} = 2(\mu_0 \mathbf{H} + \mathbf{M}(\mathbf{r})) \cdot \mathbf{S}$$

where $\mathbf{M}(\mathbf{r})$ is the magnetisation distribution in the crystal.

The kth Fourier component is

$$\mathbf{M}_\perp(\mathbf{k}) = \hat{\mathbf{k}} \times \mathbf{M}(\mathbf{k}) \times \hat{\mathbf{k}} \quad \text{with} \quad \mathbf{M}(\mathbf{k}) = \int \mathbf{M}(\mathbf{r}) \exp(-i\mathbf{k} \cdot \mathbf{r}) dr^3$$

where $\hat{\mathbf{k}}$ is a unit vector parallel to the scattering vector $\mathbf{k}$.

- $\mathbf{M}(\mathbf{k})$ is the magnetic structure factor
- $\mathbf{M}_\perp(\mathbf{k})$ is the magnetic interaction vector.
- both $\mathbf{M}(\mathbf{k})$ and $\mathbf{M}_\perp(\mathbf{k})$ are in general complex vectors.
- For pure magnetic scattering $V(\mathbf{k}) = 2\mathbf{M}_\perp(\mathbf{k}) \cdot \mathbf{S}$

Polarisation dependence of magnetic scattering

For magnetic elastic scattering the equation for the scattered intensity becomes

$$I = \tfrac{1}{2}C\mathrm{Tr}\left((\mathbf{M}_\perp^* \cdot \sigma)\ (\mathbf{M}_\perp \cdot \sigma)(\mathbf{I} + \mathbf{P} \cdot \sigma)\right)$$

Evaluating the traces gives for the intensity

$$\begin{aligned} I &= C\sum_{i,j}(M_{\perp i}^* M_{\perp j})\delta^{ij} + \sum_{i,j,k}(\imath M_{\perp i}^* M_{\perp j} P_k)\varepsilon^{ijk} \\ &= C\left(\mathbf{M}_\perp \cdot \mathbf{M}_\perp^* + \mathbf{M}_\perp^* \times \mathbf{M}_\perp \cdot \mathbf{P}\right) \end{aligned}$$

The scattered polarisation is given by

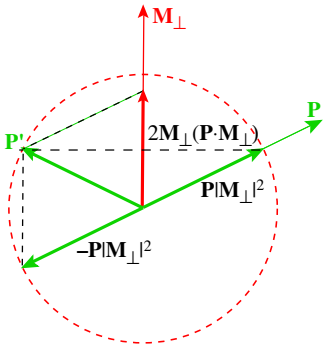
$$\mathbf{P}'I = \tfrac{1}{2}C\mathrm{Tr}\left((\mathbf{M}_\perp^* \cdot \sigma)\ \sigma\ (\mathbf{M}_\perp(\mathbf{k}) \cdot \sigma)\ (\mathbf{I} + \mathbf{P} \cdot \sigma)\right)$$

$$P_j' I = C\sum_{ik} \imath M_{\perp i}^* M_{\perp k} \varepsilon^{ijk} + M_{\perp j}^* M_{\perp k}^* P_k - M_{\perp i}^* M_{\perp i} P_j + M_{\perp i}^* M_{\perp j} P_i$$

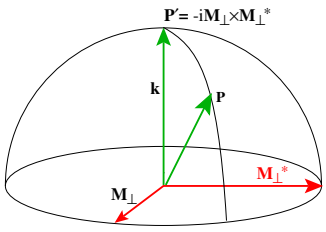
$$\mathbf{P}'I = C\left(-\imath \mathbf{M}_\perp^* \times \mathbf{M}_\perp + \mathbf{M}_\perp^*(\mathbf{M}_\perp \cdot \mathbf{P}) + \mathbf{M}_\perp(\mathbf{M}_\perp^* \cdot \mathbf{P}) - \mathbf{P}(\mathbf{M}_\perp^* \cdot \mathbf{M}_\perp)\right)$$

Simple examples

- $\mathbf{M}_\perp(\mathbf{k}) \parallel \mathbf{M}_\perp^*(\mathbf{k}), \quad \mathbf{M}_\perp^*(\mathbf{k}) \times \mathbf{M}_\perp(\mathbf{k}) = 0$
  - Part parallel to $\mathbf{P}$:- $-\mathbf{P}|\mathbf{M}_\perp(\mathbf{k})|^2$
  - Part parallel to $\mathbf{M}_\perp(\mathbf{k})$:- $2\Re(\mathbf{M}_\perp(\mathbf{k})(\mathbf{P} \cdot \mathbf{M}_\perp^*(\mathbf{k})))$
  - The scattered polarisation is rotated by 180°about the direction of $\mathbf{M}_\perp(\mathbf{k})$.



- $\mathbf{M}_\perp(\mathbf{k}) \perp \mathbf{M}_\perp^*(\mathbf{k}), \quad \mathbf{M}_\perp(\mathbf{k}) \cdot \mathbf{M}_\perp^*(\mathbf{k}) = 0$
  - The scattered polarisation is always parallel to $\mathbf{k}$
  - But the intensity is zero if $\mathbf{P}$ is parallel to $\mathbf{M}_\perp(\mathbf{k}) \times \mathbf{M}_\perp^*(\mathbf{k})$



Only neutrons with spins parallel to $\mathbf{M}_\perp^*(\mathbf{k}) \times \mathbf{M}_\perp(\mathbf{k})$ are scattered

Nuclear Scattering

- The interaction between an atomic nucleus and a neutron can be represented by the Fermi pseudo-potential, a scalar field which is zero except very close to the nuclei.
- When all spins of the nuclei are randomly oriented the neutron nuclear scattering interaction is independent of the neutron polarisation.

$$V(\mathbf{k}) = \sum_i b_i \exp(\imath \mathbf{k}\cdot\mathbf{r}_i) = N(\mathbf{k})$$

- $N(\mathbf{k})$ is the nuclear structure factor a complex scalar quantity
- The equation for the scattered intensity is then simply

$$I = \tfrac{1}{2}C\mathrm{Tr}(N^*(\mathbf{k})N(\mathbf{k})(\mathbf{I}+\mathbf{P}\cdot\sigma) = C|N(\mathbf{k})|^2$$

- The scattered polarisation is given by

$$\mathbf{P}'I = \tfrac{1}{2}C\mathrm{Tr}N^*(\mathbf{k})\ \sigma\ N(\mathbf{k})(\mathbf{I}+\mathbf{P}\cdot\sigma)$$

$$P'_iI = C|N(\mathbf{k})|^2P_i \quad \text{giving} \quad \mathbf{P}' = \mathbf{P}$$

- The polarisation is unchanged by nuclear scattering from nuclei with randomly oriented nuclear spins.

Magnetic Nuclear interference (intensity)

When both nuclear and magnetic scattering occur in the same reflections the joint interaction potential is

$$V(\mathbf{k}) = (N(\mathbf{k}) + 2\mathbf{M}_\perp(\mathbf{k})\cdot\mathbf{S})$$

The equation for the scattered intensity is then

$$I = \tfrac{1}{2}C\mathrm{Tr}(N^* + \mathbf{M}^*_\perp\cdot\sigma^\dagger)(N + \mathbf{M}_\perp\cdot\sigma)(\mathbf{I}+\mathbf{P}\cdot\sigma)$$

The extra terms are those involving products of N and $\mathbf{M}_\perp$ they are

$$\begin{aligned}\mathrm{Tr}(N^*\mathbf{M}_\perp(\mathbf{k})\cdot\sigma)(\mathbf{I}+\mathbf{P}\cdot\sigma) &= N^*\mathbf{M}_\perp\cdot\mathbf{P}\\ \text{and its complex conjugate} &\qquad N\mathbf{M}^*_\perp\cdot\mathbf{P}\end{aligned}$$

Finally

$$I = C\left(|N|^2 + 2\Re(N\mathbf{M}^*_\perp\cdot\mathbf{P}) + |\mathbf{M}_\perp|^2 - \imath\mathbf{M}^*_\perp\times\mathbf{M}_\perp\right)$$

The extra term in the intensity is non-zero when the phase difference between N and component of $\mathbf{M}_\perp$ parallel to $\mathbf{P}$ is not exactly $(2n+1)\frac{\pi}{2}$.

Magnetic Nuclear interference (polarisation)

The polarisation of the scattered beam is

$$\mathbf{P}'I = \tfrac{1}{2}C\left(N^* + \mathbf{M}_\perp^* \cdot \sigma^\dagger)\mathbf{S}(N + \mathbf{M}_\perp \cdot \sigma)(\mathbf{I} + \mathbf{P}\cdot\sigma)\right)$$

The extra terms are

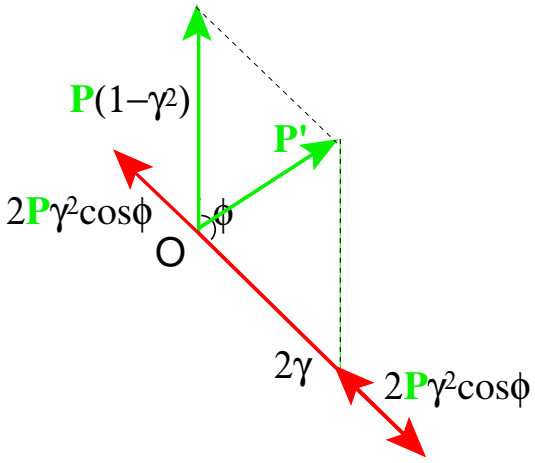
$$\begin{aligned} \mathrm{Tr}(N^*\sigma\ \mathbf{M}_\perp \cdot \sigma)(\mathbf{I} + \mathbf{P}\cdot\sigma) &= N^*\mathbf{M}_\perp + \imath N^*\mathbf{M}_\perp \times \mathbf{P} \\ \text{and their complex conjugates} &\quad N\mathbf{M}_\perp^* + \imath N\mathbf{M}_\perp^* \times \mathbf{P} \\ \text{giving} &\quad 2\Re N\mathbf{M}_\perp^* + 2\Im\mathbf{P} \times N\mathbf{M}_\perp^* \end{aligned}$$

- The real part of the product $N\mathbf{M}_\perp^*$ gives a component of scattered polarisation parallel to itself.
- It is independent of the incident polarisation and is due to the polarisation dependence of the cross-section implicit in the term $2\Re(N\mathbf{M}_\perp^*)$
- The imaginary part of the product $N\mathbf{M}_\perp^*$ rotates the scattered polarisation towards the direction perpendicular to both itself and $\mathbf{P}$.
- It only occurs when the difference in phase between the nuclear and magnetic structure factors is not an integral multiple of π.

A simple example

When $\mathbf{M}_\perp$ and N are in phase ($N\mathbf{M}_\perp^*$-$N^*\mathbf{M}_\perp$= 0).
The origin can be chosen so that both are real and ;
$\gamma = |\mathbf{M}_\perp(\mathbf{k})|/N(\mathbf{k})$ is the ratio between them.

- The component of scattered polarisation parallel to the incident polarisation has length $\mathbf{P}(1-\gamma^2)$
- The part parallel to $\mathbf{M}_\perp$ has length $2(P\cos\phi\,\gamma^2 + \gamma)$
- The scattered polarisation vector $\mathbf{P}'$ is found by completing the parallelogram
- If $\mathbf{P}$ decreases or γ approaches unity $\mathbf{P}'$ rotates towards $\mathbf{M}_\perp$.
- For $\mathbf{P} = 0$ or $\gamma = \pm 1$, $\mathbf{P}'$is parallel to $\mathbf{M}_\perp$.



The Blume Maleev Equations

The complete equation for the scattered polarisation is

$$\begin{aligned}\mathbf{P}'I &= C\Big(\mathbf{P}|N|^2 + 2\Re N\mathbf{M}_\perp^* + 2\Im\mathbf{P}\times N\mathbf{M}_\perp^* \\ &\quad -\Im(\mathbf{M}_\perp\times\mathbf{M}_\perp^*) + 2\Re(\mathbf{M}_\perp^*(\mathbf{M}_\perp\cdot\mathbf{P}) - \mathbf{P}|\mathbf{M}_\perp^*|^2\Big)\end{aligned}$$

This, together with that for the scattered intensity

$$I = C(|N|^2 + 2\Re(N\mathbf{M}_\perp^*\cdot\mathbf{P}) + |\mathbf{M}_\perp|^2 - \imath\mathbf{M}_\perp^*\times\mathbf{M}_\perp$$

comprise the Blume-Maleev equations.

These were derived, at almost the same time by Sergei Maleev and Martin Blume.

M. Blume,(1963) Phys. Rev. **130** 1670.

S.V. Maleev,V.G. Bar'yaktar and R.A.Suris,(1963) Sov. Phys. - Solid State **4** 2533.

They are the fundamental equations used to interpret polarised neutron scattering experiments.

The Blume Maleev Equations II

The scattered polarisation $\mathbf{P}'$ and scattered intensity I are given in terms of the incident polarisation $\mathbf{P}$ by

$$\begin{aligned}\mathbf{P}'I &= \mathbf{P}(|N(\mathbf{k})|^2 - \mathbf{M}_\perp(\mathbf{k})\cdot\mathbf{M}_\perp^*(\mathbf{k})) && \text{part parallel to } \mathbf{P} \\ &\quad + 2\Re[\mathbf{M}_\perp(\mathbf{P}\cdot\mathbf{M}_\perp^*(\mathbf{k}))] && \text{part parallel to } \mathbf{M}_\perp \\ &\quad + 2\Re[\mathbf{M}_\perp(\mathbf{k})N^*(\mathbf{k})] \\ &\quad + \mathbf{P}\times 2\Im(\mathbf{M}_\perp N^*(\mathbf{k})) && \text{part perpendicular to } \mathbf{P} \text{ and } \mathbf{M}_\perp \\ &\quad -\Im\mathbf{M}_\perp(\mathbf{k})\times\mathbf{M}_\perp^*(\mathbf{k})) && \text{part parallel to } \mathbf{k}\end{aligned}$$

$$\begin{aligned}I &= |N(\mathbf{k})|^2 + \mathbf{M}_\perp(\mathbf{k})\cdot\mathbf{M}_\perp^*(\mathbf{k}) && \text{polarisation independent part} \\ &\quad + 2\Re(\mathbf{P}\cdot\mathbf{M}_\perp(\mathbf{k})N^*(\mathbf{k})) && \text{polarisation dependent parts} \\ &\quad +\mathbf{P}\cdot\Im(\mathbf{M}_\perp(\mathbf{k})\times\mathbf{M}_\perp^*(\mathbf{k}))\end{aligned}$$

The polarisation tensor

The Blume Maleev equations may be written in tensor form

$$\mathbf{P}' = \mathscr{P}\mathbf{P} + \mathbf{P}'' \quad \text{or in components} \quad P'_i = \mathsf{P}_{ij}P_j + P''_i$$

$\mathbf{P}''$ is the polarisation created in the scattering process.

