The plan

- How does the neutron interact with magnetism?
- The fundamental rule of neutron magnetic scattering
- Elastic scattering, and how to understand it
- Magnetic form factors
- Inelastic scattering

How does the neutron interact with magnetism?

Neutrons have no charge, but they do have a magnetic moment.

The magnetic moment is given by the neutron's spin angular momentum:

$$-\gamma\mu_N\hat{\boldsymbol{\sigma}}$$

where:

- γ is a constant (=1.913)
- μ_N is the nuclear magneton
- $\hat{\boldsymbol{\sigma}}$ is the quantum mechanical Pauli spin operator

Normally refer to it as a spin-1/2 particle

How does the neutron interact with magnetism?

Through the cross-section!

$$\frac{d^2\sigma}{d\Omega \cdot dE} = \frac{k'}{k}\left(\frac{m_n}{2\pi\hbar^2}\right)^2 \sum_{\zeta,s} p_\zeta p_s \sum_{\zeta',s'} \left|\langle \boldsymbol{k}',s',\zeta' | \hat{V}(\mathbf{r}) | \boldsymbol{k},s,\zeta \rangle\right|^2 \delta\left(\hbar\omega + E_\zeta - E_{\zeta'}\right)$$

Probabilities of initial target state and neutron spin

Conservation of energy

The *matrix element*, which contains all the physics.

$\hat{V}(\mathbf{r})$ is the *pseudopotential*,
which for magnetism is given by:

$$\hat{V}_m(\mathbf{r}) = -\gamma\mu_N \hat{\boldsymbol{\sigma}} \cdot \mathbf{B}(\mathbf{r})$$

where $\mathbf{B}(\mathbf{r})$ is the magnetic induction.

G. L. Squires, *Introduction to the theory of thermal neutron scattering*, Dover Publications, New York, 1978

W. Marshall and S. W. Lovesey, *Theory of thermal neutron scattering*, Oxford University Press, Oxford, 1971

S. W. Lovesey, *Theory of neutron scattering from condensed matter*, Oxford University Press, Oxford, 1986

Elastic scattering

If the incident neutron energy = the final neutron energy, the scattering is *elastic*.

$$\frac{d\sigma}{d\Omega} = \left(\frac{m_n}{2\pi\hbar^2}\right)^2 \sum_{s'} p_s \left| \langle \boldsymbol{k}', s' | \hat{V}(\mathbf{r}) | \boldsymbol{k}, s \rangle \right|^2$$

Forget about the spins for the moment (*unpolarized* neutron scattering) and integrate over all **r**:

$$\langle \boldsymbol{k}' | \hat{V}(\mathbf{r}) | \boldsymbol{k} \rangle = \int \hat{V}(\mathbf{r}) e^{i\mathbf{Q}\cdot\mathbf{r}} \cdot d\mathbf{r}$$

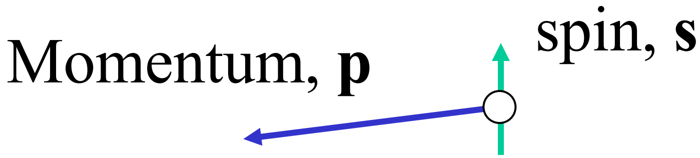
Momentum transfer $\mathbf{Q} = \boldsymbol{k} - \boldsymbol{k}'$

The elastic cross-section is then directly proportional to the *Fourier transform squared* of the potential. Neutron scattering thus works in Fourier space, otherwise called *reciprocal space.*

Evaluating $\langle \boldsymbol{k}' | \hat{V}_m(\mathbf{r}) | \boldsymbol{k} \rangle$

(Squires, chapter 7)

Magnetism is caused by unpaired electrons or movement of charge.



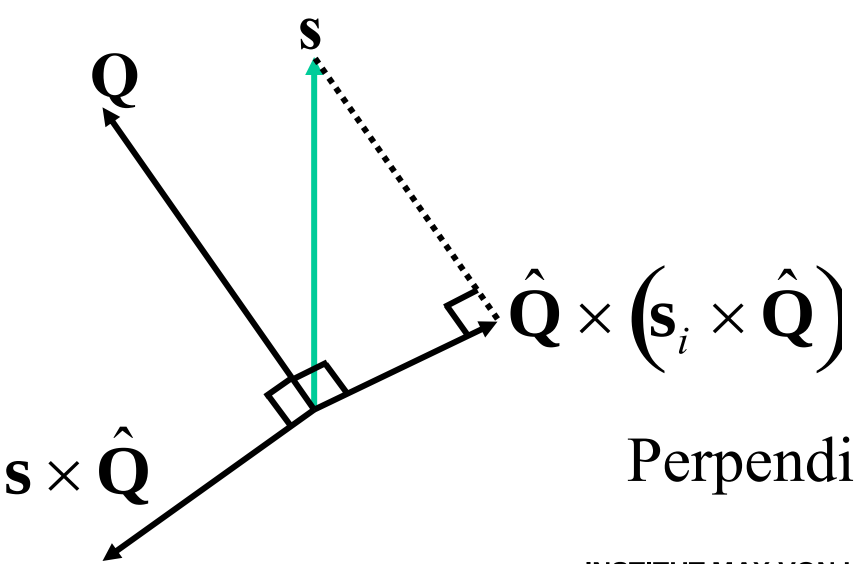
$$\langle \boldsymbol{k}' | \hat{V}_m(\mathbf{r}_i) | \boldsymbol{k} \rangle =$$

Spin:

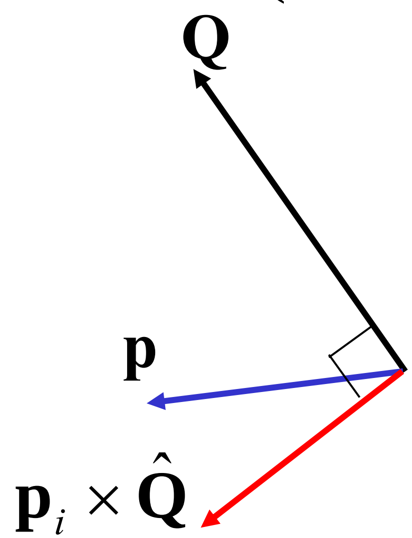
$$4\pi \exp(i\mathbf{Q}\cdot\mathbf{r}_i)\left\{\hat{\mathbf{Q}}\times(\mathbf{s}_i\times\hat{\mathbf{Q}})\right\}$$

Movement / Orbital

$$\frac{4\pi i}{\hbar Q}\exp(i\mathbf{Q}\cdot\mathbf{r}_i)(\mathbf{p}_i\times\hat{\mathbf{Q}})$$



Perpendicular to **Q**



The fundamental rule of neutron magnetic scattering

Neutrons *only ever* see the components of the magnetization that are *perpendicular* to the scattering vector!

The fundamental rule of neutron magnetic scattering

Taking elastic scattering again:

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \left(\frac{m_n}{2\pi\hbar^2}\right)^2 \left|\langle \boldsymbol{k}' | \hat{V}(\mathbf{r}) | \boldsymbol{k} \rangle\right|^2$$

Neutron scattering therefore probes the components of the sample magnetization that are *perpendicular* to the neutron's momentum transfer, **Q**.

$$\int V_m(\mathbf{r}) e^{i\mathbf{Q}\cdot\mathbf{r}} \cdot d\mathbf{r} = \mathbf{M}_\perp(\mathbf{Q})$$

and $$\frac{d\sigma_{magnetic}}{d\Omega} = \langle \mathbf{M}^*_\perp(\mathbf{Q}) \rangle \langle \mathbf{M}_\perp(\mathbf{Q}) \rangle$$

Neutron scattering measures the *correlations* in magnetization, i.e. the influence a magnetic moment has on its neighbours.

It is capable of doing this over all length scales, limited only by wavelength.

Learn your Fourier transforms!

and

Learn and understand the convolution theorem!

$$f(r) \otimes g(r) = \int f(x) g(r-x) \cdot dx$$

$$\Im\big(f(r)\big) = F(q)$$

$$\Im\big(g(r)\big) = G(q)$$

$$\Im\big(f(r) \otimes g(r)\big) = F(q) \times G(q)$$

Elastic scattering

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \left(\frac{m_n}{2\pi\hbar^2}\right)^2 \sum_{\zeta',s'} p_s \left|\langle \boldsymbol{k}', s' | \hat{V}(\mathbf{r}) | \boldsymbol{k}, s \rangle\right|^2$$

$$\propto \underbrace{\int \left|\langle \hat{V} \rangle\right|^2 e^{i\mathbf{Q}\cdot\mathbf{r}} \cdot d\mathbf{r}}_{} + \underbrace{\left(\left|\langle \hat{V}^2 \rangle\right| - \left|\langle \hat{V} \rangle\right|^2\right) \int z(\mathbf{r}) e^{i\mathbf{Q}\cdot\mathbf{r}} \cdot d\mathbf{r}}_{}$$

The contribution from deviations from the average structure: *Short-range* order

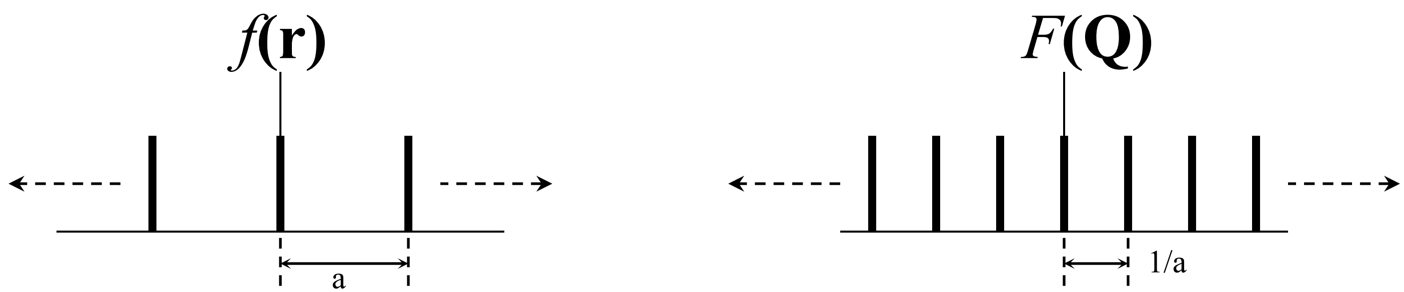
The contribution from the average structure of the sample: *Long-range* order

Magnetic structure determination

Crystalline structures

$$\frac{d\sigma}{d\Omega} \propto \int \left| \left\langle \hat{V} \right\rangle \right|^2 e^{i\mathbf{Q}\cdot\mathbf{r}} \cdot d\mathbf{r}$$

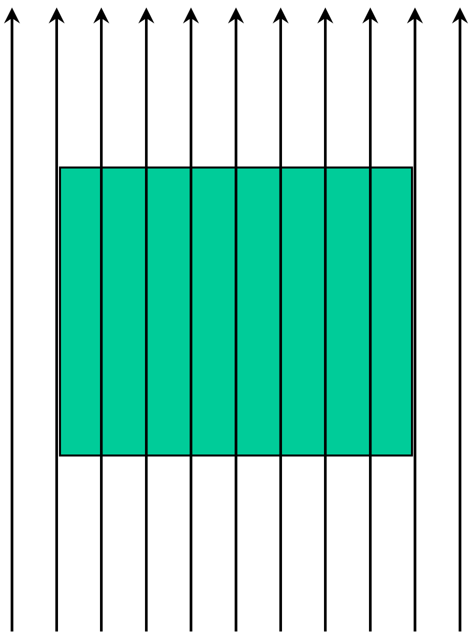
The Fourier transform from a series of delta-functions



