NEUTRONS FOR SCIENCE

Neutron Magnetic Scattering

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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
- Generalized susceptibility
- Inelastic scattering
  - Crystal fields and molecular magnets
  - Magnons
  - Spin wave continua
- Critical scattering
- Short-ranged order

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:

$$-\gamma\mu_{\mathrm{N}}\hat{\boldsymbol{\sigma}}$$

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!

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

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

NEUTRONS FOR SCIENCE

Elastic scattering

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

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

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

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

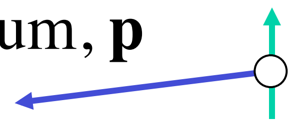
Momentum transfer $\mathbf{Q} = \boldsymbol{k} - \boldsymbol{k}'$

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*.

Learn about Fourier transforms!

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.



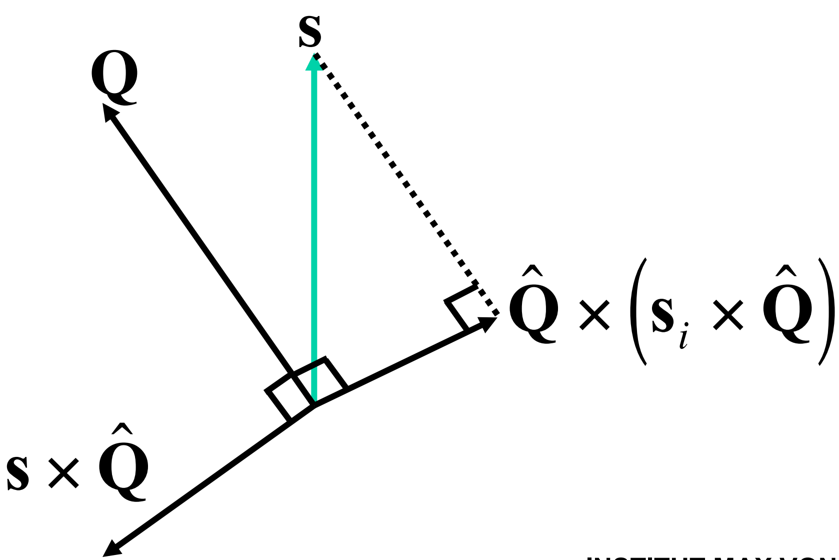
$$\langle \boldsymbol{k}' | \hat{V}_m(\mathbf{r}_i) | \boldsymbol{k} \rangle =$$

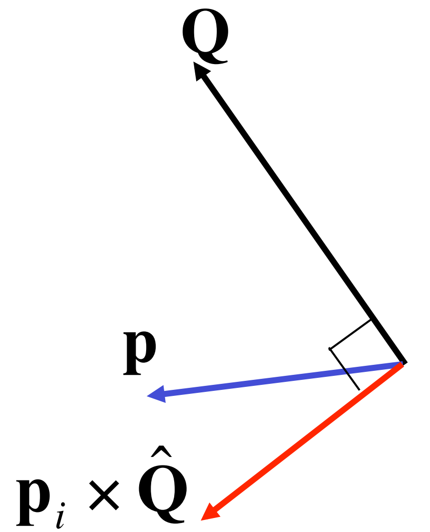
Spin:

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

Movement / Orbital

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





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:

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

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

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

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!

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

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

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

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

Fourier Transforms $F(\mathbf{Q}) = \int f(\mathbf{r}) e^{i\mathbf{Q}\cdot\mathbf{r}} \cdot d\mathbf{r}$