Polarisation axes can be defined with:

- x parallel to the scattering vector $\mathbf{k}$.
- z perpendicular to the scattering plane (vertical)
- y completing the right handed cartesian set

With this choice of axes there can be no components of $\mathbf{M}_\perp(\mathbf{k})$ parallel to x.

The polarisation tensor in polarisation coordinates

On polarisation axes this tensor equation can be can be written as:

$$\mathscr{P} = \begin{pmatrix} (N^2 - \mathbf{M}_\perp{}^2)/I_x & J_{nz}/I_x & J_{ny}/I_x \\ -J_{nz}/I_y & (N^2 - \mathbf{M}_\perp{}^2 + R_{yy})/I_y & R_{yz}/I_y \\ -J_{ny}/I_z & R_{zy}/I_z & (N^2 - \mathbf{M}_\perp{}^2 + R_{zz})/I_z \end{pmatrix}$$

$$\mathbf{P}'' = \begin{pmatrix} -J_{yz}/I \\ R_{ny}/I \\ R_{nz}/I \end{pmatrix}$$

$$\begin{aligned} I_x &= \mathbf{M}_\perp{}^2 + N^2 + P_x J_{yz} \\ I_y &= \mathbf{M}_\perp{}^2 + N^2 + P_y R_{ny} \\ I_z &= \mathbf{M}_\perp{}^2 + N^2 + P_z R_{nz} \\ I &= \mathbf{M}_\perp{}^2 + N^2 + P_x J_{yz} + P_y R_{ny} + P_z R_{nz} \end{aligned}$$

$$N^2 = N(\mathbf{k})N^*(\mathbf{k}) \qquad \mathbf{M}_\perp{}^2 = \mathbf{M}_\perp(\mathbf{k}) \cdot \mathbf{M}^*_\perp(\mathbf{k})$$

$$R_{ij} = 2\Re(M_{\perp i}(\mathbf{k})M_{\perp j}{}^*(\mathbf{k})) \qquad R_{ni} = 2\Re(N(\mathbf{k})M_{\perp i}{}^*(\mathbf{k}))$$

$$J_{ij} = 2\Im(M_{\perp i}(\mathbf{k})M_{\perp j}{}^*(\mathbf{k})) \qquad J_{ni} = 2\Im(N(\mathbf{k})M_{\perp i}{}^*(\mathbf{k}))$$

Note that when written in this simplified way $\mathscr{P}$ isn't strictly a tensor because the denominators may depend on the input polarisation direction

Francesco Ricci School, Neutron Scattering from Magnetic Systems

Neutron Polarimetry: II Polarisation Analysis

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Outline: Polarisation Analysis

Polarimetry

- A polarimetric experiment is one in which the relationship between the directions of incident and outgoing polarisations is measured.
- A neutron beam is polarised when the average over all neutrons in the beam of the expectation value of a component of spin $\langle \mathbf{S_z} \rangle$ is non-zero for some direction $\mathbf{z}$
- The polarisation direction is the one in which this average is maximised.

Neutron Polarisation

- It was shown in the previous lecture that a polarisation vector can be used to describe the polarisation of a neutron beam
- For practical purposes the component of the polarisation, parallel to an arbitrary direction $\mathbf{z}$, is given by

$$P_z = (N^+ - N^-)/(N^+ + N^-)$$

where N^+ and N^- are the number of neutrons in the beam whose spins are respectively parallel and anti-parallel to z.

- The polarisation $\mathbf{P}$ can be treated as a classical vector.

$$|\mathbf{P}| = \sqrt{{P_x}^2 + {P_y}^2 + {P_x}^2}$$

Polarisation Analysis

Neutron polarisation analysis experiments are those in which a polarised beam is incident on the sample and the numbers of scattered neutrons whose spins are parallel and anti-parallel to the direction of analysis are measured.

The results can be expressed using the generalised polarisation dependent cross-sections $\sigma^{i,j}$.

The superscripts i and j each stand for one of three orthogonal directions x, y, z.

j defines the direction of incident polarisation and i the direction of analysis.

For example: $\sigma^{z,-x}$ gives the probability that a neutron initially in a state with spin anti-parallel to x will be scattered to a state in which its spin is parallel to z.

The polarisation matrix

- The polarisation matrix P_{ij} is defined so that its component P_{ij} is the component of scattered polarisation parallel to i when the incident beam is polarised parallel to j
- The components P_{ij} can be obtained from the polarisation dependent cross-sections.

$$P_{ij} = (\sigma^{ij} - \sigma^{-i,j})/(\sigma^{ij} + \sigma^{-i,j})$$

- The polarisation dependent cross-sections contain additional intensity information.

BUT

- The P_{ij} can be measured with much higher precision than the individual cross-sections because they are obtained from ratios of intensities measured without having to move the sample.

Neutron precession in an external field (classical)

- Classically an object with moment of inertia I and magnetic moment μ inclined at an angle θ to a uniform magnetic field B will precess about the field direction at the Larmor frequency:

$$\Omega_{\mathrm{L}} = \mu B \cos\theta / I$$

- For a neutron with spin S and gyromagnetic ratio γ_{N}

$$\Omega_{\mathrm{L}} = S\gamma_{\mathrm{N}} B \cos\theta / \hbar$$

- The angle of precession ϕ depends upon the path integral $\int B\,d\ell$ of the neutron in the field.

$$\phi = 2\pi S \gamma_{\mathrm{N}} m_{\mathrm{N}} \lambda \int B\,d\ell$$

Neutron precession in an external field (quantum-mechanical)

Exactly the same result can be obtained quantum mechanically using simple perturbation theory.

- A neutron with spin wave function $\psi(0) = a\psi^{+} + b\psi^{-}$ has x and y and z components of spin $\Re(ab^{*})$, $\Im(ab^{*})$ and $\frac{1}{2}(aa^{*} - bb^{*})$ respectively.
- If a and b are real the spin is in the x-z plane inclined at an angle $\theta = 2\tan^{-1}(a/b)$ to the quantisation axis z.
- The matrix elements of the perturbing Hamiltonian due to a magnetic field B parallel to z switched on at $t = 0$ are zero for $t < 0$ and

$$\begin{array}{ll} H^{++} = -\gamma_{\mathrm{N}} a^2 B & H^{-+} = 0 \\ H^{+-} = 0 & H^{--} = \gamma_{\mathrm{N}} b^2 B \end{array} \qquad \text{for} \quad t > 0$$

Neutron precession in an external field (quantum-mechanical)

- If the unperturbed energy is E_0, the perturbed wave-function after time t becomes

$$\psi(t) = \left(a \exp \frac{\mathrm{i}\gamma_\mathrm{N} a^2 B t}{\hbar} \psi^+ + b \exp - \frac{\mathrm{i}\gamma_\mathrm{N} b^2 B t}{\hbar} \psi^- \right) \exp \frac{-\mathrm{i}E_0 t}{\hbar}$$

- the x and y components of the spin are

$$S_x = 2\Re \left(ab \exp \imath (a^2 - b^2) \frac{\gamma_\mathrm{N} B}{\hbar} t \right) = ab \cos (a^2 - b^2) \frac{\gamma_\mathrm{N} B}{\hbar} t$$

$$S_y = 2\Im \left(ab \exp \imath (a^2 - b^2) \frac{\gamma_\mathrm{N} B}{\hbar} t \right) = ab \sin (a^2 - b^2) \frac{\gamma_\mathrm{N} B}{\hbar} t$$

- The z component of the spin doesn't vary
- So the spin precesses around the field direction with angular frequency $(a^2 - b^2)\gamma_\mathrm{N} B/\hbar = \gamma_\mathrm{N} B \cos\theta/\hbar = \Omega_\mathrm{L}$.

Neutron precession in non-uniform fields

Two extreme conditions can be recognised.

1. Adiabatic approximation
   The change in field direction during one cycle of Larmor precession ($2\pi/\Omega_\mathrm{L}$) is negligibly small compared with the field itself.
   - Transitions between the two spin states take place very gradually.
   - The wave-function changes only slowly so that it always approximates to an eigenstate of the current Hamiltonian.

   The neutron polarisation follows the field direction.
2. An abrupt transition
   The field changes rapidly from one uniform value to another.
   - When the distance is much less than that needed for a complete Larmor precession.

   The neutron polarisation direction does not change at the boundary but passes immediately from one precession regime to the other.

Neutron precession in non-uniform fields

Adiabatic, and abrupt changes in the directions of magnetic fields, together with controlled precession, are the means used to manipulate the neutron polarisation in polarisation analysis experiments.

The distance travelled by a neutron, wavelength λ in time $2\pi/\Omega_{\mathrm{L}}$ is

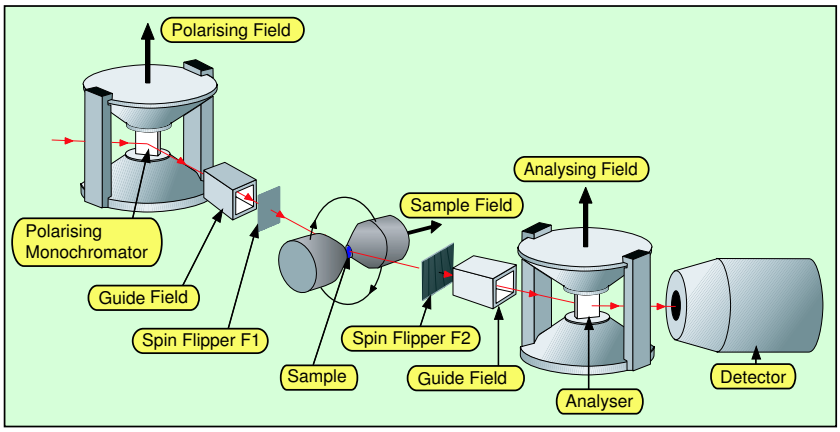
$$\lambda_L = \hbar^2/\gamma_{\mathrm{N}} m_{\mathrm{N}} \lambda B$$

For a field of 10^{-4} T (1 gauss) $\lambda_L \approx 3$ m for 1 Å neutrons

- Adiabatic conditions are achieved by separating different field regimes by distances long compared with λ_L
- An abrupt field transition, one in which the change takes place in a distance much less than λ_L is often achieved using current sheets, or by screening with sheets of mu-metal or superconducting foils.

Uni-directional polarisation analysis

The original polarisation analysis setup is that of Moon, Riste and Koehler R.M. Moon, T. Riste, and W.C. Koehler,(920) 1969 **Phys.Rev.** 181.



In its simplest arrangement all the fields are parallel to the vertical direction which is that of polarisation and analysis.
The sample field can be rotated about both vertical and horizontal axes.
The guide fields are arranged so that the neutron spins rotate adiabatically from the direction of the polariser to that of the sample field and finally to that of the analyser.

Uni-directional polarisation analysis

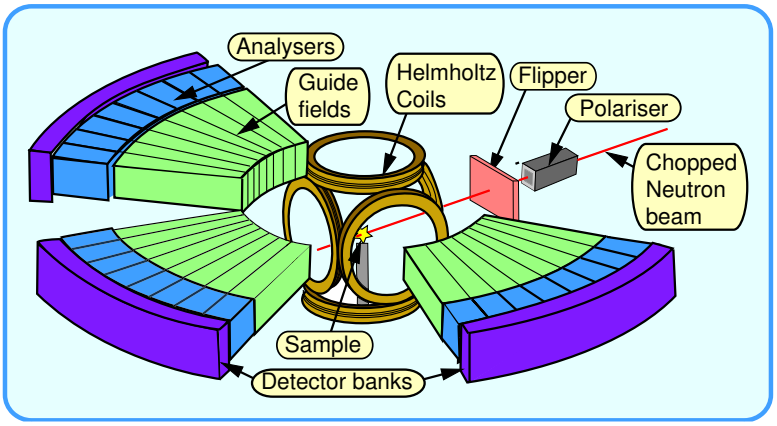
- The uni-directional technique allows four cross-sections: σ^{++}, σ^{+-}, σ^{-+} and σ^{--} to be measured.
- The first superscript indicates the direction of incident polarisation, it is + when F1 is deactivated ($\mathbf{P} \parallel \mathbf{H}$) and - when it is activated ($\mathbf{P} \parallel -\mathbf{H}$).
- The second subscript indicates the direction of analysis, switched using F2.
- These four cross-sections can be identified with four components of the general cross-sections defined previously.

$$\sigma^{++} = \sigma^{i,i}, \quad \sigma^{+-} = \sigma^{-i,i} \ldots \quad \text{etc.}$$

- For an orientation i of the sample field, only the single component P_{ii} of the polarisation matrix, will be obtained.

XYZ polarisation analysis

A more general version of the uni-directional technique allows the field at the sample to be varied without rotating a magnet.



- The efficiency of measurement can be increased by using banks of detectors.
- There is a super-mirror analyser in front of each detector.
- The direction of the field at the sample position is chosen by adjusting the currents in the three mutually perpendicular Helmholtz coils.

XYZ polarisation analysis

- The guide fields and the distances between different components must be sufficient to ensure adiabatic transitions between the field regimes at the polariser, sample and analysers.
- Any components of polarisation not parallel to the local field will precess around it.
- So only the components of polarisation parallel to the sample field are well defined.
- The XYZ technique allows 12 of the generalised cross-sections to be measured.
- They are: $\sigma^{i,i}$, $\sigma^{i,-i}$, $\sigma^{-i,i}$ and $\sigma^{-i,-i}$
- Note that if $i \neq z$ the direction i is different for each element of the detector.
- The three diagonal components P_{xx}, P_{yy} and P_{zz} of the polarisation matrix can be derived.

xyz cross-sections from XYZ data

- When using a multidetector the x and y polarisation directions differ at each element of the detector.
- A set of axes X, Y, Z are defined parallel to the axes of the Helmholtz coils.
- X is parallel to the incident beam and $Z \parallel z$ for all detector elements.
- For a detector element at scattering angle 2θ, x is at an angle $\alpha = \frac{\pi}{2} - \theta$ to X in the X–Y plane.