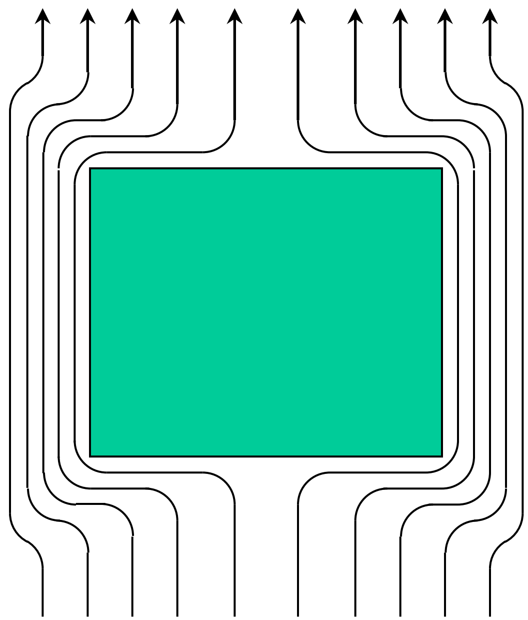
Bragg's Law: $2d\sin\theta=\lambda$

Leads to Magnetic Crystallography

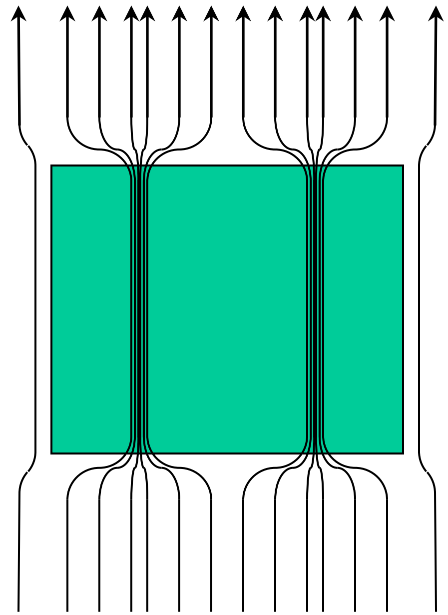
Superconductivity



Normal state



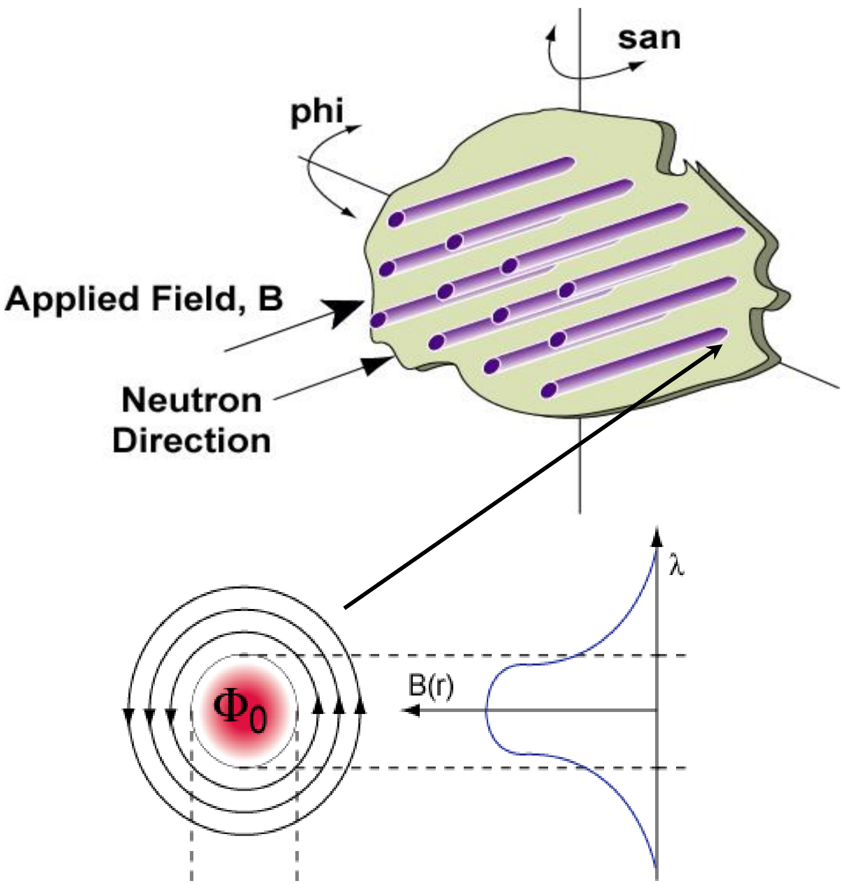
Superconducting state



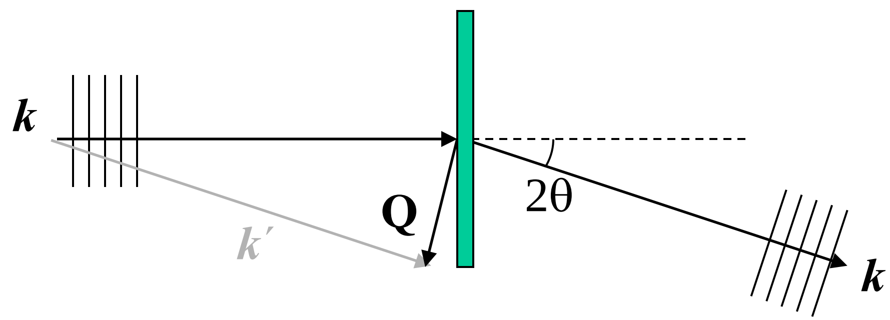
Flux line lattice

A simple example of magnetic elastic scattering

MgB_2 is a superconductor below 39K, and expels all magnetic field lines (Meissner effect). Above a critical field, flux lines penetrate the sample.



Scattering geometry

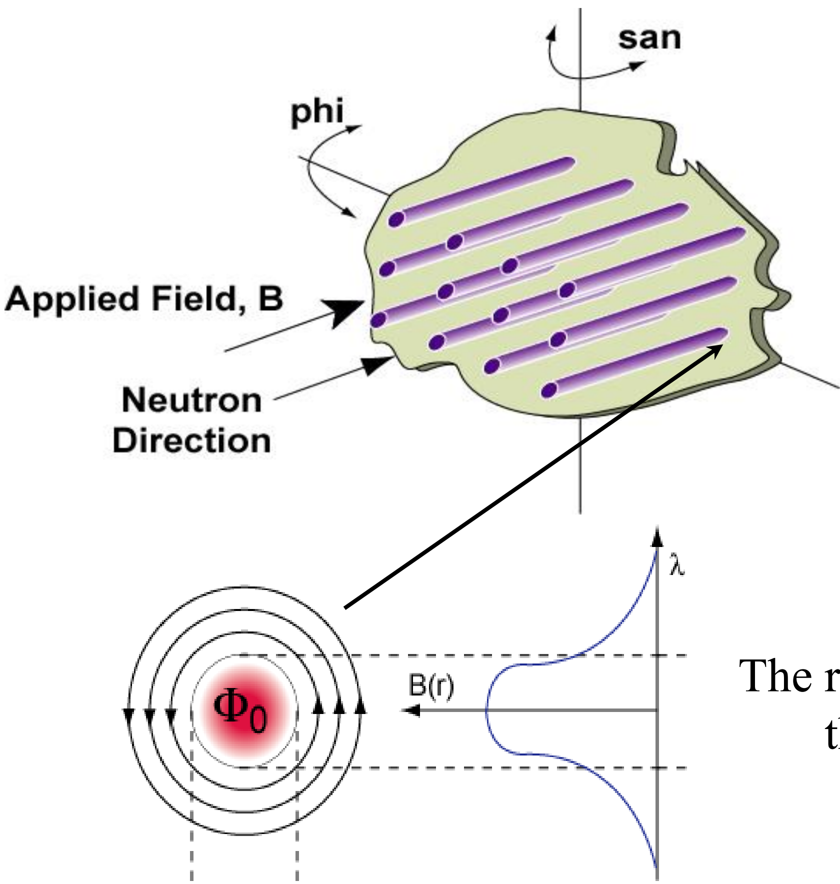


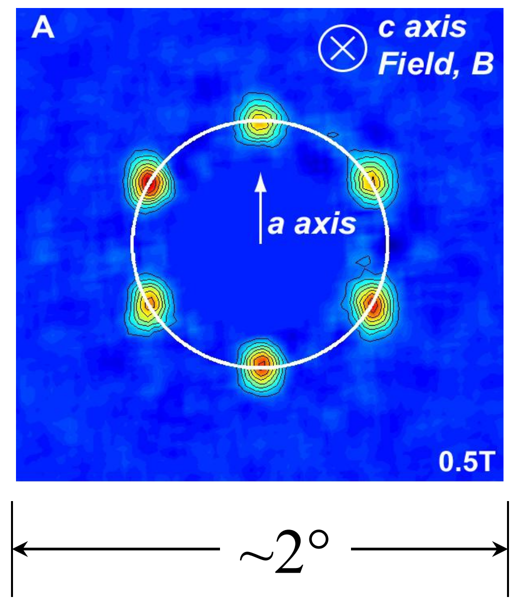
The momentum transfer, **Q**, is roughly perpendicular to the flux lines, therefore all the magnetization is seen.

(recall $\frac{d\sigma_{magnetic}}{d\Omega} = \langle \mathbf{M}^*_\perp(\mathbf{Q})\rangle\langle \mathbf{M}_\perp(\mathbf{Q})\rangle$)

A simple example of magnetic elastic scattering

MgB_2 is a superconductor below 39K, and expels all magnetic field lines (Meissner effect). Above a critical field, flux lines penetrate the sample.





Via Bragg's Law

$$2d\sin\theta = \lambda$$

$$\lambda = 10\ \text{Å}$$

$$d = 425\text{Å}$$

The reciprocal lattice has 60° rotational symmetry, therefore the flux line lattice is hexagonal

Cubitt et. al. Phys. Rev. Lett. **91** 047002 (2003)

Cubitt et. al. Phys. Rev. Lett. **90** 157002 (2003)