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

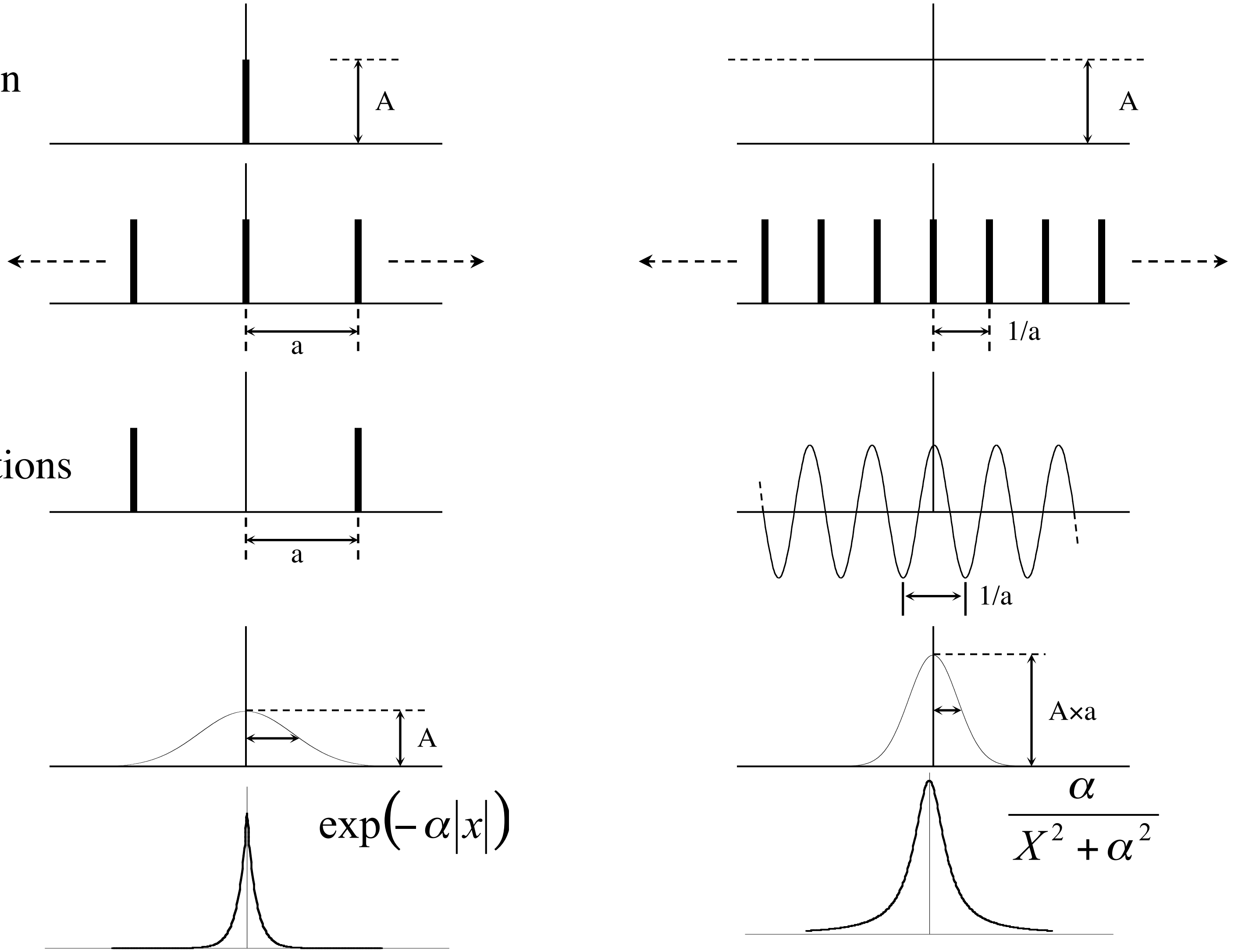
A Delta function

A series of Delta functions

Two Delta functions

A Gaussian

An exponential



Elastic scattering

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

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

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

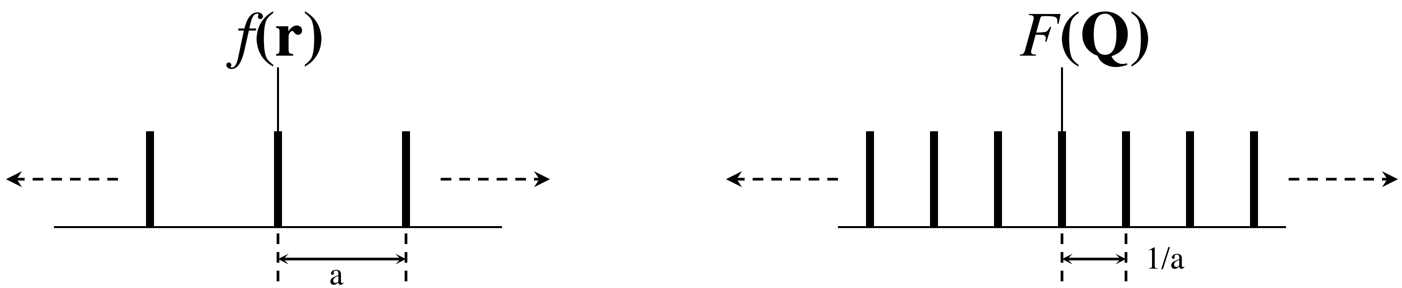
The contribution from the average structure of the sample: *Long-range* order

Magnetic structure determination

Crystalline structures

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

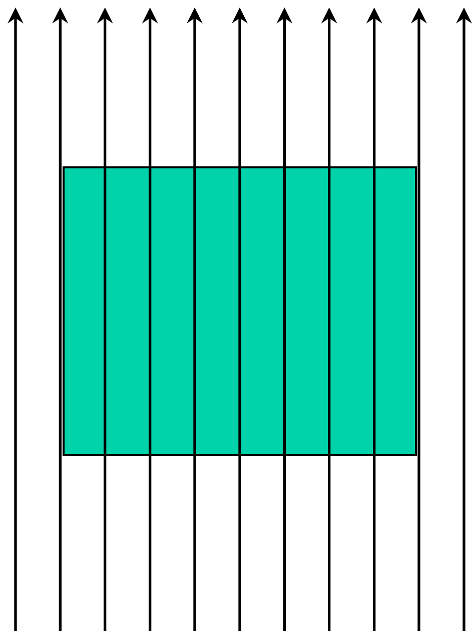
The Fourier transform from a series of delta-functions