In polarisation coordinates

$$\begin{array}{lcccc} P_X & = & P\cos\alpha & -P\sin\alpha & 0 \\ P_Y & = & P\sin\alpha & P\cos\alpha & 0 \\ P_Z & = & 0 & 0 & P \end{array}$$

$$\begin{array}{lcccc} \sigma^{X,X} & = & \sigma^{x,x}\cos\alpha & + & \sigma^{-y,-y}\sin\alpha \\ \sigma^{X,-X} & = & \sigma^{x,-x}\cos\alpha & + & \sigma^{-y,y}\sin\alpha \\ \sigma^{Y,Y} & = & \sigma^{x,x}\sin\alpha & + & \sigma^{y,y}\cos\alpha \\ \sigma^{Y,-Y} & = & \sigma^{x,-x}\sin\alpha & + & \sigma^{y,-y}\cos\alpha \end{array}$$

$\ldots$ etc.

A matrix equation relates $\sigma^{x,x}$, $\sigma^{x,-x}$, $\sigma^{y,y}$, $\sigma^{y,-y}$ etc. to $\sigma^{X,X}$, $\sigma^{X,-X}$, $\sigma^{Y,Y}$, $\sigma^{Y,-Y}$ etc.

Transverse components of polarisation

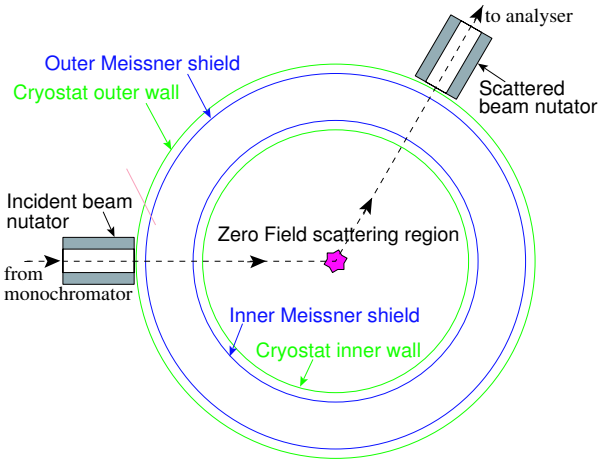
- Neither of the two previous techniques allow components of the scattered polarisation which are not parallel to the incident polarisation direction to be measured.
- This is because any such components precess around the field direction and so their direction at the analyser is undefined.
- The off-diagonal components of the polarisation matrix depend on these transverse components.
- The presence, but not the identity, of transverse components may be inferred from reduction in the size of the diagonal components (depolarisation).
- Full information about the transverse components of scattered polarisation can be obtained if the scattering sample is in zero field.
- Spherical neutron polarimetry (SNP) is the name given to polarisation analysis experiments in which all the generalised cross-sections can be measured.

SNP with CRYOPAD

One way of realising the conditions in which transverse components of polarisation can be measured is to use superconducting Meissner screens to isolate a zero-field region and provide an abrupt transition between different magnetic field regimes.

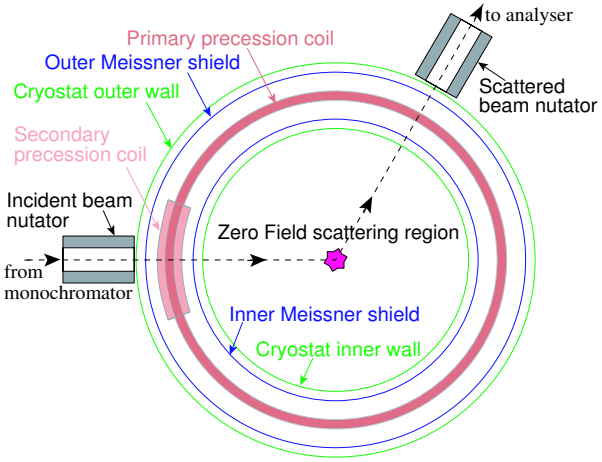
The cryostat containing two cylindrical Meissner shields is in the form of a hollow cylinder.

The sample and its independent sample environment can be placed inside



The nutator magnets align the ingoing and outgoing polarisation in the plane perpendicular to the beam at an angle θ to the vertical.

SNP with CRYOPAD



Two precession coils, wound from superconducting wire, lie between the two Meissner shields. The

The primary coil is a complete toroid.

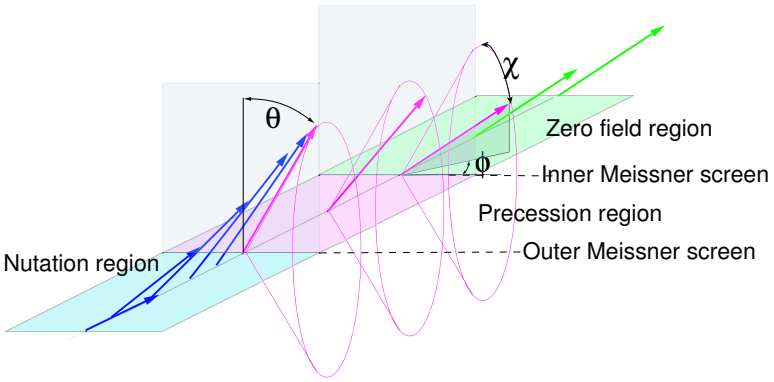
secondary coil is part of a second toroid, wound over the primary coil, in the region through which the incident beam passes.

In passing through these coils the polarisation precesses about a horizontal axis through an angle χ proportional to the currents in the coils.

F. Tasset, P.J. Brown, E. Lelièvre-Berna, T Roberts, S. Pujol, J. Alibon, and E. Bourgeat-Lami,(69) Physica B **267-268** 1999.

Rotation of the polarisation in CRYOPAD

Initially the incident beam is polarised along its direction of motion.



In the nutation region the field changes gradually from a direction parallel to the beam to one perpendicular to it at θ_{in} to the vertical. The neutron spins follow the field adiabatically.

Between the two Meissner screens the neutron spins precess through an angle χ_{in} about the horizontal axis of the precession coils.

The inner Meissner screen isolates the zero field region from the precession fields and within it the polarisation is unchanged except by interaction with the sample.

Measuring the scattered polarisation

- The field components on the scattered beam are equivalent to those in the incident beam.
- The spins in the scattered beam are guided so that those oriented with the chosen χ_{out}, θ_{out} are parallel to the field axis at the analyser.
- The angles $\theta_{in}, \theta_{out}$ are fixed by the angles of rotation of the magnetic fields in the nutators.
- The angles χ_{in}, χ_{out} are fixed by suitable adjustment of the currents in the primary and secondary precession coils.
- For a reflection with Bragg angle θ_B the directions of incident polarisation and of analysis can be made parallel to the orthogonal directions x, y, z with $x \parallel \mathbf{k}$ and z vertical by setting the angles

	θ_{in}	χ_{in}	θ_{out}	χ_{out}
x	$\frac{\pi}{2} - \theta_{\mathrm{B}}$	$\frac{\pi}{2}$	$\theta_{\mathrm{B}} - \frac{\pi}{2}$	$-\frac{\pi}{2}$
y	$-\theta_{\mathrm{B}}$	$\frac{\pi}{2}$	$-\theta_{\mathrm{B}}$	$\frac{\pi}{2}$
z	0	0	0	0

Types of experiment

- Separation of magnetic and nuclear scattering Examples
  - Weak magnetic scattering in powder diffraction
  - Paramagnetic scattering
- XYZ polarisation analysis using a multi-detector Examples
  - Magnetic defect scattering
  - Spatial correlations above T_C
- Determination of the direction of the magnetic interaction vector: Examples
  - Unique solution of complex magnetic structures
  - Studies of magneto-electric domains
  - Determination of anti-ferromagnetic form factors

The rest of this lecture will cover the first two types: the third is more complex and will be treated later.

Separation of magnetic and nuclear scattering

- Magnetic scattering will contribute to the spin-flip cross-section ($\sigma^{i,-i}$) whenever the magnetic interaction vector $\mathbf{M}_\perp(\mathbf{k})$ is not parallel polarisation direction $\mathbf{P}$ (P_i).
- Coherent nuclear scattering from disordered nuclear spins only enters the spin non-flip cross-section ($\sigma^{i,i}$).
- The magnetic interaction vectors which contribute to a reflection with scattering vector $\mathbf{k}$ from a polycrystaline sample will be distributed randomly in the plane perpendicular to $\mathbf{k}$.
- If the incident polarisation is aligned perpendicular to the scattering plane then, on average, half of the interaction vectors will be parallel and half perpendicular to it.
- Half the magnetic scattering will be spin-flip and half spin non-flip.
- If the incident polarisation is parallel to $\mathbf{k}$, all the magnetic scattering will be spin-flip.

Corrections for Polarising efficiency

Polarisation analysis instruments are never perfect, so we need to determine the corrections which must be made for

1. Incomplete polarisation of the incident beam, $P < 1$
2. Imperfect efficiency of the flippers $\varepsilon_1, \varepsilon_2 < 1$
3. Imperfect efficiency of the analyser $P' < 1$

The number of "+" neutrons scattered by the sample when F1 is off is

$$S^{++} = I_0 \left(P\sigma^{++} + (1-P)\sigma^{-+} \right)$$

The number of these analysed as "+" is

$$A^{++} = F_A P' S^{++} = I_0 F_A P' \left(P\sigma^{++} + (1-P)\sigma^{-+} \right)$$

where F_A is the reflectivity of the analyser

Similarly the number of "–" neutrons scattered by the sample when F1 is off is

$$S^{+-} = I_0 P \left(\sigma^{+-} + (1-P)\sigma^{--} \right)$$

and the number of these analysed as "+" is

$$A^{-+} = F_A(1-P')S^{+-} = I_0 F_A \left(\left(1-P'\right) \left(P\sigma^{+-} + (1-P)\,\sigma^{--} \right) \right)$$

Corrections for Polarising efficiency

The total number of "+" neutrons recorded by the analyser is

$$I^{++} = I_0 F_A \left(P' \left(P\sigma^{++} + (1-P)\sigma^{-+} \right) + (1-P') \left(P\sigma^{+-} + (1-P)\sigma^{--} \right) \right)$$

by switching F1 on we get

$$I^{-+} = I_0 F_A \left(P'(P\varepsilon_1\sigma^{-+} + (1-P\varepsilon_1)\sigma^{++} + (1-P')(P\varepsilon_1\sigma^{--} + (1-P\varepsilon_1)\sigma^{+-}) \right)$$

with F1 off and F2 on

$$I^{+-} = I_0 F_A \left(P'\varepsilon_2(P\sigma^{+-} + (1-P)\sigma^{--}) + (1-P'\varepsilon_2)(P\sigma^{++} + (1-P)\sigma^{-+}) \right)$$

and finally with both flippers on

$$I^{--} = I_0 F_A \left(P'\varepsilon_2(P\varepsilon_1\sigma^{--} + (1-P\varepsilon_1)\sigma^{+-}) + (1-P'\varepsilon_2)(P\varepsilon_1\sigma^{-+} + (1-P\varepsilon_1)\sigma^{++}) \right)$$

If all the efficiencies are known these four equations enable the four cross-sections to be determined.

Note

Further uncertainties may be introduced by errors in fixing the polarisation directions.

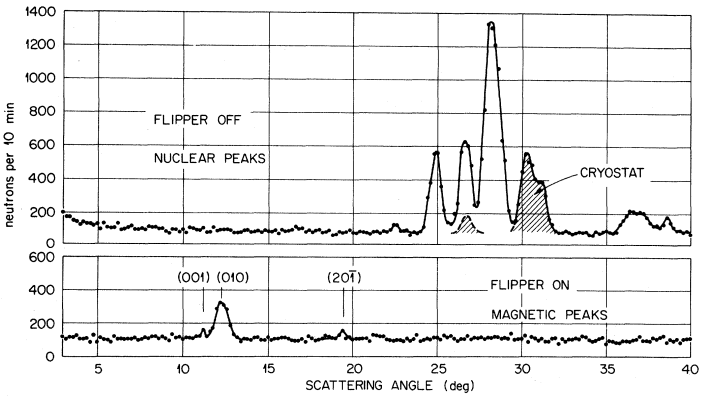
Magnetic scattering from a powder sample

PA is particularly useful for separating the magnetic ssattering when τ=0 and the moments are small.

A very early experiment on V_2O_3 by Moon provides an example

Moon R M,(1970) Phys. Rev. Letts **25** 527.