Antiferromagnetism in MnO

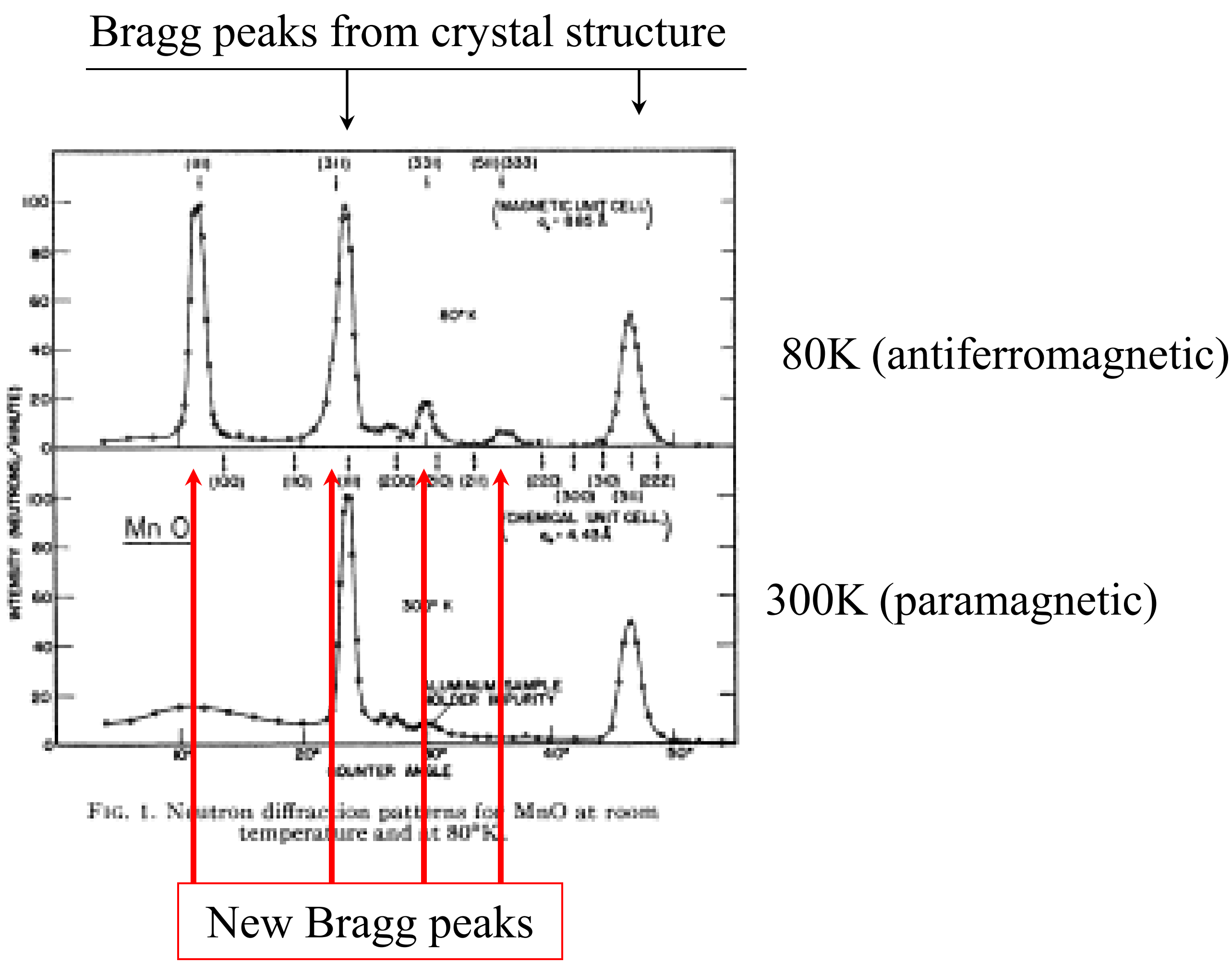


FIG. 1. Neutron diffraction patterns for MnO at room temperature and at 80°K.

C. G. Shull & J. S. Smart, Phys. Rev. **76** (1949) 1256

Antiferromagnetism in MnO

New magnetic Bragg peaks

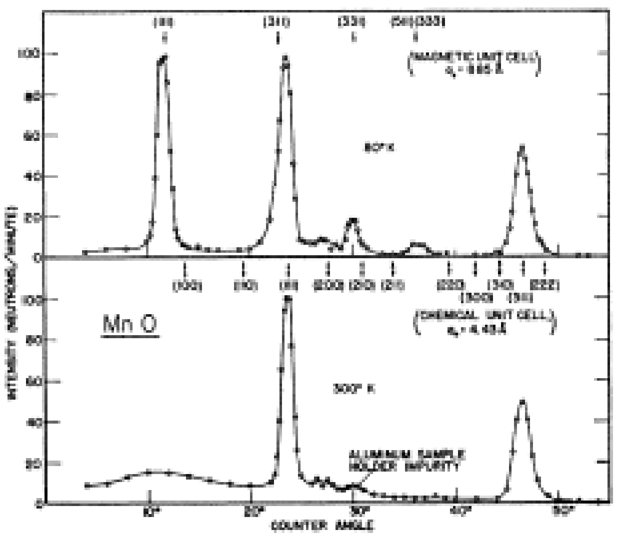
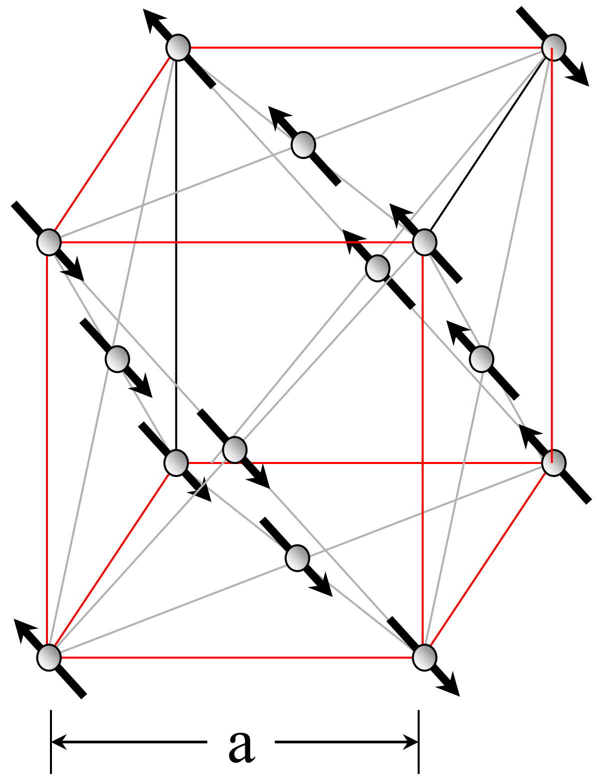


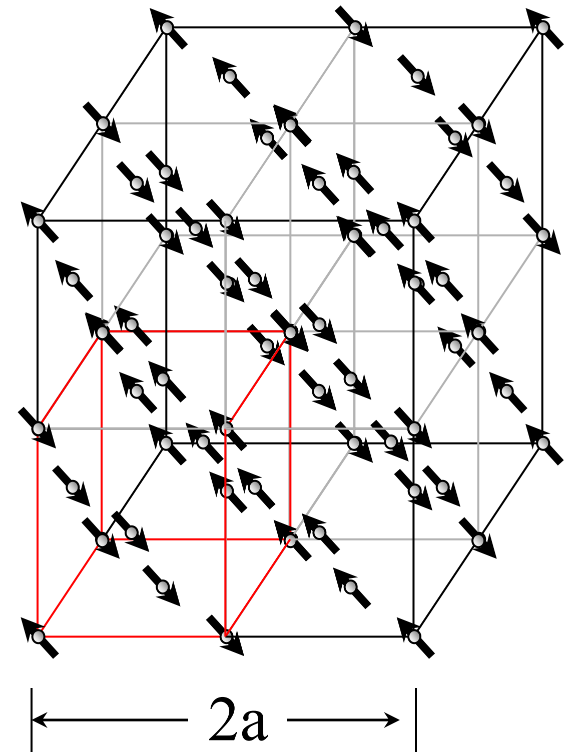
FIG. 1. Neutron diffraction patterns for MnO at room temperature and at 80°K.

C. G. Shull & J. S. Smart, Phys. Rev. **76** (1949) 1256

Magnetic structure



Magnetic unit cell



C. G. Shull *et al.*, Phys. Rev. **83** (1951) 333

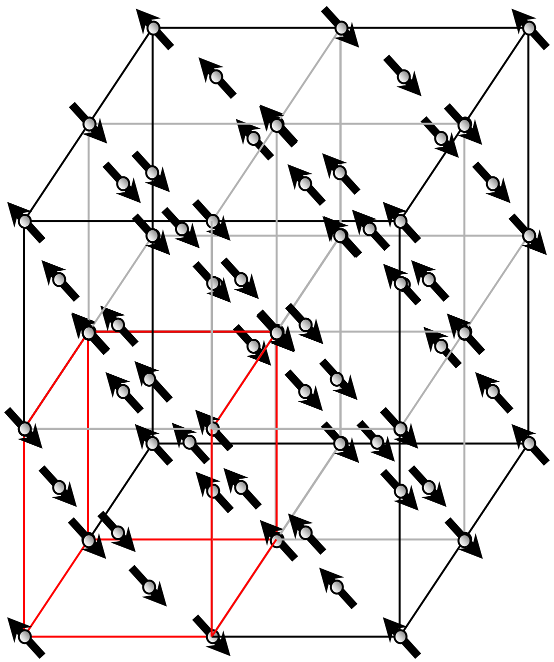
H. Shaked *et al.*, Phys. Rev. B **38** (1988) 11901

Antiferromagnetism in MnO

The moments are said to lie in the (111) plane

H. Shaked *et al*., Phys. Rev. B **38** (1988) 11901

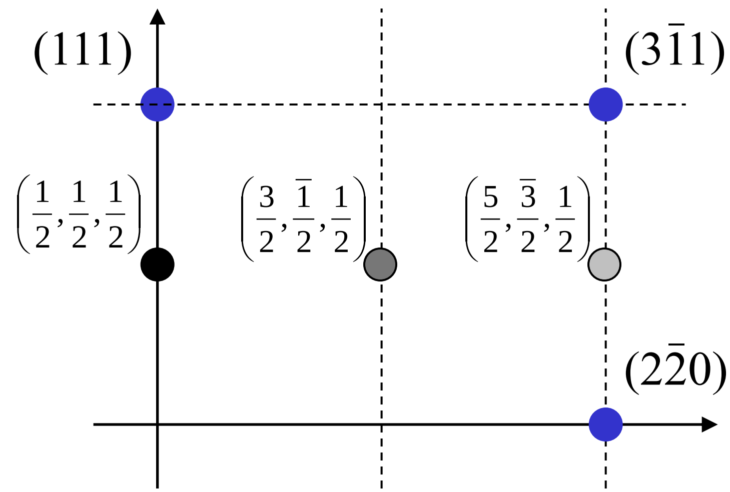
Real space



fcc lattice

(i.e. *h,k,l*) all even or all odd

Reciprocal space

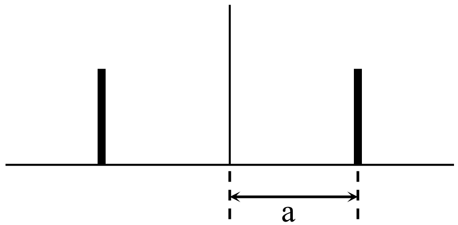


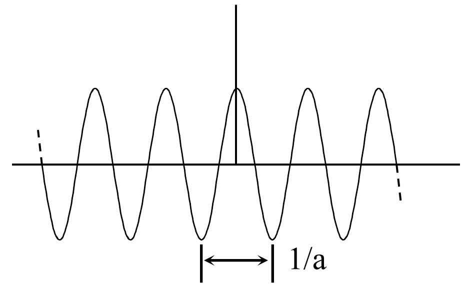
Moment direction

Antiferromagnetism in Chromium

The Fourier Transform for two Delta functions:

$F(\mathbf{Q})$ | $f(\mathbf{r})$

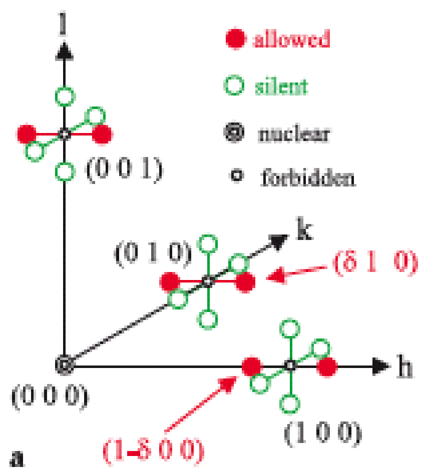


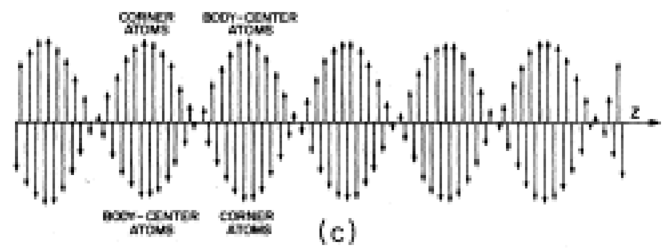


E.Fawcett, Rev. Mod. Phys. **60** (1988) 209

Chromium is an example of an *itinerant* antiferromagnet

Reciprocal space | Real space



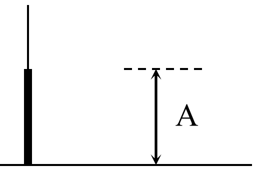


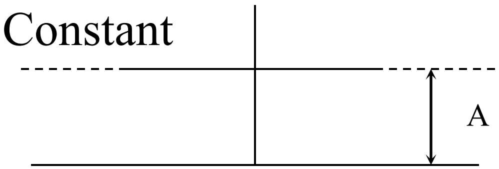
a Spin Density wave

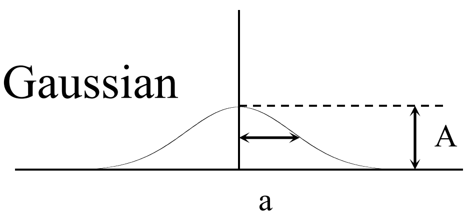
The physical meaning of $z(\mathbf{r})$

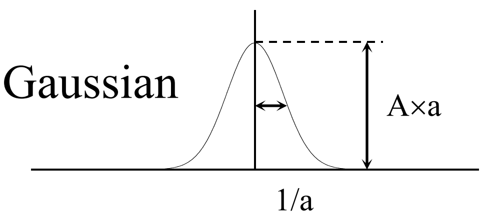
Given an atom at position $\mathbf{r}_1$,
what's the probability of finding a similar atom at position $\mathbf{r}_2$?