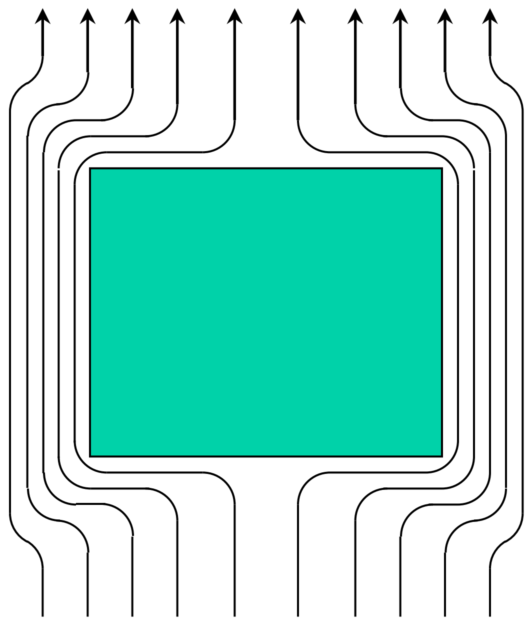
Bragg's Law: $2d\sin\theta = \lambda$

Leads to Magnetic Crystallography

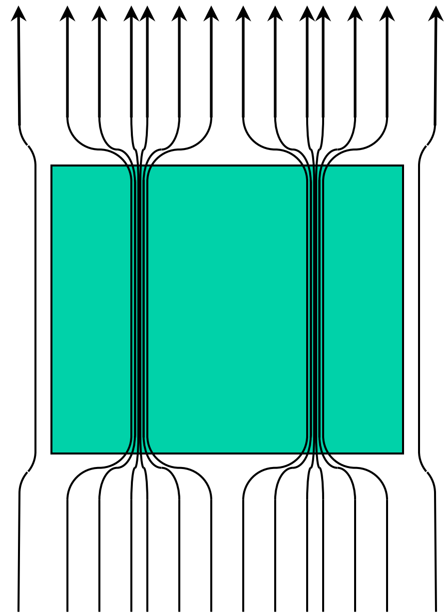
Superconductivity



Normal state



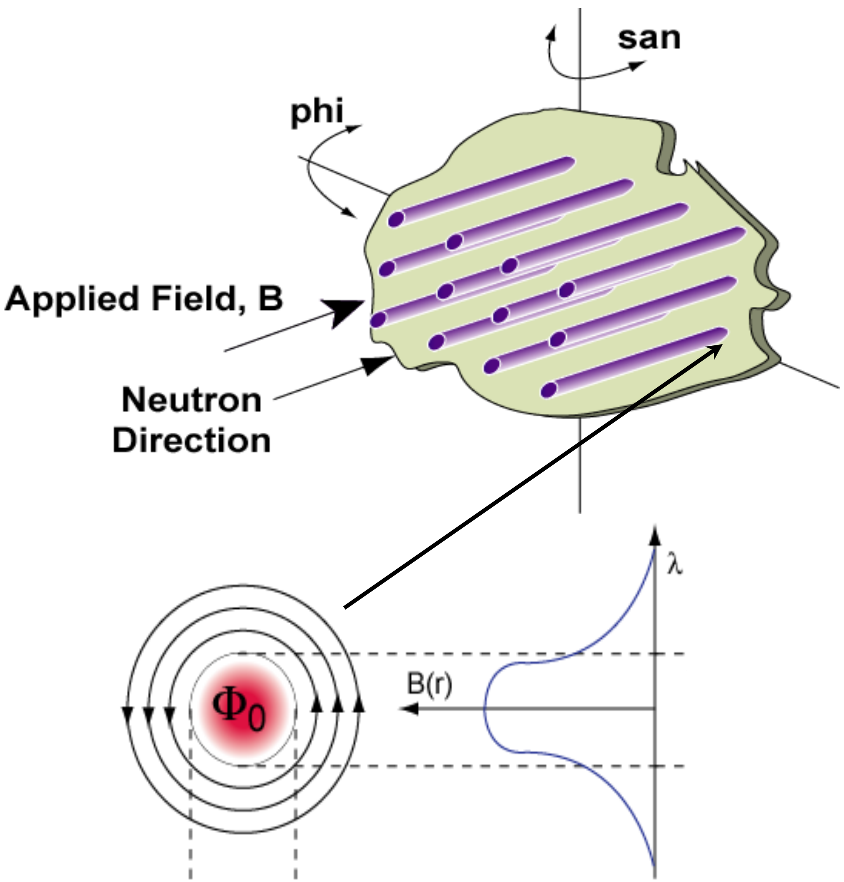
Superconducting state



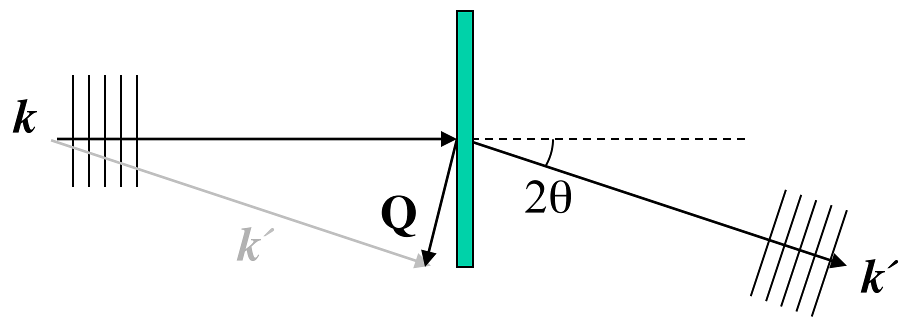
Flux line lattice

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

A simple example of magnetic elastic scattering