A horizontal field was rotated so that the polarisation at the sample was always parallel to the scattering vector



T=77 K

$\sigma^{x,x}$

$\sigma^{x,-x}$

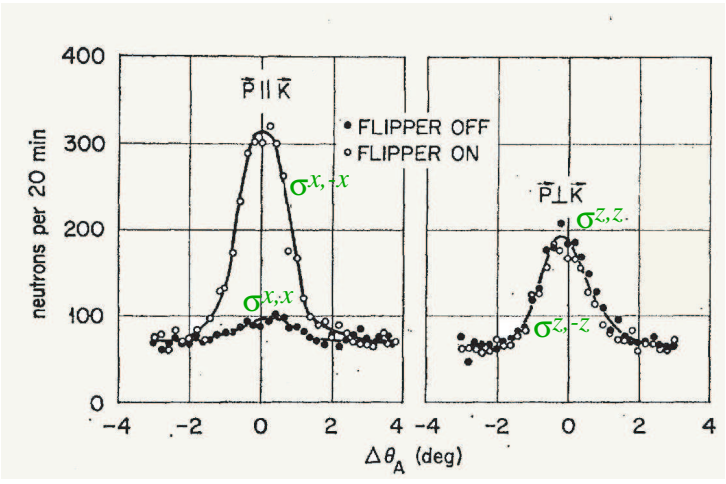
The experiment confirmed that the (001) and (100) peaks were indeed of magnetic origin

Paramagnetic scattering

- The disordered moments in a paramagnet only contribute to diffuse magnetic scattering.
- It is superposed on diffuse nuclear scattering due to thermal vibration, all types of nuclear disorder and multiple scattering.
- Only paramagnetic and nuclear spin disorder scattering contribute to the spin-flip cross-section.
- Nuclear spin scattering is distinguished from magnetic scattering because all components of the nuclear spin contribute, not just those perpendicular to the scattering vector.
- If nuclear spins are randomly oriented 2/3 always give spin-flip scattering regardless of the polarisation direction.
- When $\mathbf{P} \parallel \mathbf{k}$ $\quad \sigma^{x,-x} = \sigma_{para} + \frac{2}{3}\sigma_{nspin}$
- When $\mathbf{P} \perp \mathbf{k}$ $\quad \sigma^{z,-z} = \frac{1}{2}\sigma_{para} + \frac{2}{3}\sigma_{nspin}$
- So $\quad \sigma^{x,-x} - \sigma^{z,-z} = \frac{1}{2}\sigma_{para}$

Paramagnetic scattering from MnF_2

The polarisation dependence of paramagnetic scattering was first demonstrated in the original paper of Moon, Riste and Koehler



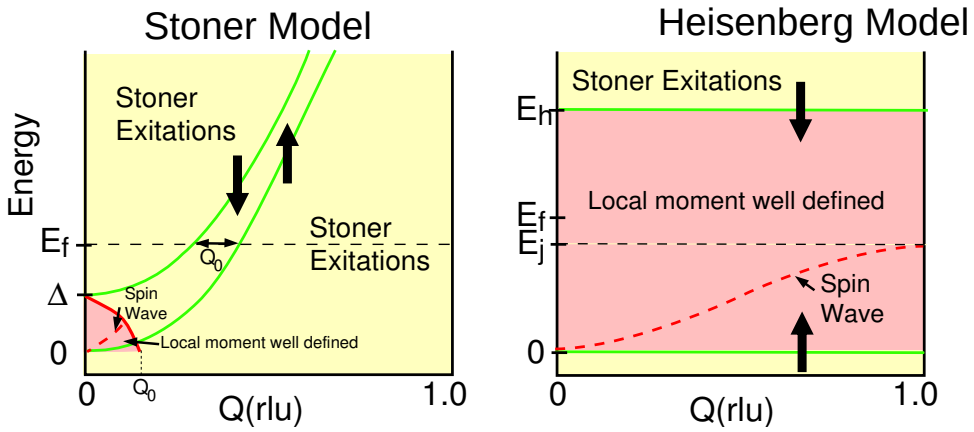
The data were obtained by rocking the analyser crystal through the elastic position

- There is no incoherent nuclear scattering from MnF_2.
- The small peak in $\sigma^{x,x}$ is due to multiple nuclear scattering.
- Multiple nuclear scattering is also responsible for the small difference between $\sigma^{z,z}$ and $\sigma^{z,-z}$.

Paramagnetic scattering from ferromagnetic metals

- The paramagnetic scattering from ferromagnetic metals is of particular interest because it can show whether or not localised moments persist in the paramagnetic state above the Curie transition.
- In ferromagnetic metals it is generally accepted that the magnetic electrons participate in the Fermi surface.
- The magnetisation is due to exchange splitting of the spin-up and spin-down bands.
- The question posed is to what extent this exchange splitting persists into the paramagnetic phase in which "up" and "down" are no longer properly defined.
- The Stoner (itinerant electron) and Heisenberg (localised moment) models represent two limiting cases.

The Stoner and Heisenberg models



Δ is the exchange splitting of the bands with $\Delta < E_f$

Atomic moments only well defined in the small range of Q–Energy space where single particle (Stoner) excitations are not excited.

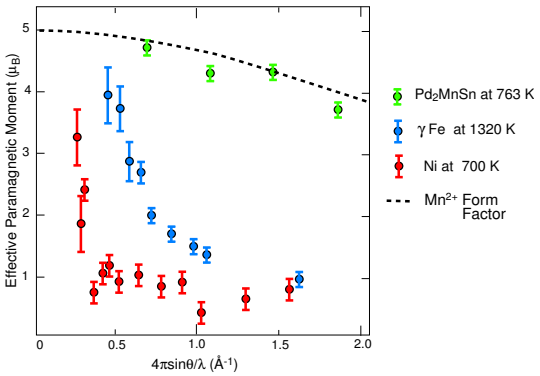
The bands are flat and separated by $\Delta = E_h$; the intra-atomic exchange(Hunds rule) energy.

The inter-atomic exchange energy E_j determines T_C and the zone-boundary spin-wave energy.

Atomic moments are well defined up to energies E_h.

Paramagnetic Scattering: 3d transition metals

Measurements made on powders and single crystals on a triple axis PA spectrometer on the ILL hot source.



- Use of hot neutrons and modest resolution ensures a wide energy acceptance
- Measurements on powders allow the intensities to be readily placed on an absolute scale

- The results for Pd_2MnSn follow the Mn^{2+} form factor as predicted by the Heisenberg model.
- For Fe and Ni the rapid fall of the effective moment with increasing Q shows that some ferromagnetic correlations persist at temperatures well above T_C.
- They have a longer range for Ni than for Fe.

Booth J G et al.,(1982) J de Physique **43** C7-363.

XYZ polarisation analysis using a multi-detector

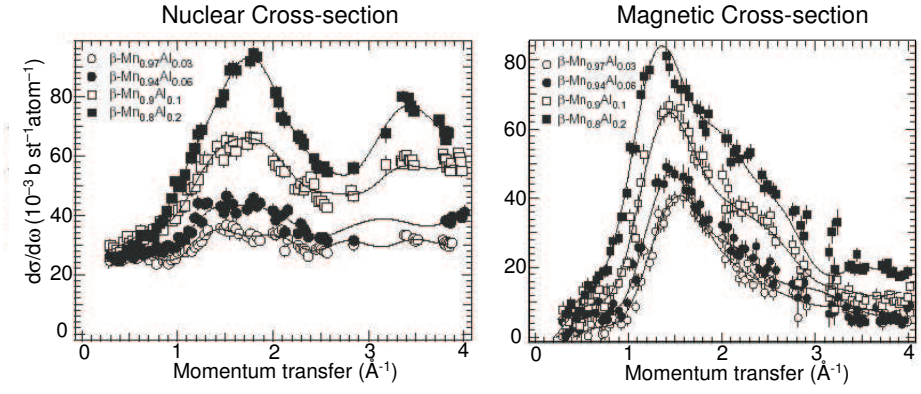
- Measurements of diffuse scattering can be made much more efficiently using a multi-detector.
- This is particularly true for experiments at long wavelength or high resolution for which the volume of phase space sampled at each point of a scan using a single detector is very small.
- The XYZ polarisation analysis technique combined with multi-detection is also more appropriate at wavelengths greater than 1.5 Å where polarising super-mirrors can be used.
- For such wavelengths the Larmor precession lengths in moderate fields will allow adiabatic changes in field direction in a reasonably compact instrument.
- The uncertainty in definition of the direction of polarisation is also inversely proportional to the wavelength.

Magnetic defect scattering

- A long wavelength is used so that very few, or even none, of the reciprocal lattice points lie inside the Ewald sphere.
- All the scattering is then incoherent and due to different types of disorder.
- The ability to separate the magnetic and nuclear contributions to the diffuse scattering allows magnetic perturbations to be distinguished from, and perhaps related to, atomic short range order.
- In dilute alloys the magnetic disorder scattering allows the perturbation in the magnetisation distribution due to individual solute atoms to be determined.
- In ferromagnetic alloys magnetic and nuclear components can be distinguished by applying saturating fields parallel and perpendicular to the scattering vector.
- For anti-ferromagnetic and paramagnetic systems the XYZ PA technique is particularly appropriate.

Example: Magnetic correlation in β–Mn

- The β phase of metallic manganese shows no long-range magnetic order.
- There is however much evidence to suggest that it is on the verge of magnetic order and moment localisation.
- XYZ polarisation analysis been used to study magnetic correlations in dilute solutions of Al in β–Mn.

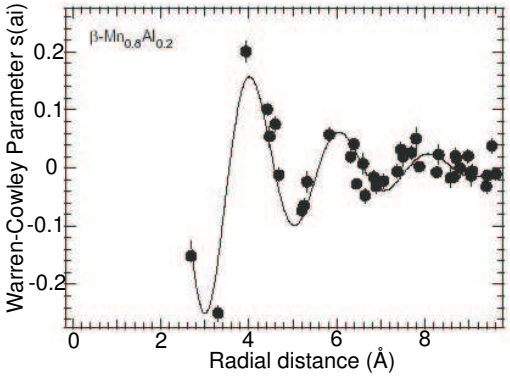


- The nuclear and magnetic cross-sections were extracted from XYZ PA data collected using D7 at ILL.

Stewart R J and Cywinski R,(2004) JMMM **272Ð276** 676.

Nuclear correlation in a β-Mn-Al alloy

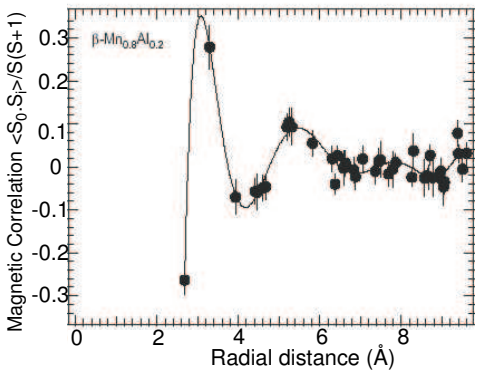
- A Monte-Carlo procedure was used to obtain the atomic short-range order parameters from the Q-dependence of the nuclear cross-section.



- The parameter $s(\alpha i)$ oscillates about zero with maxima and minima at approximately the radii of successive shells of neighbours.
- The Al atoms tend to avoid one-another.

Magnetic correlation in β-Mn

- This atomic model allows the magnetic correlation function to be deduced from the magnetic cross-section.
- It was assumed that the Mn moments are localised so that $\langle S_z \rangle^2 = S(S+1)$ for each Mn atom is well defined.



- The magnetic correlations oscillate.
- They are anti-ferromagnetic for the first and third neighbour shells and ferromagnetic for the second.

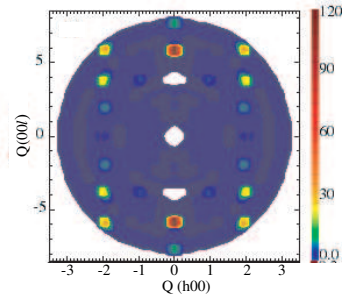
Spatial correlations above T_C

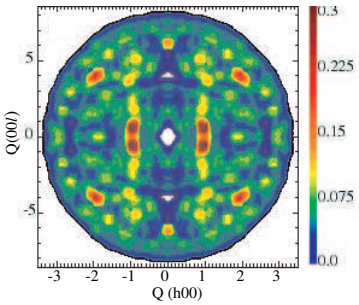
- XYZ PA experiments can yield not just the radial correlation functions but also information about the spatial anisotropy of the correlations.
- La_2CuO_4 is of interest both as the parent compound of a family of high-temperature superconductors and as a very good realization of a two-dimensional quantum Heisenberg antiferromagnet (2DQHAF).
- There is a lot of experimental evidence which suggests that the nearest-neighbor Heisenberg model is inadequate and that four-particle exchange may be significant.
- The dynamical spin correlations just above the Neél temperature have been measured using XYZ PA, to test the predictions the proposed quantum non-linear sigma model.

Dynamical spin correlations above T_C in La_2CuO_4

Neutron scattering intensity in the $h0\ell$ plane of La_2CuO_4 at room temperature measured using the multidetector on D7.

- XYZ PA allows separation of the nuclear and magnetic parts.





The coherent structural scattering

The intensity is at the reciprocal lattice nodes

The purely magnetic scattering

A rod of scattering is developing along the (10ℓ) direction showing the cross-over to 2D correlations.

Toader A M et al.,(2005) Phys. Rev. Letts **94** 197202.

Francesco Ricci School, Neutron Scattering from Magnetic Systems

Neutron Polarimetry: III Fundamentals of Spherical Polarimetry

P.J. Brown

Institut Laue Langevin, Grenoble
and
Physics Department Loughborough University

September 2006

Finding the direction of the interaction vector
Magnetic Domains
Magnetic Structure Determination using SNP

Outline: Fundamentals of Spherical Polarimetry

Limitations of structure determination from intensity measurements

To recapitulate:

The *magnetic structure factor* $\mathbf{M}(\mathbf{k}) = \int \mathbf{M}(\mathbf{r}) \exp(i\mathbf{k}\cdot\mathbf{r}) dr^3$

The *magnetic interaction vector* $\mathbf{M}_\perp(\mathbf{k}) = \hat{\mathbf{k}} \times \mathbf{M}(\mathbf{k}) \times \hat{\mathbf{k}}$

where $\hat{\mathbf{k}}$ is a unit vector parallel to the scattering vector $\mathbf{k}$.

- Both $\mathbf{M}(\mathbf{k})$ and $\mathbf{M}_\perp(\mathbf{k})$ are complex vectors
- The magnetic cross-section for unpolarised neutrons is proportional to $|\mathbf{M}_\perp(\mathbf{k})|^2$
- The only directional information comes from the fact that $\mathbf{M}_\perp(\mathbf{k})$ is the projection of $\mathbf{M}(\mathbf{k})$ onto the plane perpendicular to the scattering vector.

What can polarisation analysis add?

Whether there are components of $\mathbf{M}_\perp(\mathbf{k})$ perpendicular to the polarisation direction

- Such components will flip the neutron spin
- If the incident polarisation direction can be varied the direction of $\mathbf{M}(\mathbf{k})$ can be determined
- The ability to analyse polarisation in directions perpendicular to the incident direction is required to obtain complete information.
- hence Spherical Neutron Polarimetry (SNP)

Polarisation Matrices: The experimental result

The usual experimental strategy with SNP is to measure the scattered polarisation $\mathbf{P}'$ with the incident polarisation $\mathbf{P}$ parallel to polarisation x, y, z in turn.
This determines the polarisation matrix.

The *polarisation matrix* P_{ij} is the experimental quantity most closely related to the polarisation tensor.

The matrix element P_{ij} gives the ith component of scattered polarisation when the incident polarisation is in the jth direction.

$$\mathsf{P}_{ij} = \left\langle \frac{\mathscr{P}_{ij}P_j + P_i'')}{P_j} \right\rangle_{\text{configs}}$$

The average is over all the different configurations (structural and magnetic) present in the sample.