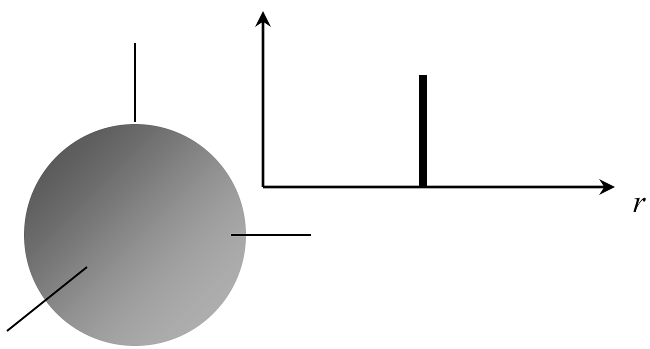
	$z(\mathbf{r})$, real space	$Z(\mathbf{Q})$, reciprocal space
Zero probability?	Delta function	Constant
Gaussian probability?	Gaussian	Gaussian
Any spherically symmetric function? e.g. a hollow sphere	Delta function at r ≠ 0	$\sin(Qr)/Qr$

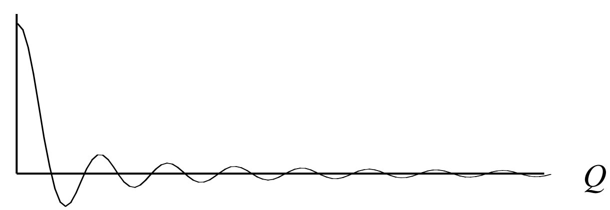






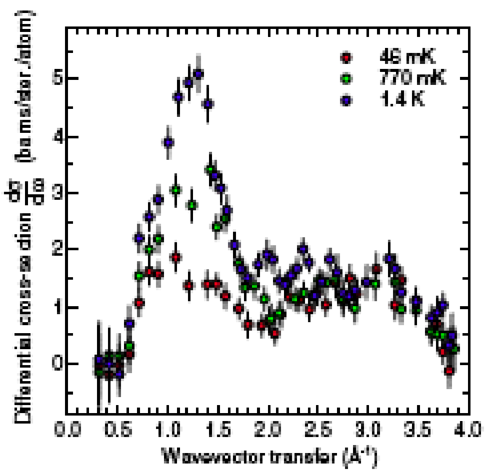




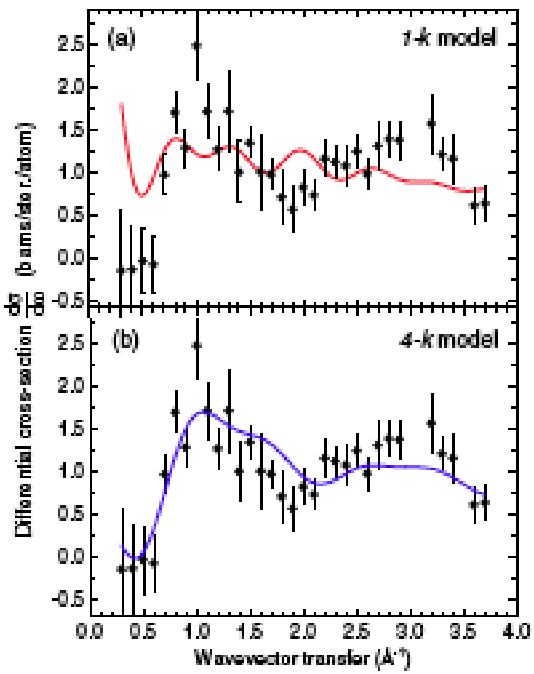


Diffuse scattering from magnetic frustration, $Gd_2Ti_2O_7$

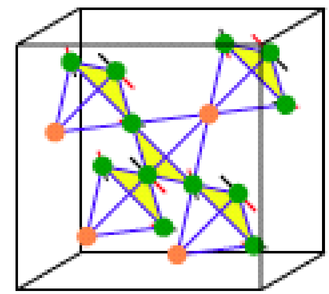
$$\frac{d\sigma}{d\Omega} \propto \sum \langle \mathbf{S}_o \mathbf{S}_r \rangle \frac{\sin(Qr)}{Qr}$$



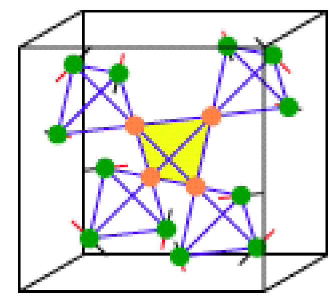
magnetic scattering



magnetic scattering at 46mK
with fits



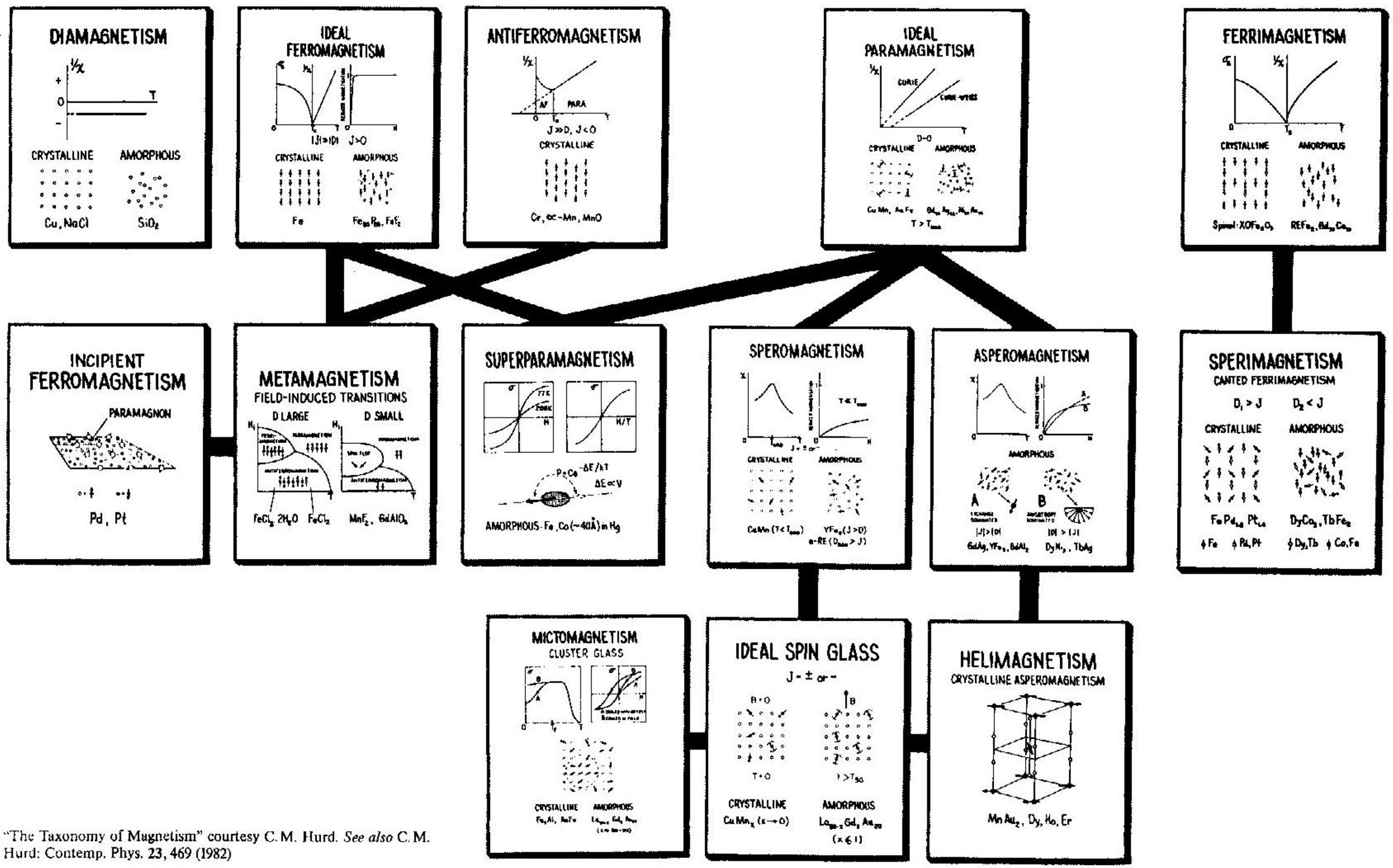
Structure model 1



Structure model 2

J. R. Stewart *et al.*, J. Phys.: Condens. Matter **16** (2004) L321

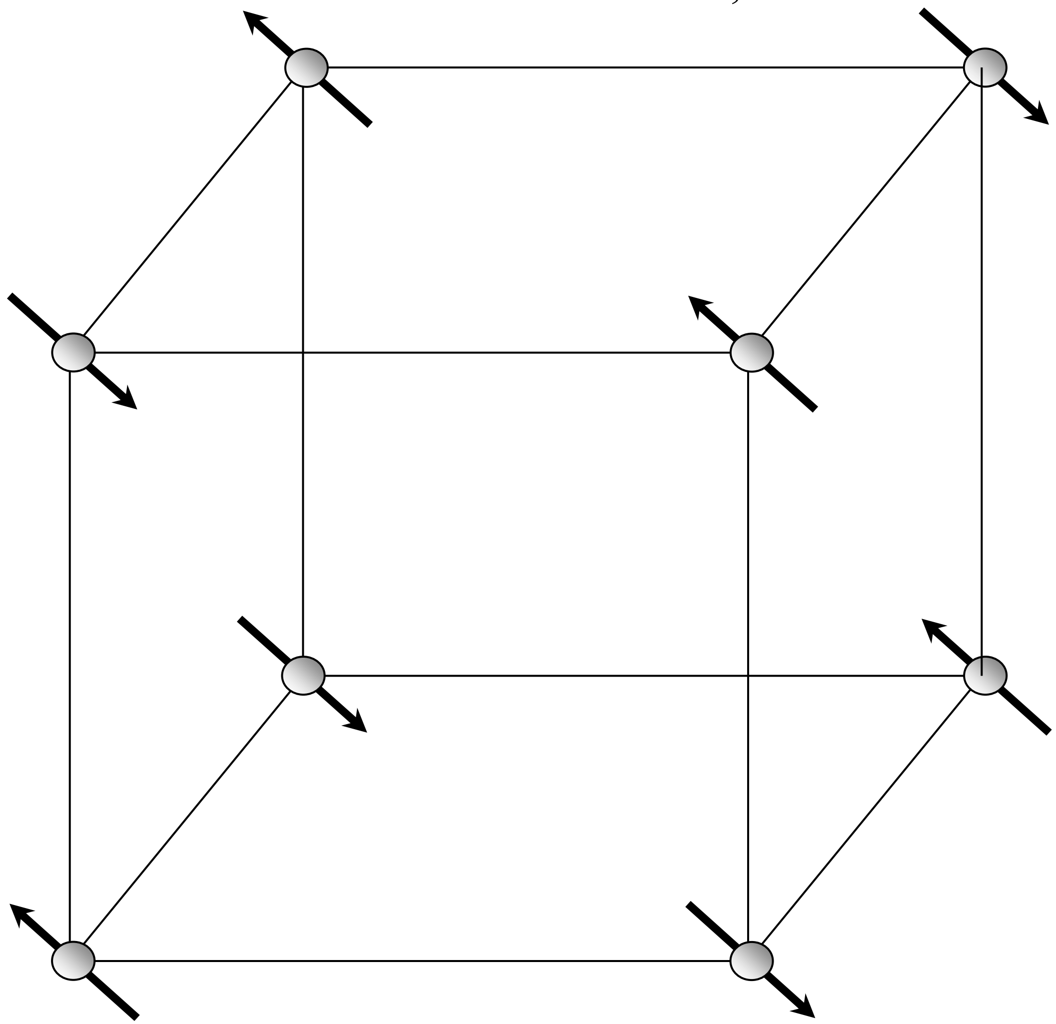
The ‘Family Tree’ of Magnetism



"The Taxonomy of Magnetism" courtesy C.M. Hurd. *See also* C.M. Hurd: Contemp. Phys. **23**, 469 (1982)