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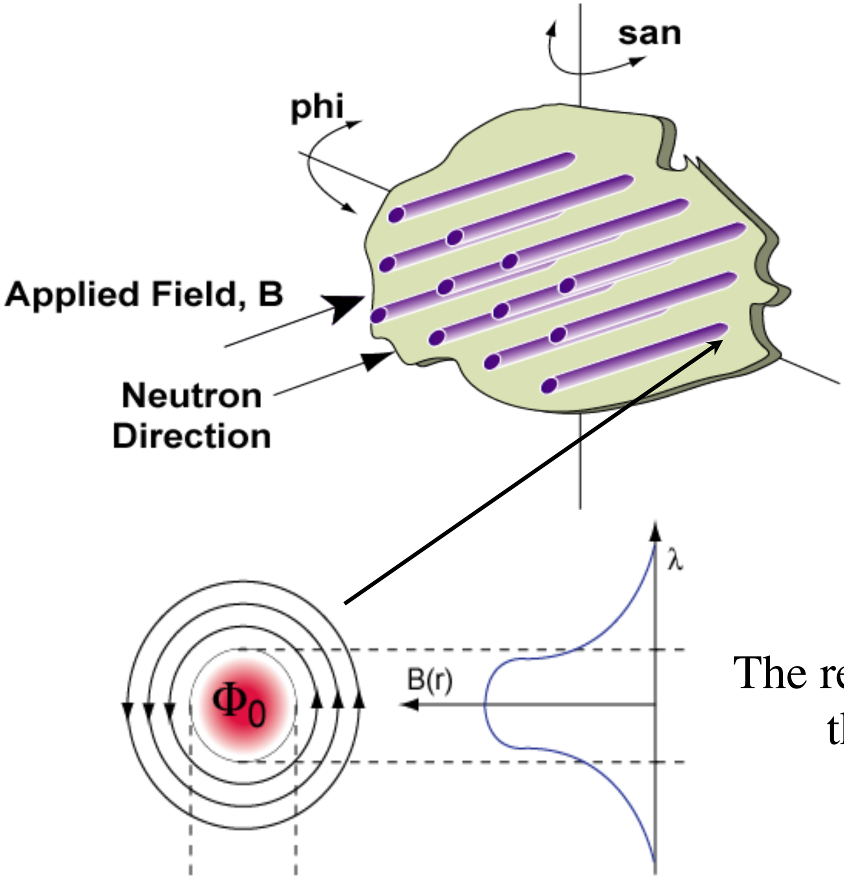
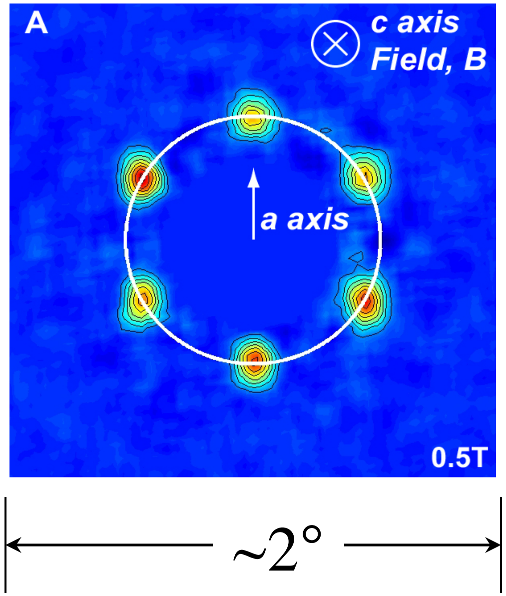




Via Bragg's Law
$2d\sin\theta=\lambda$
$\lambda = 10$ Å
$d = 425$Å

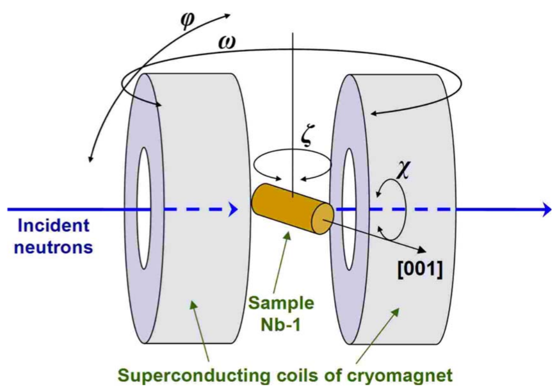
The reciprocal lattice has 60° rotational symmetry, therefore the flux line lattice is hexagonal

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

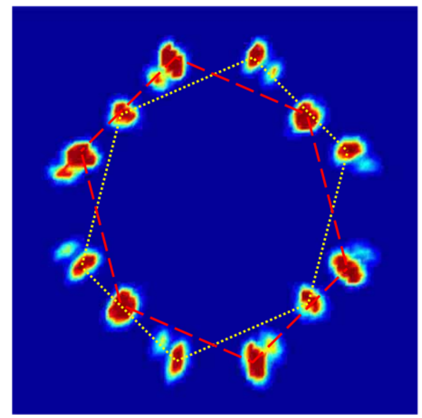
Cubitt et. al. Phys. Rev. Lett. **90** 157002 (2003)