The polarisation tensor

It is useful to recall here the form of the polarisation tensor:

$$\mathscr{P} = \begin{pmatrix} (N^2 - \mathbf{M}_\perp{}^2)/I_x & J_{nz}/I_x & J_{ny}/I_x \\ -J_{nz}/I_y & (N^2 - \mathbf{M}_\perp{}^2 + R_{yy})/I_y & R_{yz}/I_y \\ -J_{ny}/I_z & R_{zy}/I_z & (N^2 - \mathbf{M}_\perp{}^2 + R_{zz})/I_z \end{pmatrix}$$

$$\mathbf{P}'' = \begin{pmatrix} -J_{yz}/I \\ R_{ny}/I \\ R_{nz}/I \end{pmatrix}$$

$$\begin{aligned} I_x &= \mathbf{M}_\perp{}^2 + N^2 + P_x J_{yz} \\ I_y &= \mathbf{M}_\perp{}^2 + N^2 + P_y R_{ny} \\ I_z &= \mathbf{M}_\perp{}^2 + N^2 + P_z R_{nz} \\ I &= \mathbf{M}_\perp{}^2 + N^2 + P_x J_{yz} + P_y R_{ny} + P_z R_{nz} \end{aligned}$$

$$N^2 = N(\mathbf{k})N^*(\mathbf{k}) \qquad \mathbf{M}_\perp{}^2 = \mathbf{M}_\perp(\mathbf{k}) \cdot \mathbf{M}_\perp(\mathbf{k})$$
$$R_{ij} = 2\Re(M_{\perp i}(\mathbf{k})M_{\perp j}{}^*(\mathbf{k})) \qquad R_{ni} = 2\Re(N(\mathbf{k})M_{\perp i}{}^*(\mathbf{k}))$$
$$J_{ij} = 2\Im(M_{\perp i}(\mathbf{k})M_{\perp j}{}^*(\mathbf{k})) \qquad J_{ni} = 2\Im(N(\mathbf{k})M_{\perp i}{}^*(\mathbf{k}))$$

Rotation of the polarisation

Off-diagonal terms in the polarisation matrix correspond to rotation of the polarisation direction.

They are of two kinds.

1. P_{yz} and P_{zy} which depend upon $R_{yz} = 2\Re(M_{\perp y}(\mathbf{k})M_{\perp z}{}^{*}(\mathbf{k}))$

   They can be reduced to zero by choosing either the y or z axis parallel to $\mathbf{M}_{\perp}$.
2. Elements P_{xy}, P_{xz},P_{yx} and P_{zx} which represent rotations towards, or away from, the scattering vector.

   They are always present when nuclear and magnetic scattering occur together with a phase difference which is neither 0 or π.

Direction of Polarisation Rotation

When the scattered polarisation is rotated with respect to the incident polarisation direction it is important to understand what determines the direction of rotation,

- For rotations in the x–y plane (P_{yz}, P_{zy}) it is the orientation of $\mathbf{M}_{\perp}$ within that plane.
  If $\mathbf{M}_{\perp}$ is inclined at an angle ϕ to y measured towards positive z; both P_{yz} and P_{zy} will be positive for $0 < \phi < \frac{\pi}{2}$, $\pi < \phi < \frac{3\pi}{2}$ and negative for $\frac{\pi}{2} < \phi <= \pi$, $\frac{3\pi}{2} < \phi < 2\pi$
- For rotations towards or away from the scattering vector it is the phase angle ψ between the nuclear and magnetic structure factors which determines the direction of rotation. The signs of P_{yx},$-P_{xy}$,P_{zx} and $-P_{xz}$ are given by that of $\sin\psi$

Note that when there is a configuration which gives polarisation rotation in a particular sense, there is very often a degenerate configuration which will give rotation in the opposite one.

Depolarisation

- The squared modulus of the scattered polarisation $\mathbf{P}'$ obtained from the Blume-Maleev equations is always greater than or equal to $|\mathbf{P}|^2$
- The amplitude of the polarisation is either increased or unchanged by scattering from any pure target state.
- Real depolarisation of the scattered beam is an indication that a mixed state consisting of more than one type of magnetic domain is present in the target.
- The ability to distinguish depolarisation from rotation of the polarisation away from the axis of analysis is one of the features which makes SNP more powerful than axial polarisation analysis.

Types of Domain

An understanding of the types of magnetic domain which occur and the kinds of depolarisation to which they give rise is fundamental in interpreting polarimetric data.

- Magnetic domains can occur whenever the symmetry of the ordered magnetic structure is less than that of the paramagnetic phase.
- If the order of the paramagnetic space group is p and that of the magnetic space group m, there will be p/m different domains.
- The domains can be classified according to the type of symmetry elements that are lost on magnetic ordering
  (a) Configuration domains: translational symmetry
  (b) 180° domains: Time inversion symmetry
  (c) Orientation domains: Rotation symmetry
  (d) Chirality domains: Centro-symmetry
- The effects produced by the presence of each of these kinds of domains on the scattered polarisation are quite distinct.

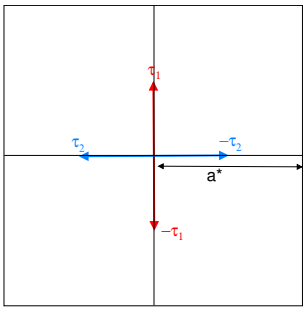
Configuration domains

- Configuration domains exist if the propagation vector τ of the magnetic structure is not transformed either into itself, or itself plus a reciprocal lattice vector, by all the symmetry operators of the paramagnetic group.
- Operating with the paramagnetic symmetry elements on τ generates a set of inequivalent vectors which form the star of τ.
- Each vector in the star generates a different configuration domain.
- Each configuration domain gives a completely separate set of magnetic reflections at positions $\pm\tau$ from the reciprocal lattice nodes.
- Each reflection belongs to a distinct configuration domain, hence effectively to a single state.
- Configuration domains do not give rise to depolarisation.

Example: Space Group $P4/mmm$ $\tau = 0, \frac{1}{2}, 0$

There are 16 operators in the paramagnetic group
$E, 4_z, 2_z, -4_z, 2_x, 2_y, 2_{x+y}, 2_{x-y}, I, 4_z, m_z, -4_z, m_x, m_y, m_{x+y}, m_{x-y}$

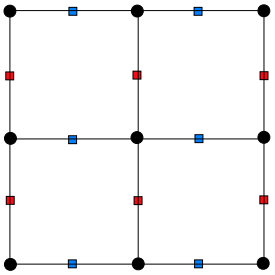
Operators	
$E,\ 2_y,\ m_x,\ m_z$	$\tau_1 \Longrightarrow$ itself $(0, \frac{1}{2}, 0)$
$I,\ 2_x,\ 2_z,\ m_y$	$\tau_1 \Longrightarrow -\tau_1 = (0, -\frac{1}{2}, 0)$
$4_z,\ -4_z,\ 2_{x+y},\ m_{x-y}$	$\tau_1 \Longrightarrow \tau_2 = (-\frac{1}{2}, 0, 0)$
$-4_z,\ 4_z,\ 2_{x-y},\ m_{x+y}$	$\tau_1 \Longrightarrow -\tau_2 = (\frac{1}{2}, 0, 0)$



There are two distinct configuration domains

The $hk0$ layer of reciprocal space:

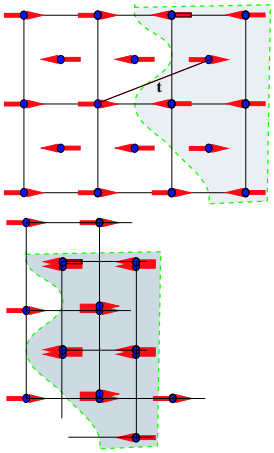
- The nuclear reflections
- Magnetic reflections due to τ_1
- Magnetic reflections due to τ_2
- The complete diagram



180° domains

Regions in which all the moment directions in one domain are reversed with respect to those in the other.

- $\mathbf{M}_\perp$ points in opposite directions in the two domains. (Phase difference of π).
- The two domains are related by the time inversion operator.
- Ferromagnetic domains provide a simple example.



In a structure with non-zero propagation vector ($\tau \neq 0$) 180° domains cannot be distinguished except by the defects associated with the domain walls.

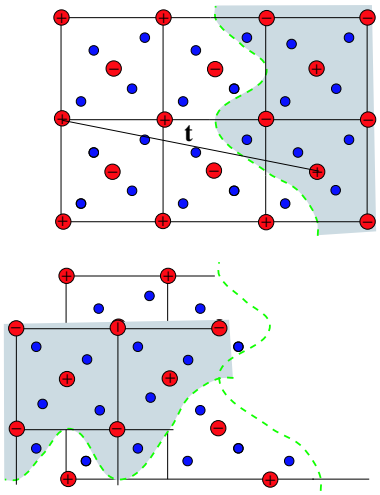
One domain can be transformed into the other by a translation **t** such that $\tau \cdot \mathbf{t} = (2n+1)/2$.

The intensity and the polarisation scattered by the two domains are identical.

180° domains τ=0

When τ=0 atoms with opposite spins are related by a rotation as well as a translation.

When the rotation is a proper one (not combined with inversion):

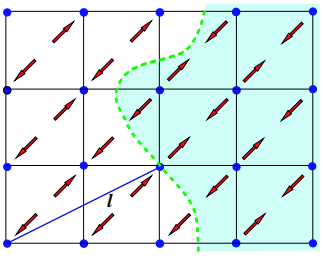


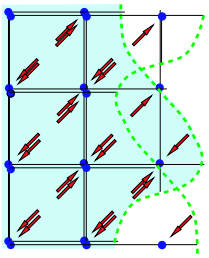
- Atoms with + and – spins are related by a rotation of $\frac{\pi}{2}$ and a translation $\mathbf{u} = \frac{1}{2}, \frac{1}{2}, 0$
- N and $\mathbf{M}_\perp$ are both real: $\psi_{NM} = 0, \frac{\pi}{2}$
- The terms $R_{ni} = 2\Re(N\mathbf{M}_\perp^*)$ in the polarisation matrix are non-zero.
- The 180° domains are related by a rotation of $\frac{\pi}{2}$ and a translation of $\mathbf{t} = \boldsymbol{l} + \mathbf{u}$
- If $\mathbf{M}_\perp$ is positive for one domain it is negative for the other
- The R_{ni} terms have opposite signs for the two domains.

These domains do not lead to depolarisation, but inhibit the creation of polarisation parallel to $\mathbf{M}_\perp$

180° domains τ=0 ($\psi_{NM} = \pm\frac{\pi}{4}$)

When the symmetry element relating atoms with oppositely oriented spins involves inversion (improper rotation), $\psi_{NM} = \pm\frac{\pi}{4}$.





- In this example atoms with opposite spins are related by a centre of symmetry.
- N is real and $\mathbf{M}_\perp$ imaginary. (N and $\mathbf{M}_\perp$ in quadrature)
- The terms $J_{ni} = 2\Im(N\mathbf{M}_\perp^*)$ in the polarisation matrix are finite.
- They turn the polarisation towards the direction perpendicular to both $\mathbf{P}$ and $\mathbf{M}_\perp$
- The two 180° domains can be superposed by inversion and translation by a lattice vector $\boldsymbol{l}$.
- J_{ni} changes sign and will rotate the polarisation in the opposite sense.

This type of 180° domain leads to depolarisation of the all components not parallel to $\mathbf{M}_\perp$.

Orientation domains (s-domains)

Occur when the magnetic space group is not congruent with the group describing the configurational symmetry.

- If $\mathscr{P}$ is a sub-group of the configurational symmetry $\mathscr{G}$, congruent with the magnetic space group $\mathscr{M}$, then $\mathscr{G} = \mathscr{P} \times \mathscr{S}$
- The sub-group $\mathscr{S}$ is made up of operators contained in $\mathscr{G}$ which are not in the magnetic group.
- If $\mathscr{S}$ is of order s there are s possible orientation domains related to one another by the elements of $\mathscr{S}$.
- The magnetic interaction vectors for reflections related by the elements of $\mathscr{S}$ are different.

$$\mathbf{M}_\perp(\mathbf{k}) \neq \mathbf{M}_\perp(\mathbf{R}_s\mathbf{k}) \quad \text{but} \quad \mathbf{M}_{\perp s}(\mathbf{k}) = \mathbf{M}_\perp(\mathbf{R}_s\mathbf{k})$$

$\mathbf{R}_s$ is an operator in $\mathscr{S}$ and $\mathbf{M}_{\perp s}(\mathbf{k})$ is the interaction vector for the domain generated by $\mathbf{R}_s$.

- For collinear structures the magnetic structure factors of reflections related by the elements of $\mathscr{S}$ are equal:

$$\mathbf{R}_s\mathbf{M}(\mathbf{k}) = \mathbf{M}(\mathbf{R}_s\mathbf{k})$$

but this is not true in the general case.

Orientation domains and symmetry elements

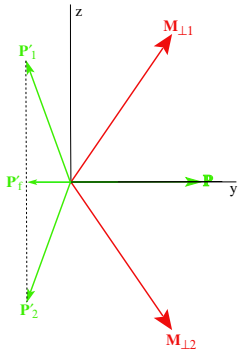
- If the configurational symmetry possesses a symmetry axis of order higher than 2:

either the moments lie parallel to this axis,
or the structure is non collinear,
or the symmetry axis is not in the magnetic space group.

- In a collinear structure,

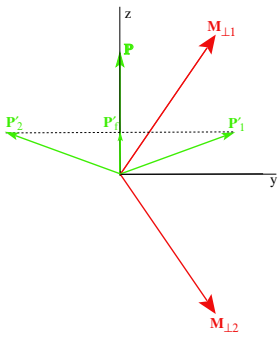
either the moments lie parallel to any mirror planes and diad axes.
or they are perpendicular to them
or the mirror plane or diad axis is not in the magnetic space group.

Depolarisation by s domains



The two orientation domains with interaction vectors $\mathbf{M}_{\perp 1}$ and $\mathbf{M}_{\perp 2}$ are related by a diad axis parallel to y

- When $\mathbf{P}$ is parallel to y
- $\mathbf{P}$ is rotated to $\mathbf{P}'_1$ by domain 1
- It is rotated to $\mathbf{P}'_2$ by domain 2.
- The final polarisation is parallel to $\mathbf{P}'_f$.
- The z components are depolarised



The two orientation domains with interaction vectors $\mathbf{M}_{\perp 1}$ and $\mathbf{M}_{\perp 2}$ are related by a mirror plane perpendicular to z

- When $\mathbf{P}$ is parallel to z
- $\mathbf{P}$is rotated to $\mathbf{P}'_1$ by domain 1
- It is rotated to $\mathbf{P}'_2$ by domain 2.
- The final polarisation is parallel to $\mathbf{P}'_f$.
- The y components are depolarised.

Orientation domains can depolarise the y and z, but not the x components

Chiraity domains

Occur whenever the paramagnetic space group is centro-symmetric but the magnetic structure is not.

They are related by the inversion operator.