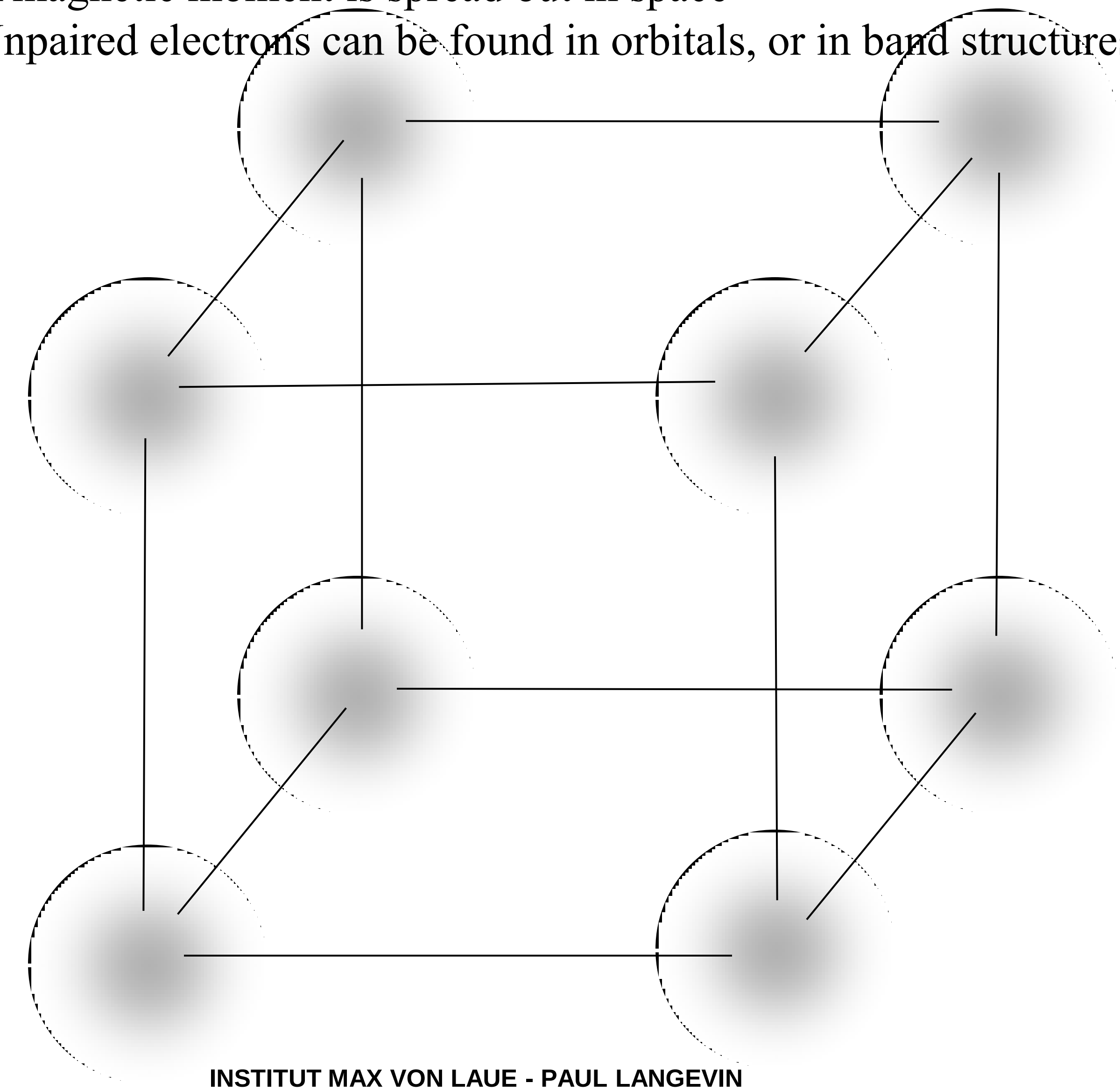
Magnetic form factors

A magnetic moment is spread out in space
Unpaired electrons can be found in orbitals, or in band structures



A magnetic moment is spread out in space

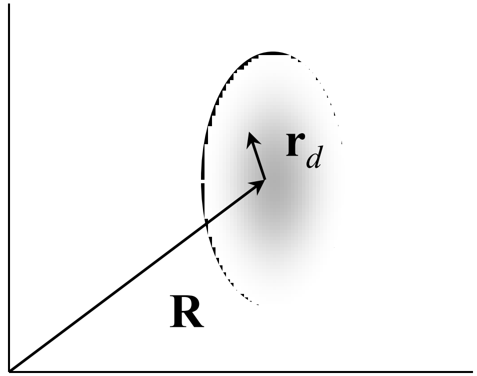
Unpaired electrons can be found in orbitals, or in band structures



Magnetic form factors

A magnetic moment is spread out in space
Unpaired electrons can be found in orbitals, or in band structures

e.g.
Take a magnetic ion with total spin **S** at position **R**
The (normalized) density of the spin is $s_d(\mathbf{r})$
around the equilibrium position



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

$$\propto \int s_d e^{i\mathbf{Q}\cdot\mathbf{r}_d} \cdot d\mathbf{r}_d \int S(\mathbf{R}) e^{i\mathbf{Q}\cdot\mathbf{R}} \cdot d\mathbf{R}$$

$$= f(Q) \int S(\mathbf{R}) e^{i\mathbf{Q}\cdot\mathbf{R}} \cdot d\mathbf{R}$$

$$f(Q) = \int s_d e^{i\mathbf{Q}\cdot\mathbf{r}_d} \cdot d\mathbf{r}_d$$

$f(Q)$ is the *magnetic form factor*
It arises from the *spatial distribution* of *unpaired electrons* around a magnetic atom

Magnetic form factors

f(*Q*) is the *magnetic form factor*
It arises from the *spatial distribution* of *unpaired electrons* around a magnetic atom

$$\frac{d\sigma_{magnetic}}{d\Omega} = \left\langle \mathbf{M}_{\perp}^{*}(\mathbf{Q}) \right\rangle \left\langle \mathbf{M}_{\perp}(\mathbf{Q}) \right\rangle$$
$$\propto f^{2}(Q) \int S_{\perp}(\mathbf{R}_i) S_{\perp}^{*}(\mathbf{R}_j) e^{i\mathbf{Q}\cdot(\mathbf{R}_i - \mathbf{R}_j)} \cdot d\mathbf{R}$$

There is no form factor for nuclear scattering, as the nucleus can be considered as a point compared to the neutron wavelength

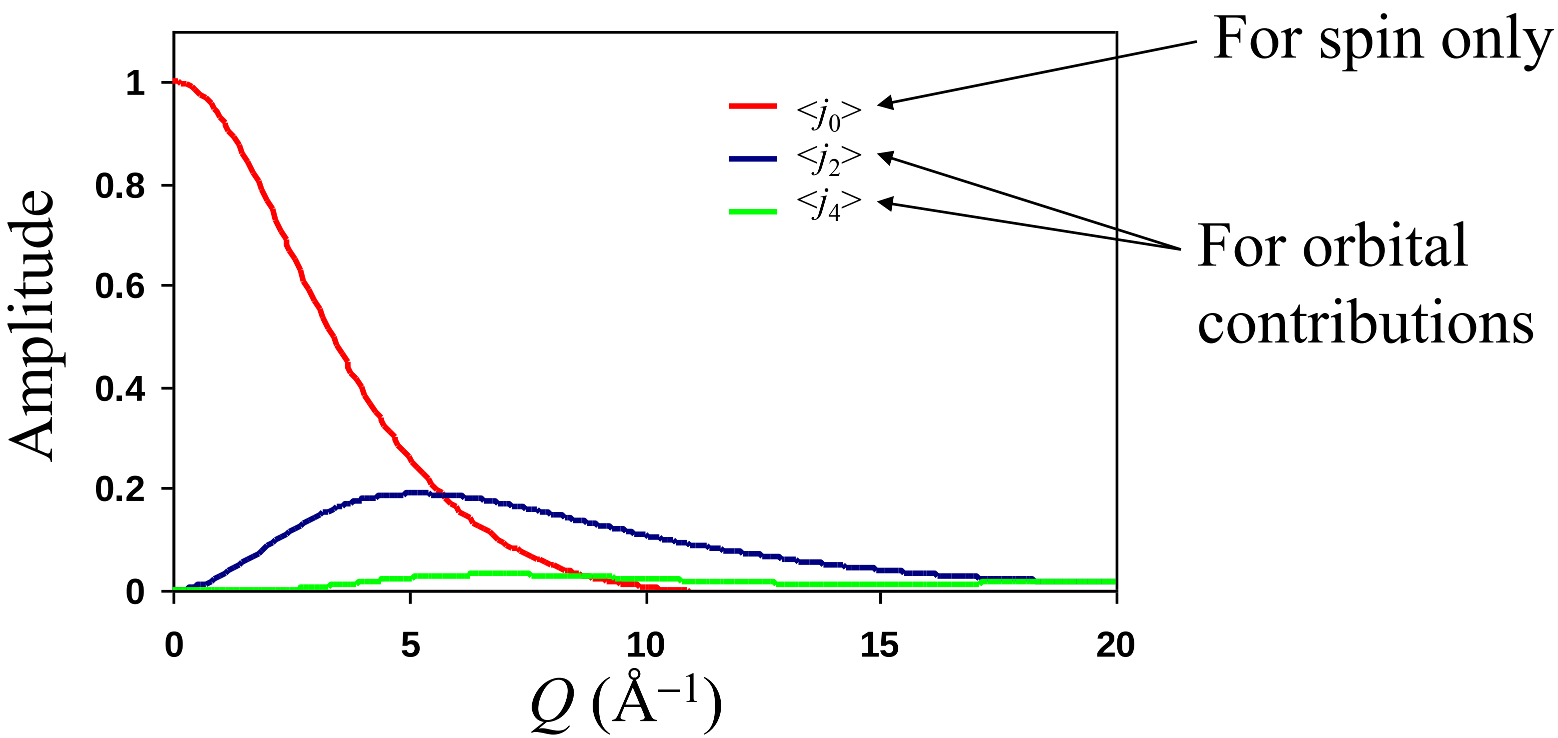
Magnetic form factors

Approximations for the form factors are tabulated

(P. J. Brown, International Tables of Crystallography, Volume C, section 4.4.5)