Flux line lattices

Pure Niobium

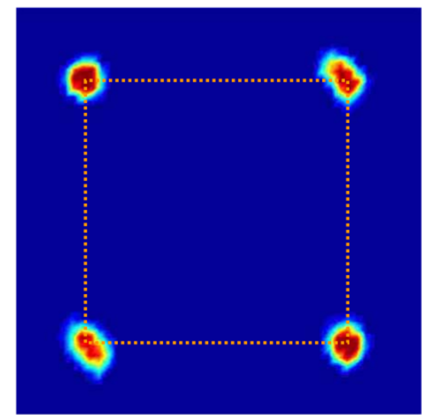


200 mT

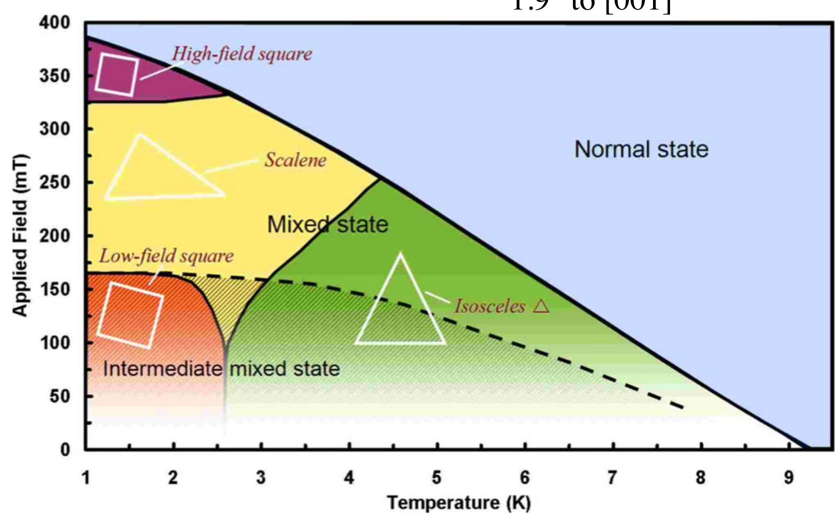


0.1° to (110)
1.9° to [001]

350 mT



0.1° to (110)
1.9° to [001]



M. Laver et. al. Phys. Rev. B **79** 014518 (2009)

Antiferromagnetism in MnO

Bragg peaks from crystal structure

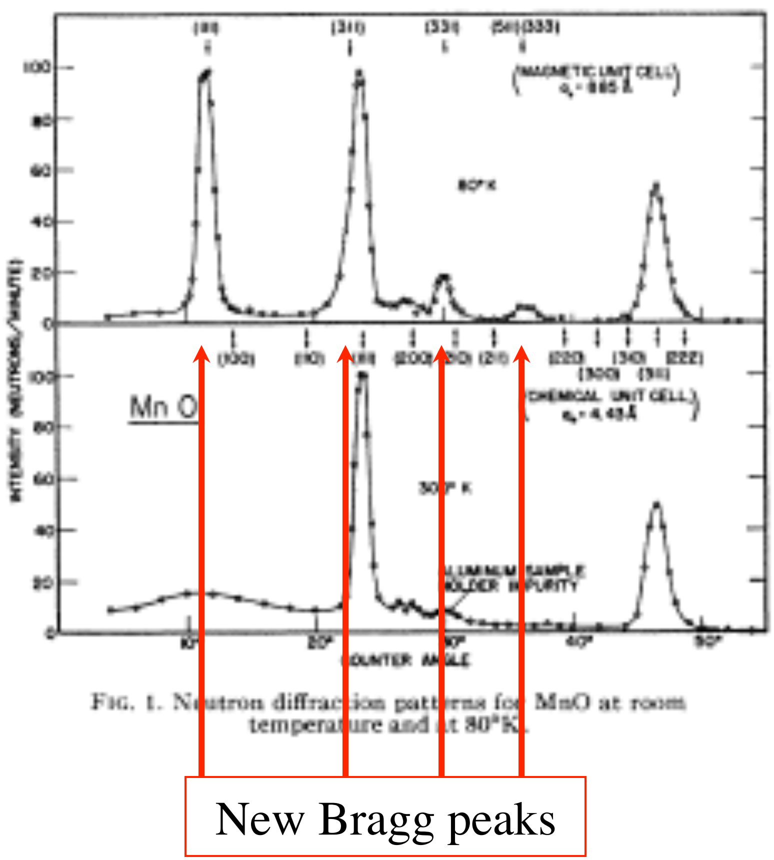
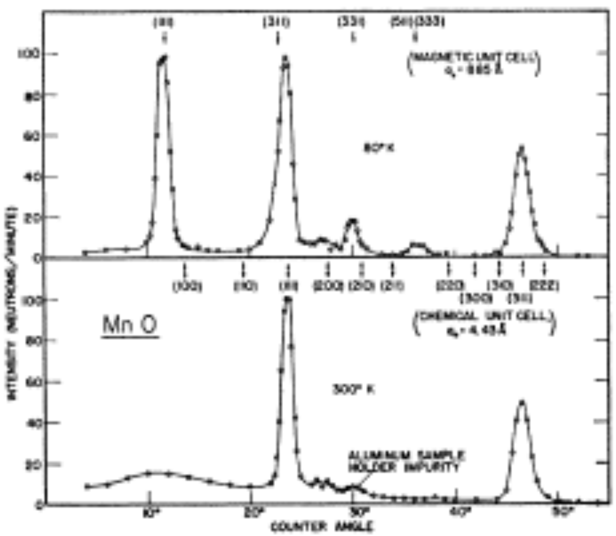


Fig. 1. Neutron diffraction patterns for MnO at room temperature and at 80°K.