This happens when either

1. Magnetic moments on centro-symmetrically related sites are not parallel.

   or

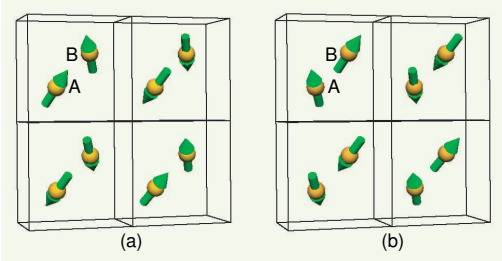
2. 2τ is not a reciprocal latice vector so the configurational group is acentric.
   The two chirality domains correspond to $\pm\tau$. They both give reflections at $\mathbf{g}\pm\tau$ with

$$\mathbf{M}_{\perp\tau}(\mathbf{g}+\tau) = -\mathbf{M}_{\perp\tau}{}^{*}(\mathbf{g}-\tau) = -\mathbf{M}_{\perp-\tau}{}^{*}(\mathbf{g}+\tau)$$

   Such structures include helices and cycloids.

Chirality domains: Examples

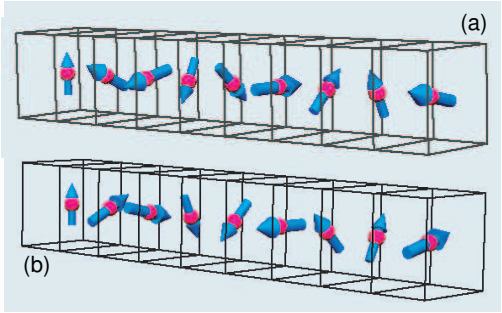
The centre of symmetry is not in the magnetic group



The atoms A and B at $\pm(xyz)$ have non-parallel moments.
$\mathbf{M}_{\perp}(\mathbf{k})$ is not parallel to $\mathbf{M}^{*}_{\perp}(\mathbf{k})$.

The moment on A in domain (a) is parallel to B in domain (b)
$\mathbf{M}_{\perp(a)}(\mathbf{k}) = \mathbf{M}^{*}_{\perp(b)}(\mathbf{k}) = \mathbf{M}_{\perp(b)}(-\mathbf{k})$
$\tau = (\frac{1}{2}\,\frac{1}{2}0) \quad 2\tau = (110) = \mathbf{g}$

The centre of symmetry is not in the configuration group



$\tau = (0.15,0,0) \quad 2\tau = (0.3,0,0) \neq \mathbf{g}$
$\mathbf{M}_{\perp}(\mathbf{k})$ is not parallel to $\mathbf{M}^{*}_{\perp}(\mathbf{k})$.

In the (b) domain $\tau = (-0.15,0,0)$ and the spiral turns in the opposite sense.

Chirality domains: Polarisation

- $\mathbf{M}_\perp$ is not parallel to $\mathbf{M}_\perp^*$ in either type of chiral structure.
- The term $J_{ij} = \Im(M_{\perp i} M_{\perp j}^*)$ in the polarisation matrix is non-zero.
- J_{ij} is of opposite sign for the two chiralities.
- If the chirality domains are unequally populated
  - The intensity will depend on the x component of $\mathbf{P}$ due to the term $\mathbf{P} \cdot J_{ij}$.
  - if the component of $P_x \parallel J_{ij} < 1$ it will be increased in the scattered beam.
  - This is not due to rotation, but is because the unfavourable polarisation is not scattered.
- Chirality domains do not lead to depolarisation of the x component of $\mathbf{P}$.
- They lead to depolarisation in the y and z components because the chiral component analyses the polarisation parallel to x which is zero when $\mathbf{P}$ is parallel to y or z.

Experimental strategy

SNP cannot be used in isolation to determine magnetic structure.

- The magnetic propagation vector τ must be known.
- If $\tau \neq 0$ intensity measurements are needed to determine the absolute magnitudes of the moments
- With the current geometry τ must be in the scattering plane.
- It is advantageous to orient the crystal so that a component of magnetisation is perpendicular to the scattering plane.
- Analysis of rather few magnetic reflections is then usually sufficient to determine the structure.

The usual experimental strategy is to measure the scattered polarisation $\mathbf{P}'$ with the incident polarisation $\mathbf{P}$ parallel to polarisation x, y, z in turn.
This determines the polarisation matrix.

$$\mathsf{P}_{ij} = \left\langle \frac{P_i \mathscr{P}_{ij} + P_j'')}{P_i} \right\rangle_{\text{domains}}$$

Structures with $\tau \neq 0$

- For structures with $\tau = 0$; $N(\mathbf{k})$ is zero at the positions of magnetic reflections.
- The terms R_{ny}, R_{nz}, J_{ny} and J_{nz} in the polarisation tensor are all zero.
- If the configuration group is centrosymmetric J_{yz} is also zero so $\mathbf{P}''$=0 and the phases can be chosen to make $\mathbf{M}_\perp(\mathbf{k})$ real.

Suppose $\mathbf{M}_\perp$ is inclined at an angle α to z (measured clockwise about x) then :

$$\mathscr{P} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -\cos 2\alpha & -\sin 2\alpha \\ 0 & -\sin 2\alpha & \cos 2\alpha \end{pmatrix}$$

If $\mathbf{M}_\perp$ is parallel to either y or z the matrix is diagonal

$$Q \parallel y \qquad \mathscr{P} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \qquad Q \parallel z \qquad \mathscr{P} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

When s domains with different values of α are present any off-diagonal elements are reduced

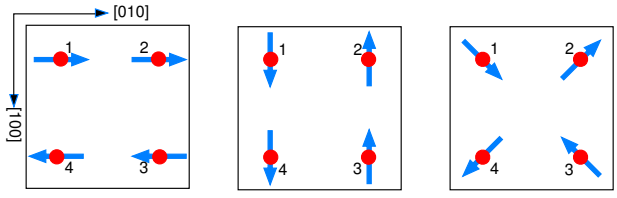
A commensurate tetragonal structure $\tau = 0, 0, \frac{1}{2}$

An imaginary structure will be used to show how SNP can distinguish between canted and collinear models.

There are 4 magnetic atoms per cell,The spins S lie in the 001 plane.

A1 at $(x, x, 0)$;
A2 at $(-x, x, 0)$
A3 at $(-x, -x, 0)$
A4 at $(x, -x, 0)$
with $x \approx 0.2$.

Possible configurations of the plane at $z = 0$



(a) mm'm' (b) m'mm' (c) 4'/m'mm'

The Magnetic Structure Factors $\mathbf{M}(\mathbf{k})$ for $h, k, \frac{1}{2} + l$ reflections			
Component	Model (a)	Model (b)	Model (c)
$M_{[100]}$	0	$4Ss(h)c(k)$	$2\sqrt{2}Ss(h)c(k)$
$M_{[010]}$	$4Ss(k)c(h)$	0	$2\sqrt{2}Ss(k)c(h)$
Intensity	$(4Ss(k)c(h))^2$	$(4Ss(h)c(k))^2$	$8S^2(s^2(h)c^2(k) + s^2(k)c^2(h))$
Domain Average	$8S^2(s^2(h)c^2(k) + s^2(k)c^2(h))$		
$c(h) = \cos 2\pi hx \quad s(h) = \sin 2\pi hx \quad c(k) = \cos 2\pi kx \quad s(k) = \sin 2\pi kx$			

Magnetic structure factors for 3 models

The Magnetic Structure Factors $\mathbf{M}(\mathbf{k})$ for $h,k,\frac{1}{2}+l$ reflections			
Component	Model (a)	Model (b)	Model (c)
$M_{[100]}$	0	$4Ss(h)c(k)$	$2\sqrt{2}Ss(h)c(k)$
$M_{[010]}$	$4Ss(k)c(h)$	0	$2\sqrt{2}Ss(k)c(h)$
Intensity	$(4Ss(k)c(h))^2$	$(4Ss(h)c(k))^2$	$8S^2(s^2(h)c^2(k)+s^2(k)c^2(h))$
Domain Average	$8S^2(s^2(h)c^2(k)+s^2(k)c^2(h))$		
$c(h)=\cos 2\pi hx \quad s(h)=\sin 2\pi hx \quad c(k)=\cos 2\pi kx \quad s(k)=\sin 2\pi kx$			

- The average intensity scattered by the two orthorhombic domains is exactly the same as that scattered by the tetragonal structure.
- The tetragonal structure gives a unique $\mathbf{M}(\mathbf{k})$ for each reflection. SNP can determine its direction.
- A mixture of orthorhombic domains will give depolarisation when $\mathbf{P}$ is perpendicular to $\mathbf{k}$ because the structure factors for the two domains are not parallel.

Polarisation matrices for the model structures

In an SNP experiment to distinguish the models the crystal would be mounted so as to have the $h,0,\frac{1}{2}+l$ reflections in the scattering plane: [010] parallel to polarisation z.

The magnetic interaction vectors for $(h,0,\frac{1}{2}+l)$ reflections are:

Component	Model (a)	Model (b)	Model (c)
$M_{\perp y}$	0	$2F'\sin\alpha$	$\sqrt{2}F'\sin\alpha$
$M_{\perp z}$	$2F$	0	$\sqrt{2}F$
Intensity $\lvert\mathbf{M}_\perp\rvert^2$	$4F^2$	$4F'^2\sin^2\alpha$	$2(F^2+F'^2\sin^2\alpha)$

$F=S\sin 2\pi hx \qquad F'=S\cos 2\pi hx$

α is the angle between [001] and the normal to $(h,0,\frac{1}{2}+l)$

The corresponding polarisation matrices are:

Model (a)

$$\mathsf{P}_{ij}=\begin{pmatrix}-1&0&0\\0&-1&0\\0&0&1\end{pmatrix}$$

Model (b)

$$\mathsf{P}_{ij}=\begin{pmatrix}-1&0&0\\0&1&0\\0&0&-1\end{pmatrix}$$

Distinction between the model structures

From all these results

The mean from equal volumes of domains (a) and (b) is

$$P_{ij} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -(F'^2 - F^2 \sin^2\alpha)/I & 0 \\ 0 & 0 & (F'^2 - F^2 \sin^2\alpha)/I \end{pmatrix}$$

Model (c)

$$P_{ij} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -(F'^2 - F^2 \sin^2\alpha)/I & (2FF' \sin\alpha)/I \\ 0 & (2FF' \sin\alpha)/I & (F'^2 - F^2 \sin^2\alpha)/I \end{pmatrix}$$

Only the off-diagonal terms differ.

They would be measured in the SNP experiment.

Francesco Ricci School, Neutron Scattering from Magnetic Systems

Neutron Polarimetry: IV Experiments with SNP

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Institut Laue Langevin, Grenoble
and
Physics Department Loughborough University

September 2006

Outline: Experiments with SNP

Structures with non-zero propagation vector
- Commensurate structures
- Incommensurate structures
- SNP with sinusoidally modulated structures
- The incommensurate structure of CuO
- Magnetic structure of UPtGe

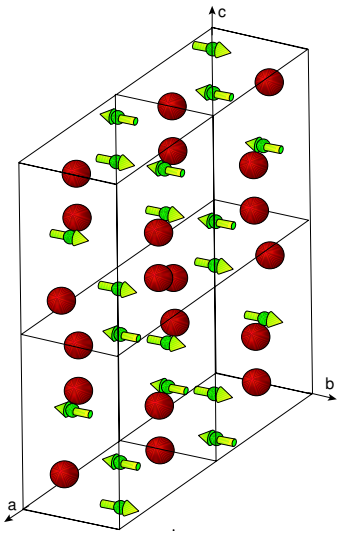
Magnetic structures with zero propagation vector
- Nuclear magnetic interaction terms
- The magnetic structure of $U_{14}Au_{51}$
- Magneto-electric and Multi-Ferroic materials
- Simple magneto-electrics: Cr_2O_3

Determination of precise magnetic structure factors using SNP
- Magnetic structure factors from rotation of polarisation
- Experimental considerations
- Determination of the Cr^{3+} form factor in Cr_2O_3

The commensurate structure of CuO

The low temperature magnetic structure of cupric oxide provides a simple example.

- Below 213 K cupric oxide, CuO, (space group C2/c) is antiferromagnetic with $\tau = \frac{1}{2}, 0, -\frac{1}{2}$.
- Magnetic reflections $h0l \pm \tau$ with $h+l$ odd are absent.
- So the spins on copper atoms related by the n glide-plane perpendicular to [010] are parallel.
- The reflection intensities suggest that the spin-direction is [010]



SNP measurements confirm this structure

Polarisation matrices were measured for the $\frac{1}{2}, 0, \overline{\frac{1}{2}}$ $\overline{\frac{1}{2}}, 0, \frac{1}{2}$ $\frac{3}{2}, 0, \overline{\frac{3}{2}}$ and $\frac{3}{2}, 0, \overline{\frac{1}{2}}$ reflections.

Within experimental error, they were all diagonal with P_{xx}=P_{yy}=-1, P_{zz}=1

This proves that the structure is collinear with spins parallel to polarisation $z = [010]$.

Incommensurate structures

SNP has been used rather successfully in determining the details of incommensurate structures such as helices, cycloids and spin-density waves.

It also often allows these types of structures to be distinguished

To study incommensurate structures some thought must be given to the crystal orientation.

- The propagation vector must lie in the scattering plane,
- A component of moment should be perpendicular to the scattering plane, because
  - If both components of the moment lie in the scattering plane, then $\mathbf{M}_\perp$ is parallel to polarisation y for all the accessible reflections.
  - When $\tau \neq 0$, it is only the direction and not the magnitude of $\mathbf{M}_\perp$ which is measured by SNP, so measuring different reflections in the zone gives no additional information.
- If the orientation is chosen so that a component of moment is parallel to polarisation z then the full potential of SNP can be realised.

Sinusoidally modulated structures

The magnetic moment distribution in a sinusoidally modulated structure with lattice vectors $\boldsymbol{l}$ and propagation vector τ can be written as

$$\mathbf{M}(\mathbf{r}+\boldsymbol{l}) = \hat{\mathbf{p}} M_p(\mathbf{r}) \cos \boldsymbol{l}\cdot\tau + \hat{\mathbf{q}} M_q(\mathbf{r}) \sin \boldsymbol{l}\cdot\tau$$

where $\hat{\mathbf{p}}$ and $\hat{\mathbf{q}}$ are perpendicular unit vectors.

- When either $M_p(\mathbf{r})$ or $M_q(\mathbf{r})$ is zero the equation describes a spin-density wave.
- When τ lies in the plane of $\hat{\mathbf{p}}$ and $\hat{\mathbf{q}}$ it describes a cycloid.
- When both are perpendicular to τ it describes a right helix.