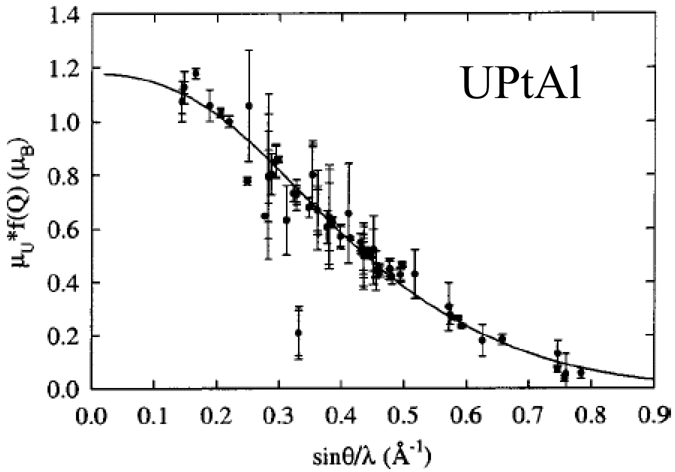
$$f(Q) = C_1\langle j_0(Q/4\pi)\rangle + C_2\langle j_2(Q/4\pi)\rangle + C_4\langle j_4(Q/4\pi)\rangle + \dots$$

Form factors for iron



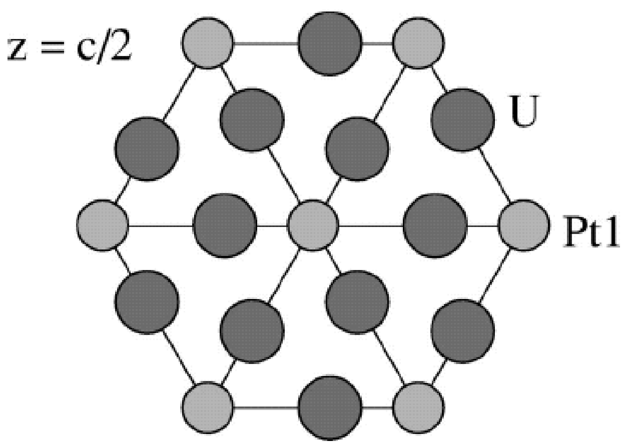
Magnetic electron density

$$f(Q) = \int s_d e^{i\mathbf{Q}\cdot\mathbf{r}_d} \cdot d\mathbf{r}_d$$

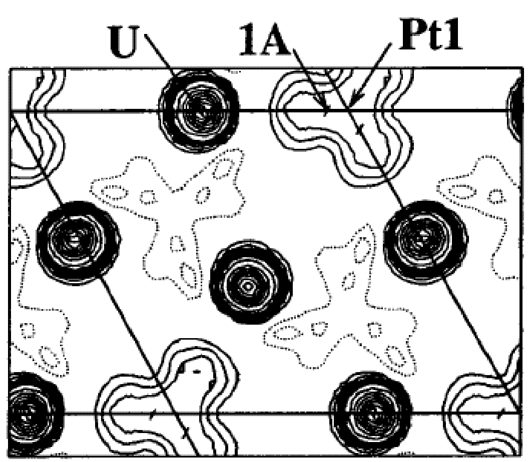


P. Javorsky *et al*., Phys. Rev. B **67** (2003) 224429

From the form factors, the magnetic moment density in the unit cell can be derived



crystal structure



magnetic moment density

NEUTRONS FOR SCIENCE

Magnetic electron density

Nickel

H. A. Mook., Phys. Rev. **148** (1966) 495

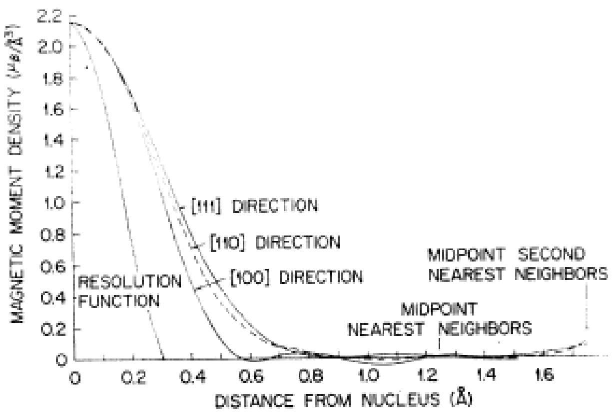


FIG. 1. Distribution of magnetic moment density along the three major crystallographic directions.

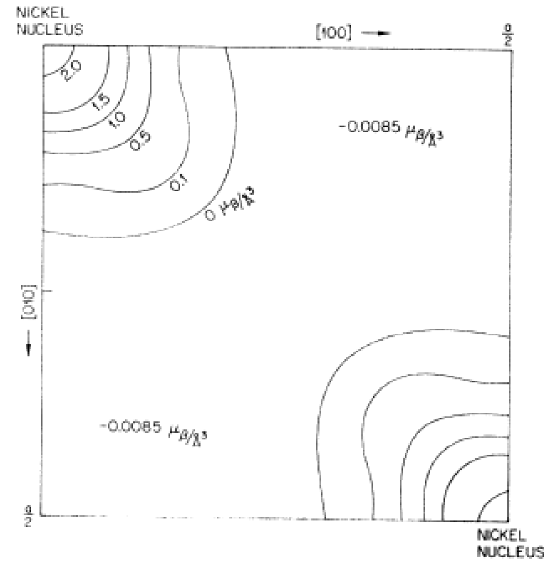


FIG. 4. The magnetic moment distribution in the [100] plane.

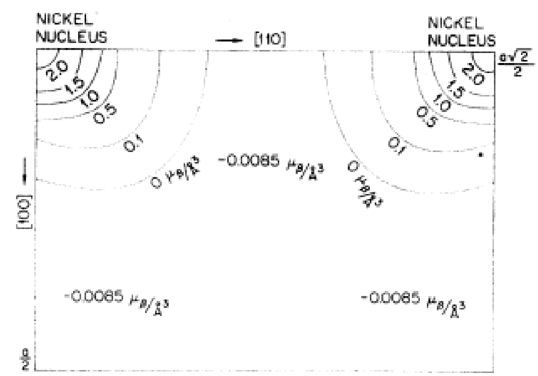


FIG. 5. The magnetic moment distribution in the [110] plane.

Neutron inelastic scattering

Magnetic fluctuations are governed by a wave equation:

$$H\psi=E\ \psi$$

The Hamiltonian is given by the physics of the material.

Given a Hamiltonian, *H*, the energies *E* can be calculated.
(this is sometimes very difficult)

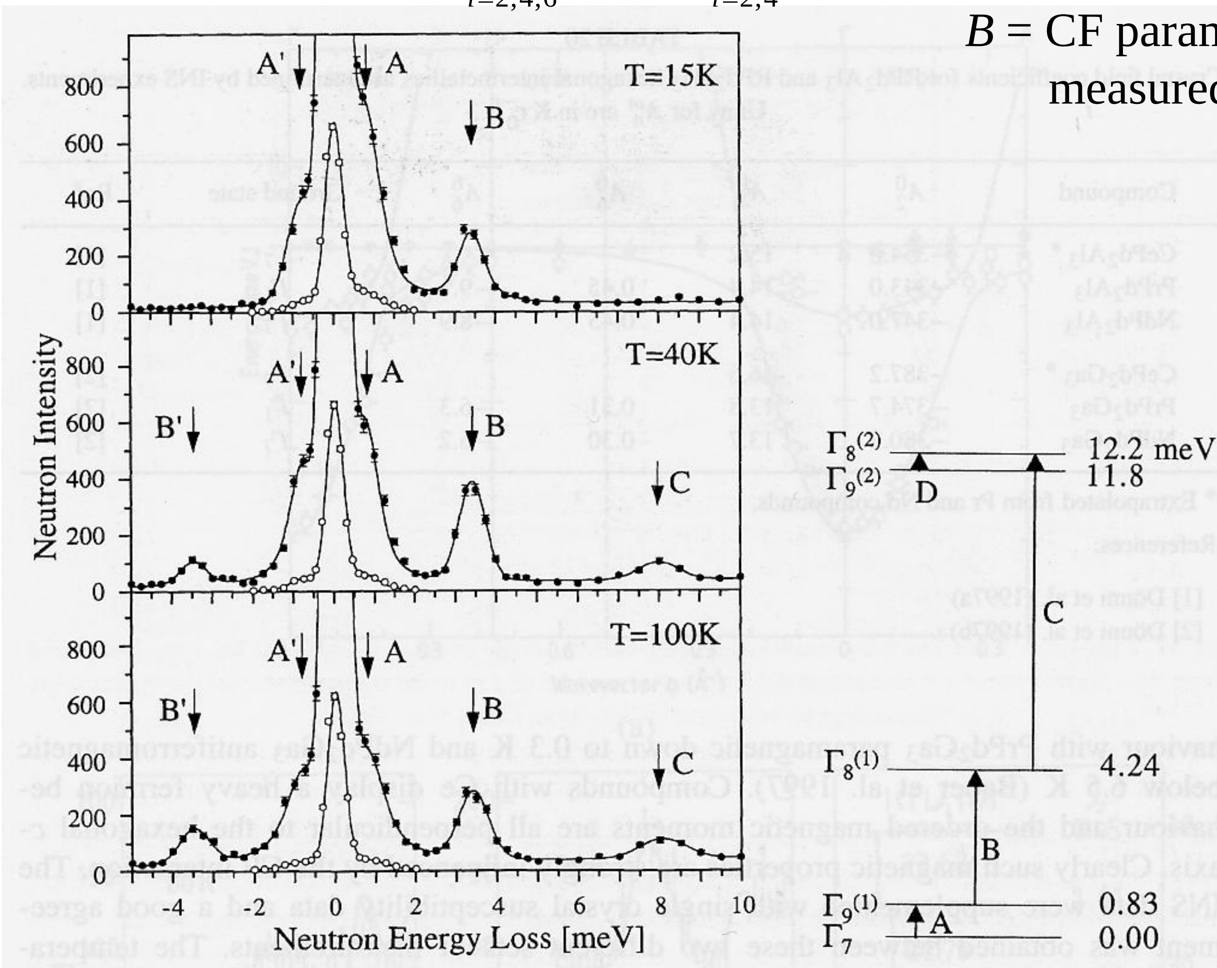
Neutrons measure the energy, *E*, of the magnetic fluctuations, therefore probing the free parameters in the Hamiltonian.