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

Antiferromagnetism in MnO

New magnetic Bragg peaks



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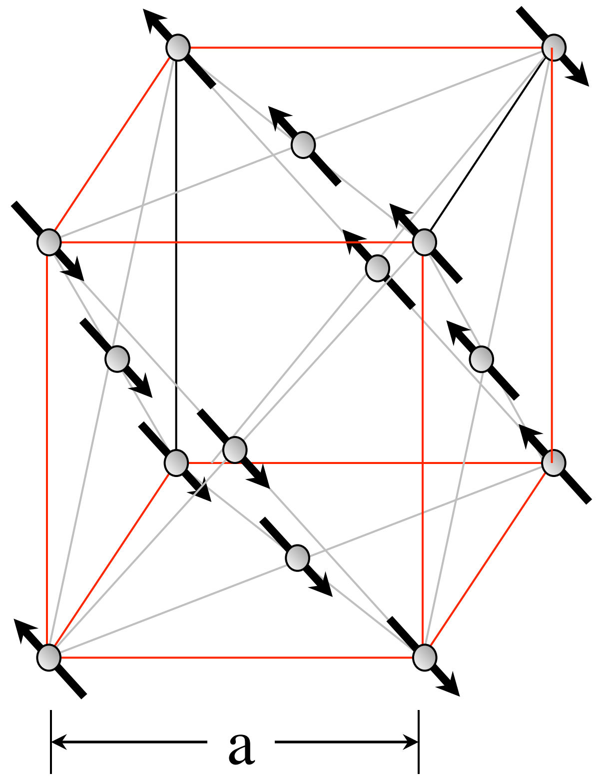
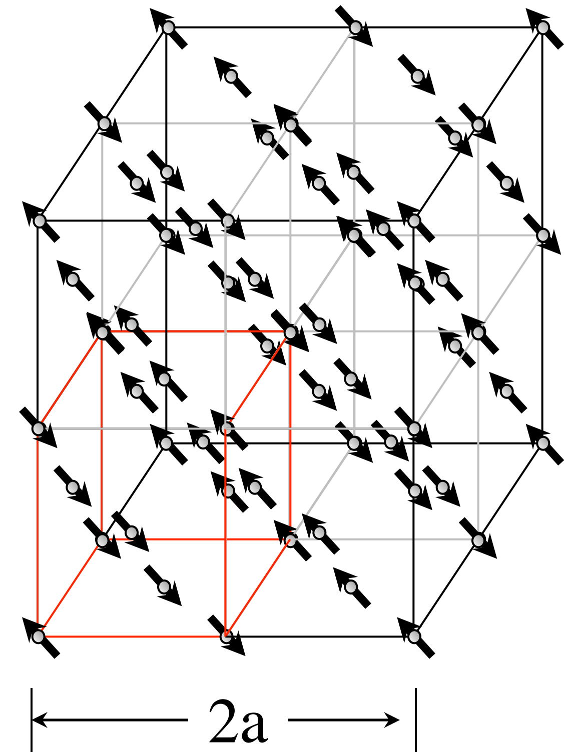
C. G. Shull & J. S. Smart, Phys. Rev. **76** (1949) 1256

Magnetic structure



Magnetic unit cell



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

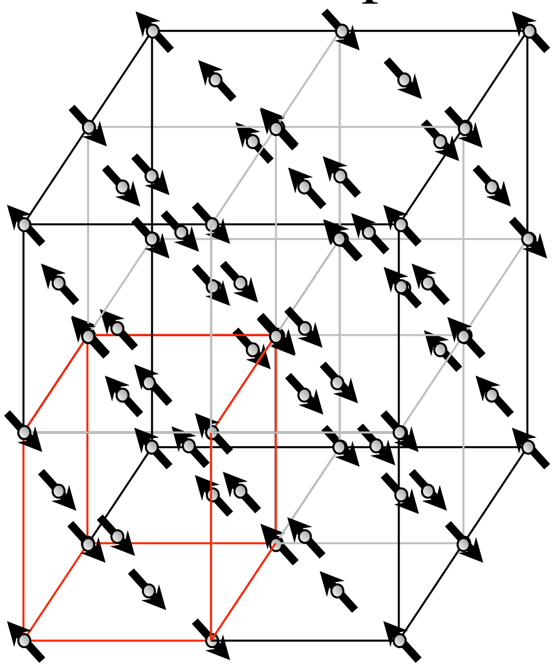
H. Shaked *et al.*, Phys. Rev. B **38** (1988) 11901