The magnetic scattering from such a modulated structure is given by

$$\begin{aligned}\mathbf{M}_\perp(\mathbf{k}) &= (\mathbf{p}_\perp M_p(\mathbf{k}) - \imath\mathbf{q}_\perp M_q(\mathbf{k}))\delta(\mathbf{g}+\tau-\mathbf{k}) \\ &+ (\mathbf{p}_\perp M_p(\mathbf{k}) + \imath\mathbf{q}_\perp M_q(\mathbf{k}))\delta(\mathbf{g}-\tau-\mathbf{k})\end{aligned}$$

where $\mathbf{p}_\perp$ and $\mathbf{q}_\perp$ are the components of $\hat{\mathbf{p}}$ and $\hat{\mathbf{q}}$ perpendicular to $\mathbf{k}$.

The structure factors for sinusoidally modulated structures

In the equation for the interaction vector

$$M_{p,q}(\mathbf{k}) = \int_{\text{unit cell}} M_{p,q}(\mathbf{r}) \exp -(\mathbf{k}.\mathbf{r}) \mathrm{d}r^3$$

are the unit cell structure factors for the two perpendicular magnetic moment distributions.

- A structure with propagation vector τ gives reflections at both $\mathbf{g}+\tau$ and $\mathbf{g}-\tau$.
- For structures for which $M_{p,q}(\mathbf{k})$ are real, ie the magnetisation distributions themselves are centrosymmetric $\mathbf{M}_\perp\tau(\mathbf{k}) = \mathbf{M}^*_\perp{}_{-\tau}(\mathbf{k})$
- The term which creates polarisation along x:

  $$J_{ij} = 2\Re\left(M_p(\mathbf{k}){M_q}^*(\mathbf{k})\right) p_{\perp i} \times q_{\perp j}$$

  is finite if neither $p_{\perp i}$, $q_{\perp j}$ or either structure factor $M_{p,q}(\mathbf{k})$ is zero.

SNP with sinusoidally modulated structures

An example will show how SNP measurements determine the structure when $M_{p,q}(\mathbf{k})$ are real.

The crystal will be aligned with τ in the scattering plane. Suppose for simplicity that $\hat{\mathbf{p}}$ is perpendicular to the scattering plane so that $\hat{\mathbf{q}}$ lies in it.

For reflections in the scattering plane; $\mathbf{p}_\perp \parallel z$ is constant, whilst $\mathbf{q}_\perp \parallel y$ varies from 0 when $\hat{\mathbf{q}} \parallel \mathbf{k}$ to a maximum when $\hat{\mathbf{q}} \perp \mathbf{k}$.

The polarisation matrices which would be obtained are:

$$\mathrm{P}_{ij} = \begin{pmatrix} -1 & 0 & 0 \\ B & A & 0 \\ B & 0 & -A \end{pmatrix} \quad \text{for } \mathbf{k} \parallel \hat{\mathbf{q}} \qquad \text{with } A = \frac{M_p(\mathbf{k})^2 - M_q(\mathbf{k})^2}{M_p(\mathbf{k})^2 + M_q(\mathbf{k})^2}$$

$$\text{and } B = \frac{2M_p(\mathbf{k})M_q(\mathbf{k})}{M_p(\mathbf{k})^2 + M_q(\mathbf{k})^2}$$

$$\mathrm{P}_{ij} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \text{for } \mathbf{k} \perp \hat{\mathbf{q}}$$

$$\mathrm{P}_{ij} = \begin{pmatrix} -1 & 0 & 0 \\ -B & A & 0 \\ -B & 0 & -A \end{pmatrix} \quad \text{for } \mathbf{k} \parallel \hat{\mathbf{q}} \quad \text{for the other chirality}$$

SNP with sinusoidally modulated structures

- $\mathrm{P}_{xx} = -1$ in all three cases; in fact this is true for any structure with $\tau \neq 0$.
- For $\mathbf{P} \perp \mathbf{k}$ there is no y component of $\mathbf{M}_\perp(\mathbf{k})$ and so the behaviour is the same as for a collinear structure with $\mathbf{M}_\perp(\mathbf{k}) \parallel \mathbf{z}$.
- For $\mathbf{P} \parallel \mathbf{k}$; $\mathrm{P}_{yy} = -\mathrm{P}_{zz} = A$ gives the ellipticity of the helix.

$$A = \frac{M_p(\mathbf{k})^2 - M_q(\mathbf{k})^2}{M_p(\mathbf{k})^2 + M_q(\mathbf{k})^2}$$ is zero if the envelope is circular.

- The off-diagonal terms P_{xy}, P_{xz} depend on

$$B = \frac{2M_p(\mathbf{k})M_q(\mathbf{k})}{M_p(\mathbf{k})^2 + M_q(\mathbf{k})^2}$$ which changes sign for the opposite chirality

The intensity scattered by the domain for which B is positive will be greater than that for which B is negative.

- if the two chirality domains are equally populated the components $\mathrm{P}_{xy} = \mathrm{P}_{xz}$ will average to zero giving a diagonal polarisation matrix.

The incommensurate structure of CuO

At its Néel temperature, 230 K, CuO orders magnetically with an incommensurate structure τ= 0.506, 0, -0.483 which remains constant on further cooling down to a lock-in transition at 213 K.

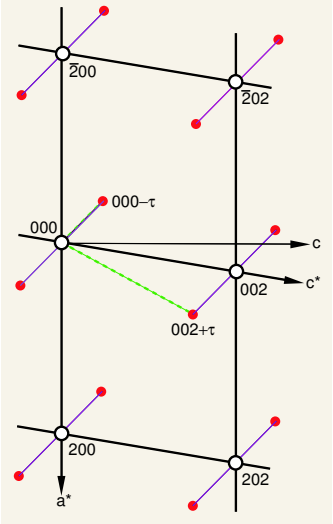
- The systematically absent magnetic reflections follow the same rules as in the low temperature phase
- This suggests that the coupling between moments in the two phases is nearly the same.
- Integrated intensity measurements were not able to distinguish clearly between different possible models for the modulation.

  Forsyth J B, Brown P J and Wanklyn B M,(1988) J. Phys. C **21** 2917.
- SNP measurements of a few $h0l \pm \tau$ reflections were able to resolve the problem.

  Brown P J *et al.*,(1991) J. Phys. Condens. Matter **3** 4281.

The incommensurate structure of CuO: SNP

The $h0l$ reciprocal lattice layer

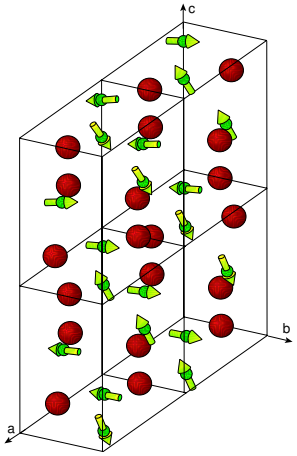


- The scattering vectors for the $002 + \tau$ and $000 - \tau$ reflections are nearly perpendicular.
- The polarisation matrix for $002 + \tau$ was similar to those measured in the commensurate phase (diagonal with P_{zz} positive).
- Therefore for $002 + \tau$, $\mathbf{M}_{\perp}$ is parallel to [010].
- The matrix obtained for $000 - \tau$ was very different.

The incommensurate structure of CuO: SNP

$$P_{ij}(000-\tau) = \begin{pmatrix} -1.00(2) & 0.00(2) & -0.04(2) \\ -0.08(2) & -0.07(2) & 0.00(2) \\ -0.08(2) & 0.00(2) & 0.06(2) \end{pmatrix}$$

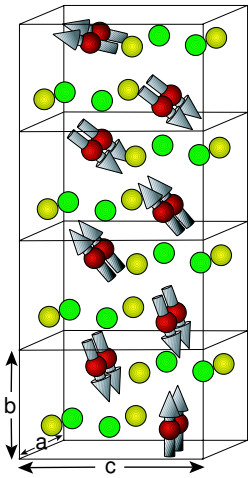
- The full polarisation is only transmitted for the x direction.
- The small values of the off-diagonal components indicate chirality domains.
- The small values of P_{yy} and P_{zz} show that for this reflection $A \approx 0$ so $M_{\perp p}$ and $M_{\perp q}$ are nearly equal.

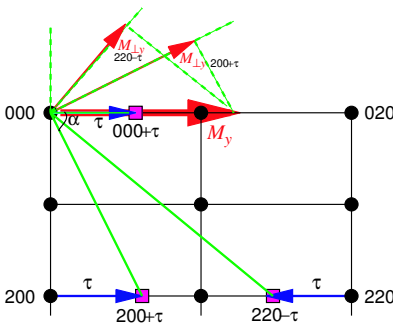


These results are only consistent with a helical structure in which the spins rotate in a plane containing the [010] axis and the normal to $002+\tau$.

Magnetic structure of UPtGe

The orthorhombic intermetallic compound UPtGe is reported to order magnetically at 51 K to a cycloidal structure with propagation vector $\tau = 0, 0.554, 0$ and the U spins rotating in the **b**-**c** plane. Robinson R *et al.*,(1993) Phys. Rev. B **47** 6138.
The plausibility of such a structure was queried because of the huge magnetic anisotropy found for U in other UTX compounds.



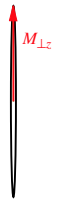


The proposed structure has been verified by measuring the polarisation matrices for magnetic reflections in the $hk0$ plane

Magnetic structure of UPtGe: SNP

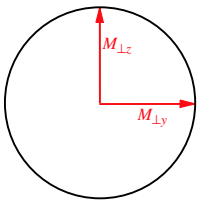
$$P_{ij}(000+\tau) = \begin{pmatrix} -0.98 & 0.00 & 0.00 \\ 0.00 & -0.99 & 0.00 \\ 0.00 & 0.00 & 1.00 \end{pmatrix}$$

shows $\mathbf{M}_\perp \parallel z$



$$P_{ij}(200+\tau) = \begin{pmatrix} 0.50 & 0.00 & 0.00 \\ 1.02 & 0.00 & 0.00 \\ 1.02 & 0.02 & 0.04 \end{pmatrix}$$

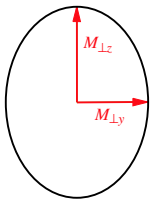
gives $\mathbf{P}' \parallel x$ for all $\mathbf{P}$



With $\mathbf{P} \parallel x$ the scattered intensity was very small and P_{xx} poorly determined

$$P_{ij}(220-\tau) = \begin{pmatrix} -0.98 & 0.05 & -0.05 \\ -0.98 & -0.10 & -0.02 \\ -0.98 & 0.01 & 0.17 \end{pmatrix}$$

$\mathbf{P}' \parallel -x$ with small P_{zz}



Magnetic structure of UPtGe: SNP

Structures with non-zero propagation vector
Commensurate structures
Incommensurate structures
SNP with sinusoidally modulated structures
The incommensurate structure of CuO
Magnetic structure of UPtGe
Magnetic structures with zero propagation vector
Determination of precise magnetic structure factors using SNP

These results are characteristic of a nearly single domain cycloid structure in which the populated domain has $\tau \parallel -x$.

D. Mannix *et al.*,(2000) Phys. Rev. B **62** 3810.

The ellipticity of the envelope

$$\varepsilon = \frac{M_{[010]}}{M_{[001]}} = \frac{\text{major axis}}{\text{minor axis}}$$

and the orientation of the major axis of the cycloid were obtained by fitting

$$P_{yy}(\mathbf{k}) = -P_{zz}(\mathbf{k}) = \pm\frac{\varepsilon^2 \sin^2\phi_{\mathbf{k}} - 1}{\varepsilon^2 \sin^2\phi_{\mathbf{k}} + 1}$$

where $\phi_{\mathbf{k}}$ is the angle between the major axis and $\mathbf{k}$

for a set of magnetic reflections;

Magnetic structures with zero propagation vector

When the magnetic propagation vector is zero magnetic and nuclear scattering can occur in the same reflections.

The terms

$$J_{ni} = 2\Im(N(\mathbf{k})M_{\perp i}{}^{*}(\mathbf{k})) \quad \text{and} \quad R_{ni} = 2\Re(N(\mathbf{k})M_{\perp i}{}^{*}(\mathbf{k}))$$

in the polarisation matrix can be non-zero.

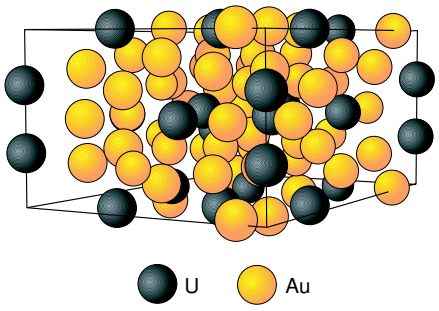
- Finite R_{ni} results in a polarisation dependent cross-section. The scattered beam is polarised parallel to $\mathbf{M}_{\perp}$.
  - This occurs when the phase angle between $\mathbf{M}_{\perp}(\mathbf{k})$ and $N(\mathbf{k}) \neq \frac{(2n+1)\pi}{2}$.
  - It is the term used to polarise neutrons and to determine magnetic structure factors from *flipping ratios*.
- Finite J_{ni} leads to rotation of the scattered polarisation towards the direction perpendicular to both $\mathbf{M}_{\perp}$ and $\mathbf{P}$.
  - It is finite when the phase angle between $\mathbf{M}_{\perp}(\mathbf{k})$ and $N(\mathbf{k}) \neq n\pi$.
  - It is the only term which can lead to depolarisation with $\mathbf{P} \parallel x$

$U_{14}Au_{51}$:The crystal structure

$U_{14}Au_{51}$ has the hexagonal $Gd_{14}Ag_{51}$ structure with space group P6/m.

The uranium atoms occupy three different crystallographic sites

U1 6(k) $(x_1, y_1, \frac{1}{2})$
U2 6(j) $(x_2, y_2, 0)$
U3 2(e) $(0, 0, z_3)$



Susceptibility, specific heat and resistivity indicate an antiferromagnetic phase transition at 22 K.

Powder diffraction suggested a structure with moments $\parallel [001]$.

No moment on U3 because of close U3-U3 distance.

Dommann A *et al.*,(1990) J. Less-Comm. Metals **160** 171.

Single crystal intensity measurements were not compatible with this structure.