Crystal fields in $NdPd_2Al_3$

$$H = \sum_{l=2,4,6} B_l^0 O_l^0 + \sum_{l=2,4} B_l^4 O_l^4$$

O = Stevens parameters
(K. W. Stevens, Proc. Phys. Soc A**65** (1952) 209)

B = CF parameters, measured by neutrons

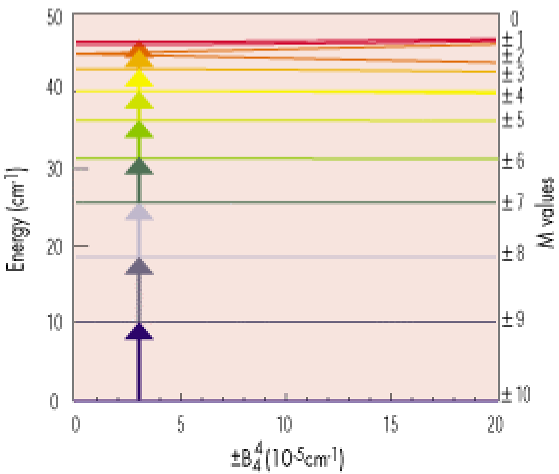


A. Döni *et al.*, J. Phys.: Condens. Matter **9** (1997) 5921

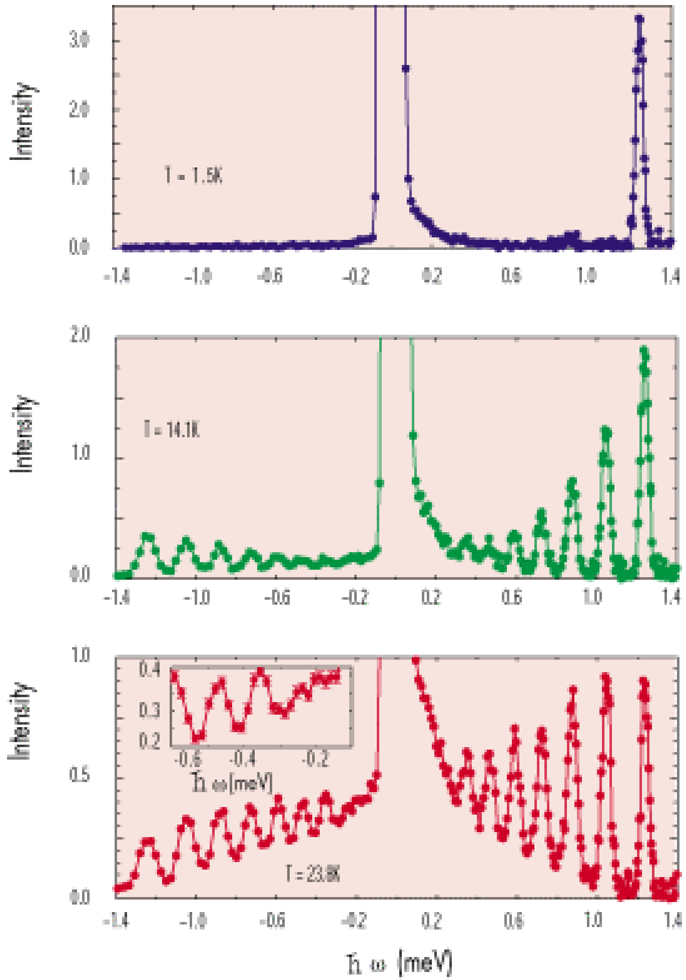
O. Moze., *Handbook of magnetic materials* vol. 11, 1998 Elsevier, Amsterdam, p.493

Quantum tunneling in Mn_{12}-acetate

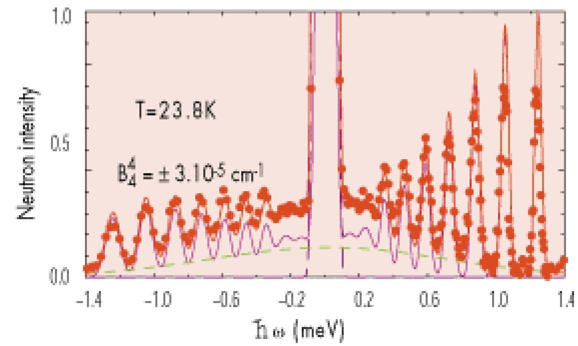
$$H = \sum_{l=2,4,6} B_l^0 O_l^0 + \sum_{l=2,4} B_l^4 O_l^4$$



Calculated energy terms



Neutron spectra



Fitted data with scattering from:

- energy levels
- elastic scattering
- incoherent background

I. Mirebeau *et al.*, Phys. Rev. Lett. **83** (1999) 628

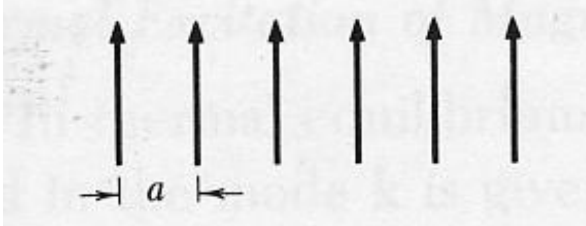
Spin waves and magnons

A simple Hamiltonian for spin waves is:

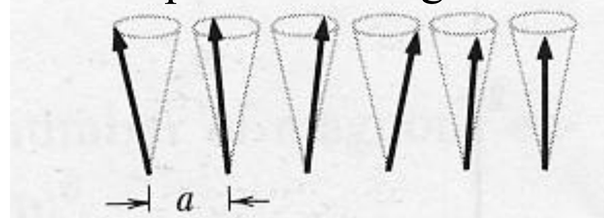
$$H = -J\sum_{i,j} \mathbf{s}_i \mathbf{s}_j$$

J is the magnetic exchange integral, which can be measured with neutrons.

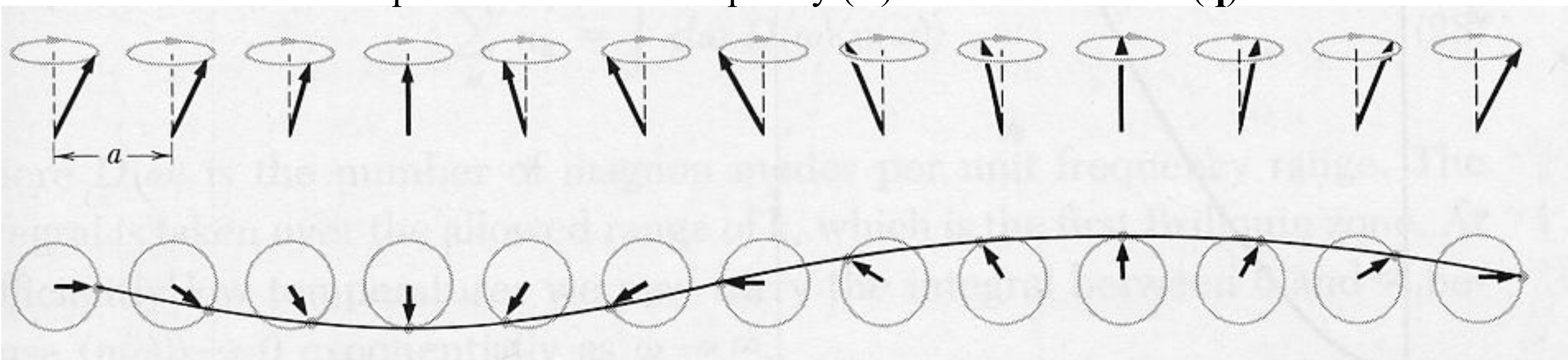
Take a simple ferromagnet:



The spin waves might look like this:

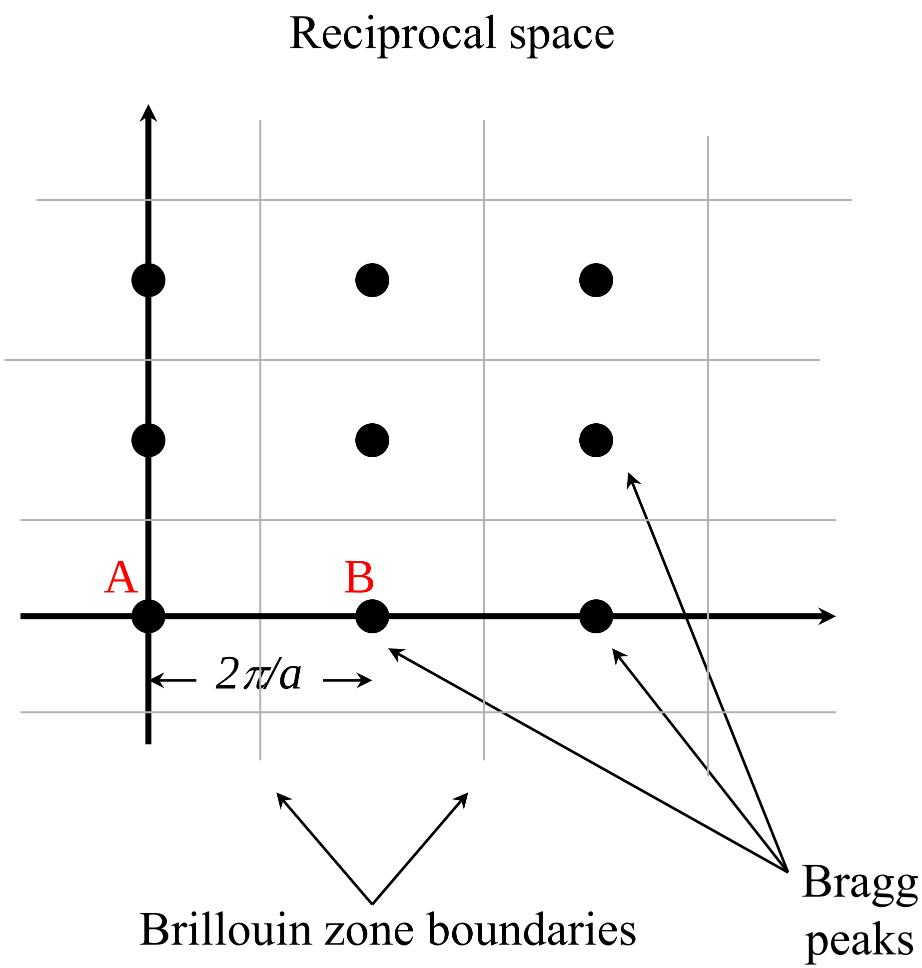


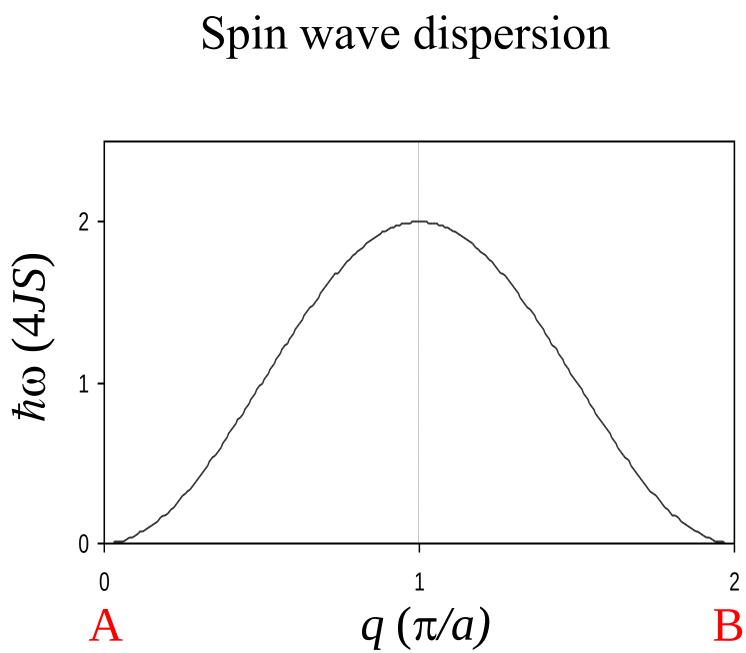
Spin waves have a frequency (ω) and a wavevector (**q**)



The frequency and wavevector of the waves are *directly measurable* with neutrons

Magnons and reciprocal space





$$\hbar\omega = 4JS(1-\cos qa)$$

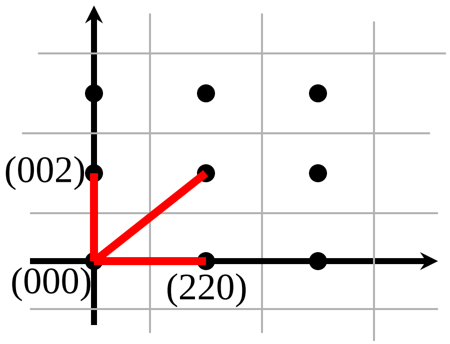
$$= Dq^2 \quad (\text{for } qa << 1)$$

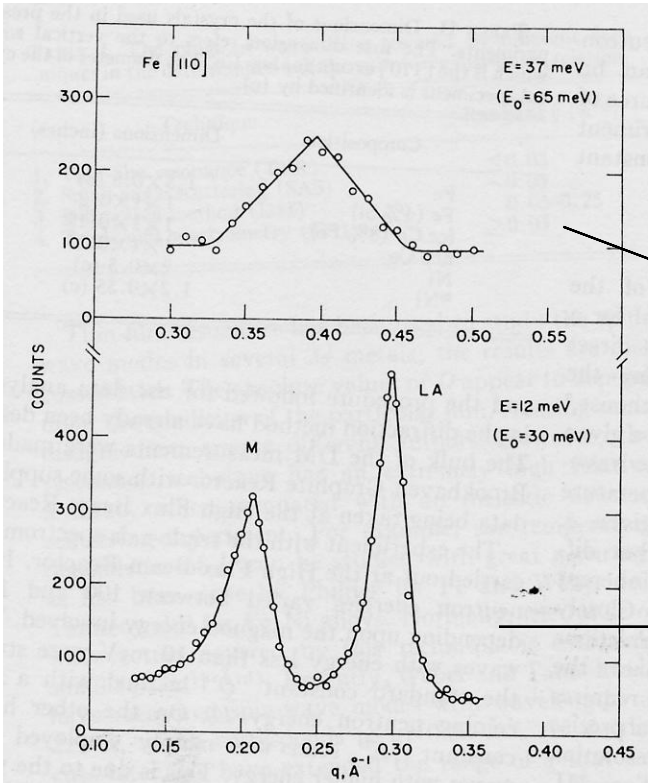
$$D = 2JSa^2$$

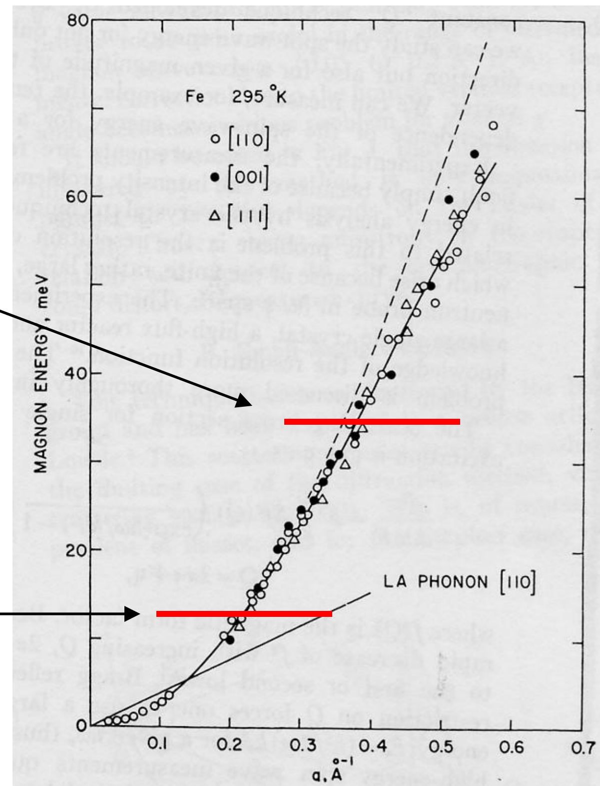
C. Kittel, *Introduction to Solid State Physics*, 1996, Wiley, New York

F. Keffer, *Handbuch der Physik* vol 18II, 1966 Springer-Verlag, Berlin

Magnons in crystalline iron



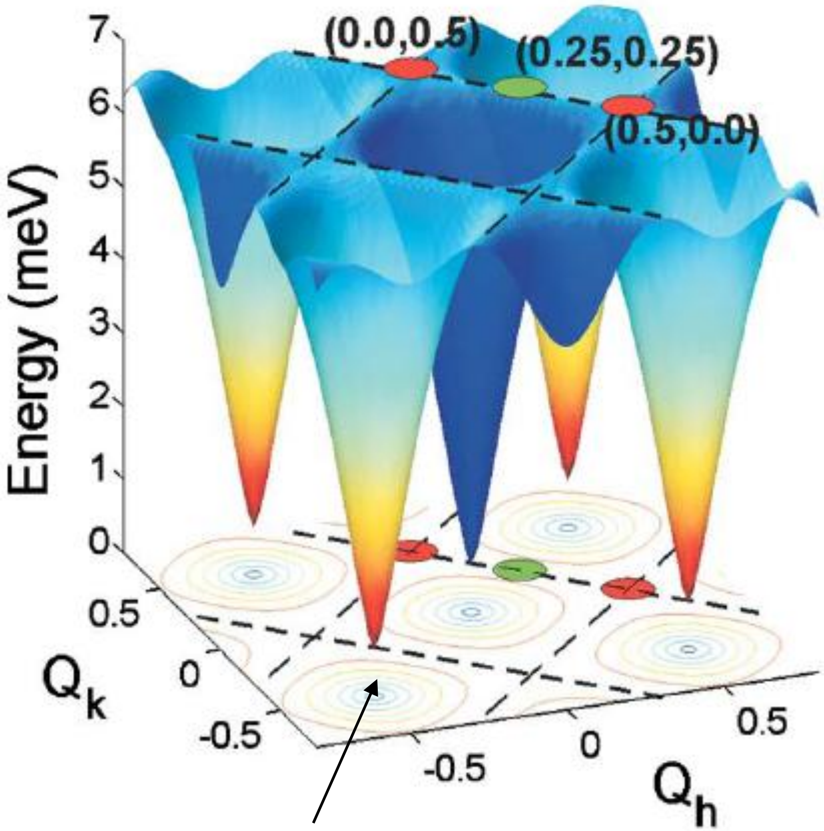


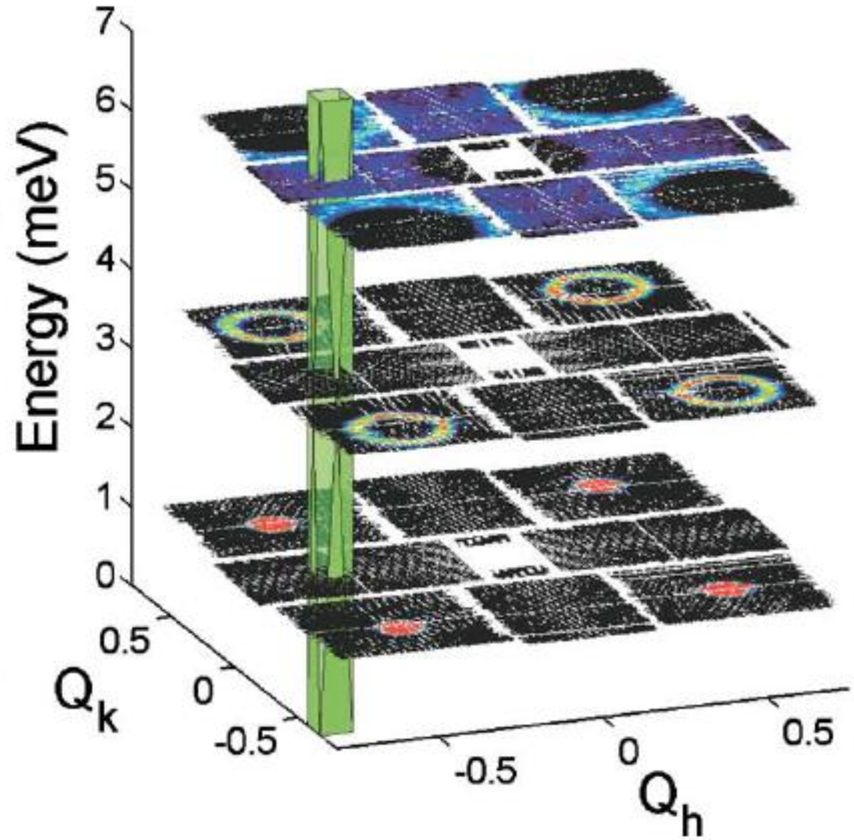


G. Shirane *et al*., J. Appl. Phys. **39** (1968) 383

Spin-waves in Rb_2MnF_4

A quasi-two dimensional antiferromagnetic system

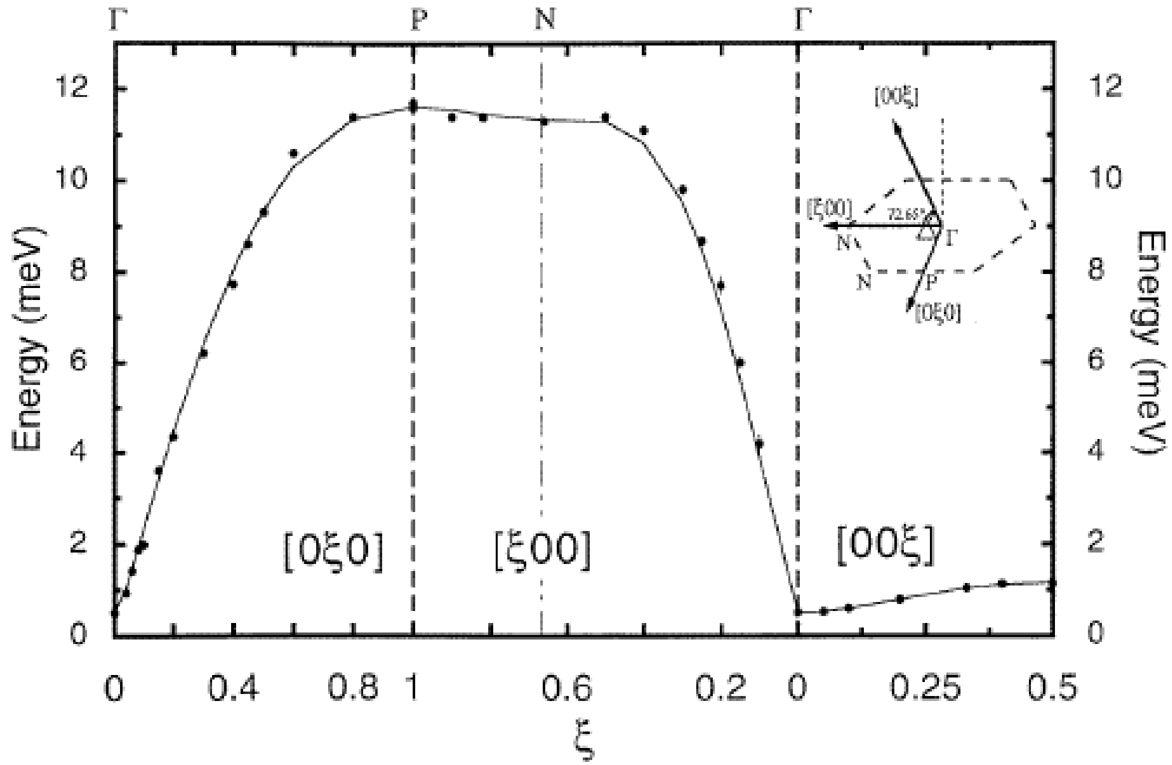




Gap in dispersion due to magnetic anisotropy

T. Huberman *et al*., Phys. Rev. B **72** (2005) 014413

Spin-waves in $MnPS_3$



A. R. Wildes *et al.*, JPCM **10** (1998) 6417

Other magnetic Hamiltonians

Model magnetic systems (one, two and three dimensions)
Superconductivity
Giant and colossal magnetoresistance
Quantum magnetic fluctuations
Heavy fermion materials
Overdamped excitations in amorphous materials
Multiple magnon scattering
Slow relaxation in spin glasses
Fluctuations in Fractals and percolation theory
etc. etc. etc.

Conclusions:

- Neutrons only ever see the components of the magnetization,**M**, that are *perpendicular* to the scattering vector, **Q**
- Magnetization is distributed in space, therefore the magnetic scattering has a *form factor*