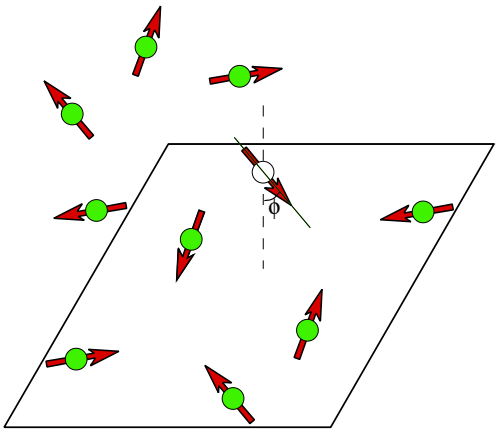
$U_{14}Au_{51}$: Spherical polarisation analysis results

hkl	$i\backslash j$	x	y	z
200	x	-0.86	0	0
	y	0	-0.83	0
	z	0	0	0.98
201	x	-0.28	0	0
	y	0	-0.62	0.38
	z	0	0.37	0.73
101	x	-0.54	-0.08	-0.07
	y	-0.08	0.98	-0.12
	z	0.01	-0.05	-0.55

- The P_{xx} terms are negative and $|P_{xx}| < 1$.
  The magnetic scattering is in quadrature with and greater than the nuclear scattering ($J_{ni} \neq 0$).
- For 200 P_{ij} is diagonal and $P_{zz} \approx 1$
  $\mathbf{M}_\perp(200) \parallel$ polarisation z
  [010]:- No significant moment $\parallel$ [001].
- For 201 there are off-diagonal terms $P_{yz} \approx P_{zy}$.
  Since $\mathbf{k}$ has a component on polarisation z, this is consistent with all moments in the (001) plane
- The depolarisation for P_x is greater than for either P_y or P_z.
  There are no orientation domains so the magnetic structure probably retains full symmetry

$U_{14}Au_{51}$: The layer motif

These constraints determine the motif in both the U1 and U2 layers



Only the magnetic moments and the values of ϕ in the U1 and U2 layers, remain to be determined

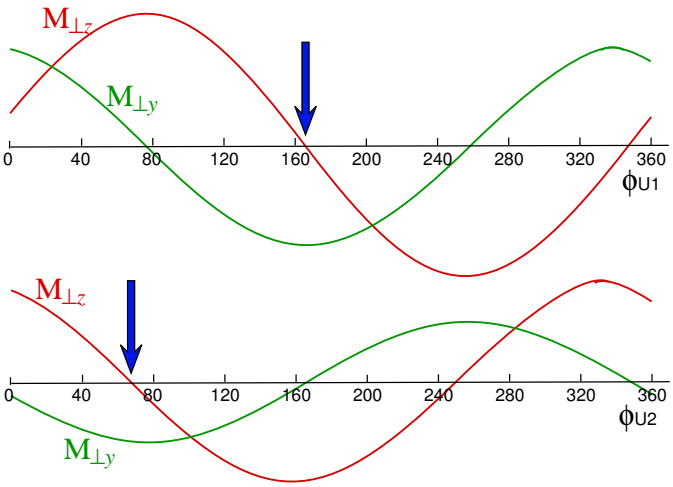
$U_{14}Au_{51}$: Angles within the layers

For the 101 reflection $P_{yy} \approx 1$

$\mathbf{M}_\perp(101)$ is nearly parallel to y: $M_{\perp z}$ small and $M_{\perp y}$ large

it is the sum of contributions from the U1 and U2 layers.

The y and z components of $\mathbf{M}_\perp(101)$ can be computed separately as a function of ϕ.



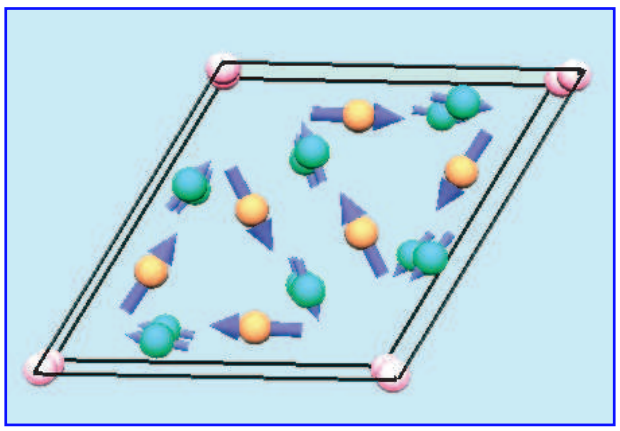
There is only a small range in which a pair of ϕ's exist for which the $M_{\perp z}$ for U1 and U2 cancel whilst their $M_{\perp y}$ reinforce one another.

$U_{14}Au_{51}$: The Magnetic structure

These initial values provided an adequate starting point for a least squares refinement of the structure using both SNP and integrated intensity data.

U1 $\mu = 2.28(6)\ \mu_B$
$\phi = 88(2)^\circ$

U2 $\mu = 1.48(8)\mu_B$
$\phi = 139(2)^\circ$



Brown P J *et al.*,(1997) J. Phys. Condens. Matter **9** 4729.

Magneto-electric and Multi-Ferroic materials

- Multi-ferroic is the name give to materials which possess more than one polar property. They are nowadays exciting a lot of interest as possible electronic components.
- Polarimetry is particularly useful to study such materials when one of the polar properties is magnetic: a ferromagnetic moment, and the other structural, for instance ferro-electric polarisation or peizo-electric displacement.
- The ability of SNP to determine the relative phases of nuclear and magnetic scattering allows the precise relationship between the structural and magnetic polarisations to be determined.
- Magneto-electric materials are closely related to magnetic multi-ferroics; in both the presence of a ferromagnetic polarisation implies a magnetic structure with zero propagation vector, or at least a component of the structure which propagates with $\tau = 0$.

The magneto-electric effect

- The property of magneto-electricity in centro-symmetric crystals is restricted to those having antiferromagnetic structures with zero propagation vector the centre of symmetry must invert the spins.
- In this case the J_{ni} are finite giving rise to off-diagonal terms $P_{xz} = -P_{zx}$ and $P_{xy} = -P_{yx}$ in the polarisation matrix.
- The magnitudes and even the signs of magnetoelectric (ME) susceptibilities are specimen dependent.
  but
- their temperature dependencies are unique to each material.
- The variability is due to the existence of 180°domains which have opposite ME effects.

The magneto-electric effect: rotation of the polarisation

The measured and intrinsic ME susceptibilities are related by

$$\chi_{obs} = \eta\chi_0 \quad \text{with} \quad \eta = \frac{v_1 - v_2}{v_1 + v_2}$$

v_1 and v_2 are the volumes of crystal belonging to each of the the two 180° domains.

η can be determined using SNP

If the moments are parallel to polarisation z

$$P_{ij} = \begin{pmatrix} \beta & \eta\xi & 0 \\ -\eta\xi & \beta & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \text{with} \quad \begin{aligned} \beta &= (1-\gamma^2)/(1+\gamma^2) \\ \xi &= 2q_z\gamma/(1+\gamma^2) \\ \gamma &= \mathbf{M}_\perp(\mathbf{k})/N(\mathbf{k}) \end{aligned}$$

q_z is $+1$ if $\mathbf{M}(\mathbf{k})$ is parallel to $\mathbf{z}$ and -1 if it is antiparallel.

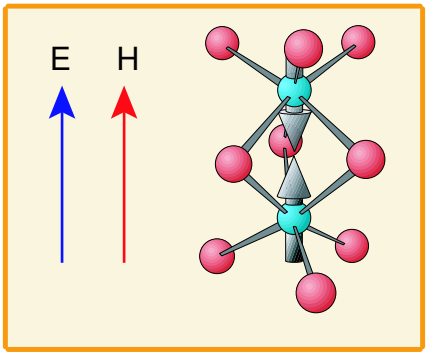
The magneto-electric effect: 180° domain populations

- Measurement of the polarisation matrix allows both η and γ to be determined.
- The effects of electric and magnetic fields on the domain population can be studied.
- When $\eta \neq 0$ the absolute directions of rotation of the neutron spins determine the magnetic configuration of the more populous domain.
- The results shed light on the fundamental mechanisms leading to the ME effect.

The magneto-electric effect: Cr_2O_3

- Cr_2O_3 is perhaps the best known ME material.
- The Cr^{3+} ions are octahedrally coordinated by oxygen. with pairs of octahedra, sharing a common face.
- The double octahedra are linked by sharing free vertices.

Electric and magnetic fields, applied parallel to one another and to the c-axis while cooling through the Néel transition, stabilise the domain in which the moments point towards the shared face.



Magnetic structure factors from polarisation rotation

When the magnetic and nuclear scattering are in quadrature the terms $P_{xi}\ P_{ix}$ $(i = y, z)$ depend just on the ratio γ between the magnetic and nuclear structure factors and on the imbalance η in the populations of the two 180° domains.

This property can be exploited to obtain precise values for the magnetic structure factors and hence for the antiferromagnetic form factor.

The polarisation matrix allows two independent estimates of γ to be made.

For $\mathbf{M}_\perp \parallel z$:

(a) $P_{xz} = -P_{zx} = \eta\xi = \dfrac{\eta q_z \gamma}{1+\gamma^2}$ (b) $P_{xx} = P_{zz} = \beta = \dfrac{1-\gamma^2}{1+\gamma^2}$

(a) Is only useful if there is an imbalance η in the population of 180° domains.

Experimental considerations

The precision with which γ can be determined depends on the statistical error in the determination of P_{ij}.

In this case, since the cross-section is not polarisation dependent, the recorded counting rate, summed over the two polarisation states, is constant and independent of either the incident or the scattered polarisation direction.

- The polarisation measured by the analyser is given by:

$$P = (I^+ - I^-)/(I^+ + I^-)$$

where I^+ and I^- are the counting rates in the two detector channels.

- The variance in the measurement of a component of polarisation due to counting statistics is

$$V_P = \frac{(1-P^2)^2}{4}\left(\frac{1}{N^+} + \frac{1}{N^-}\right)$$

where N^+ and N^- are the counts recorded in each channel.

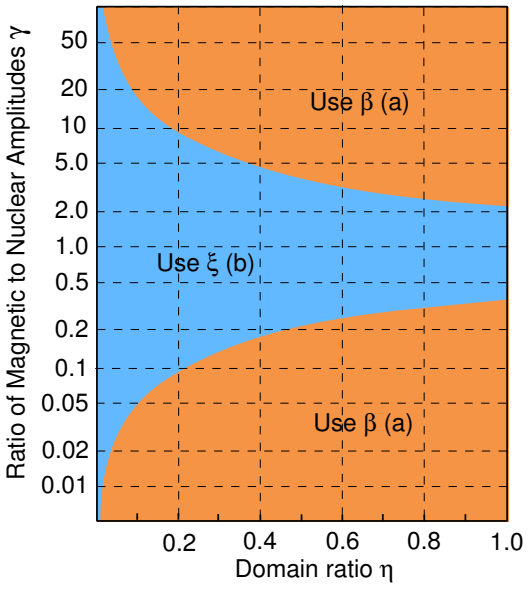
Variance in measurement of P′

- The variance is minimised by dividing the measuring time available in the ratio $t^+/t^- = (1-P)/(1+P)$.
- With this division, for a total N neutrons counted, the variance is $V_P = (1-P^2)/N$
- The variances in the values of γ derived from the equations for ξ (a) and β (b) are:

(a) $$V_\gamma = \frac{(1+\gamma^2)^4}{16\gamma^2}V_P$$

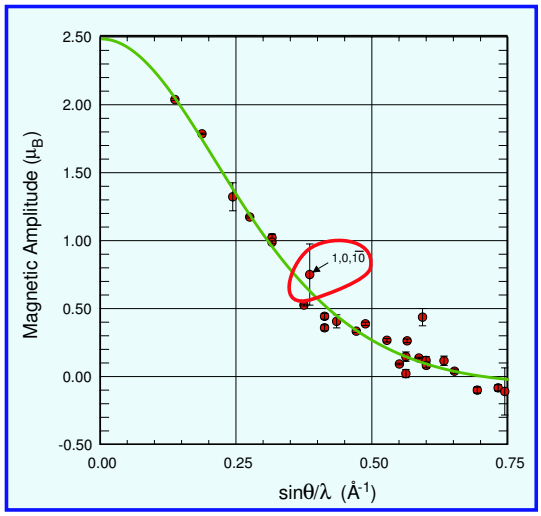
(b) $$V_\gamma = \frac{(1+\gamma^2)^4}{4\eta^2(1-\gamma^2)^2}V_P$$

If η is small or γ is close to unity use (a)
For very small or very large γ use (b) so long as η is not small.



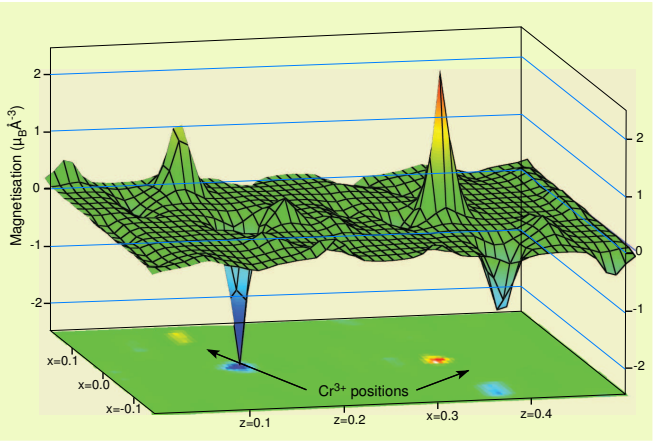
The Cr^{3+} form factor in Cr_2O_3

- The polarisations scattered by $h0l$ reflections from Cr_2O_3 were studied.
- Measurements were made with the crystal in several states with different domain populations produced by field cooling.
- Values for the Cr^{3+} form factor for each reflection were derived form the experimental γ's.
- For most reflections an extremely good precision was obtained.
- Exceptions are:
  $2,0,2$ for which N is very small so that $\gamma >> 1$.
  and $1,0,10$ for which the the Cr geometric structure factor is small so the reflection is insensitive to the form factor.



The magnetisation distribution in Cr_2O_3

The data can be used to make a maximum entropy reconstruction of the antiferromagnetic magnetisation distribution projected down [010].



The coefficients of the reconstruction are differences between the observed structure factors and those calculated for an antiferromagnetic arrangement of Cr^{3+} ions with t_{2g} symmetry in the Cr_2O_3 structure

The difference density has a a gradient of magnetisation at the Cr^{3+} positions.

This may be the signature of the ME property.