Antiferromagnetism in MnO

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

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

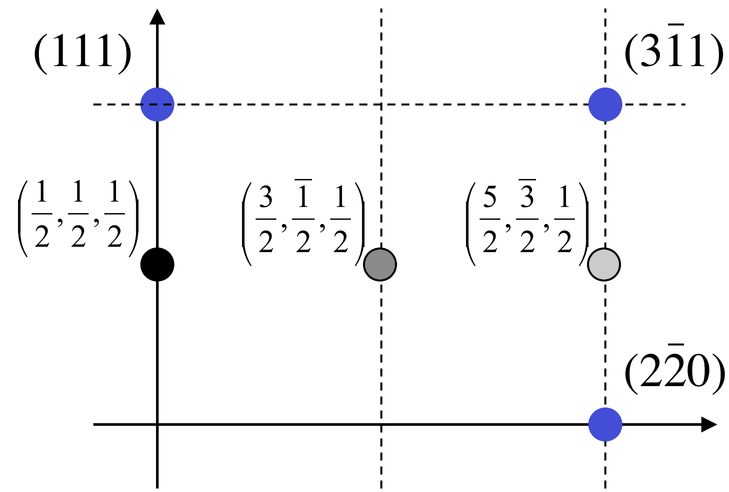
Real space



fcc lattice

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

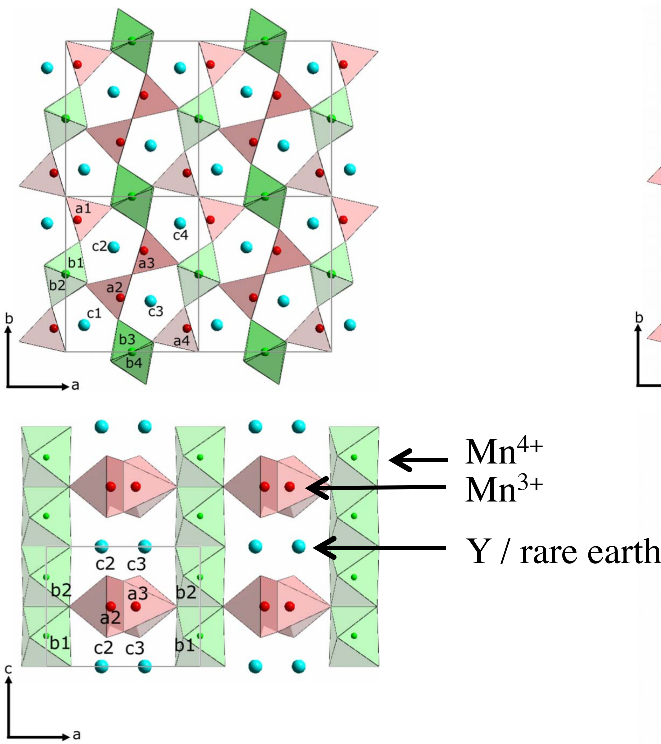
Reciprocal space



Moment direction

The magnetic structure of YMn_2O_5

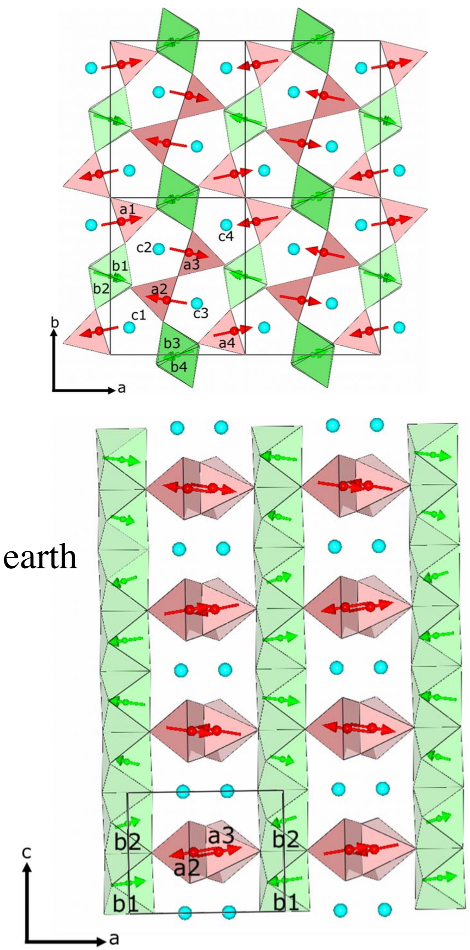
Crystal structure

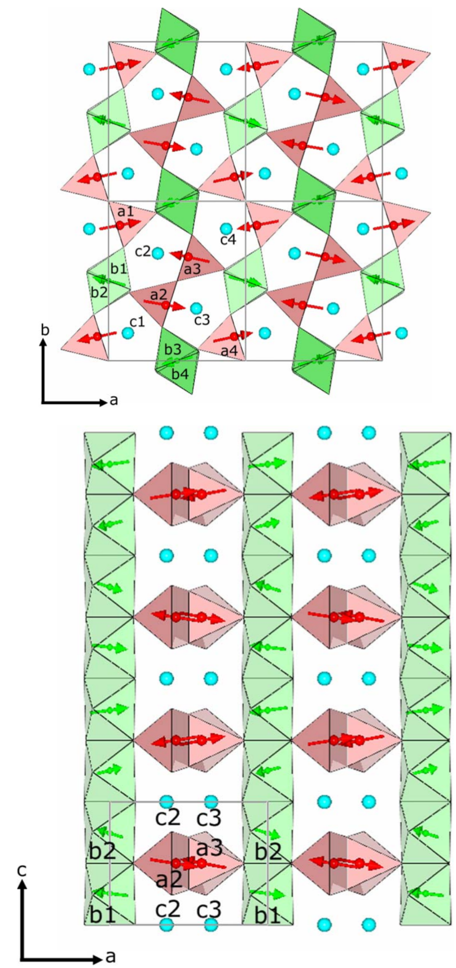


C. Vecchini *et al*., PRB **77** (2008) 134434

Domain 1 | Domain 2

(domains are related by inversion symmetry)



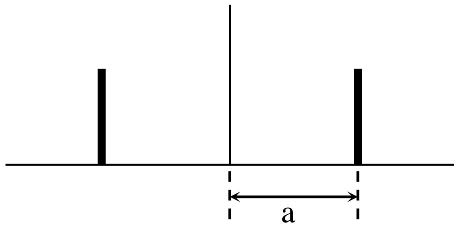


YMn_2O_5 has a *commensurate* magnetic structure

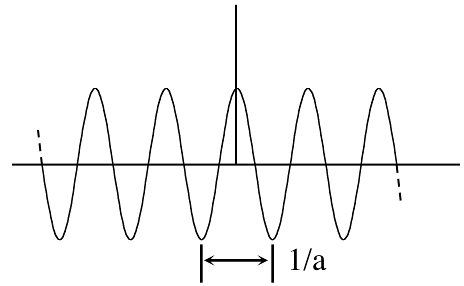
Antiferromagnetism in Chromium

The Fourier Transform for two Delta functions:

$F(\mathbf{Q})$



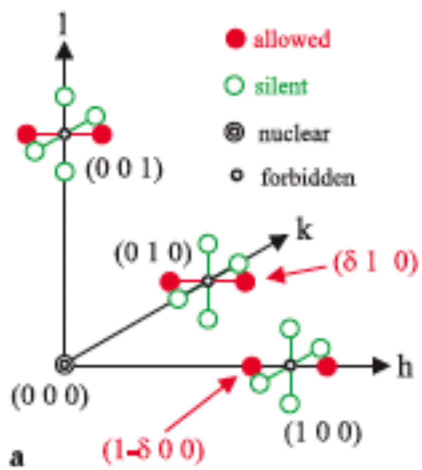
$f(\mathbf{r})$



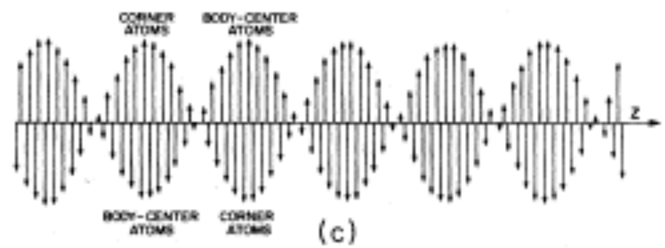
E.Fawcett, Rev. Mod. Phys. **60** (1988) 209

Chromium is an example of an *itinerant* antiferromagnet

Reciprocal space



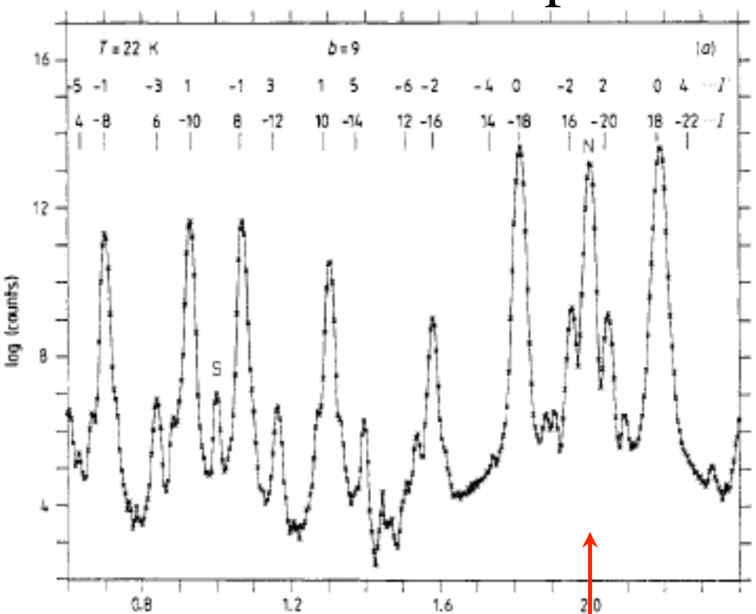
Real space



a Spin Density wave

Magnetic structure of Holmium

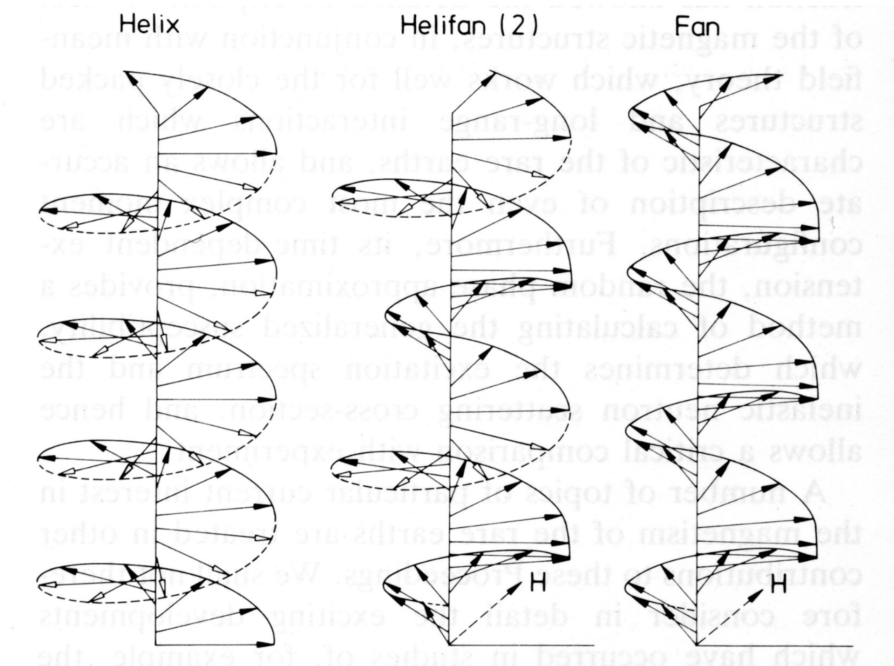
Scan along [00*l*], incommensurate peaks



l (rlu)

Nuclear peak

Real space structures

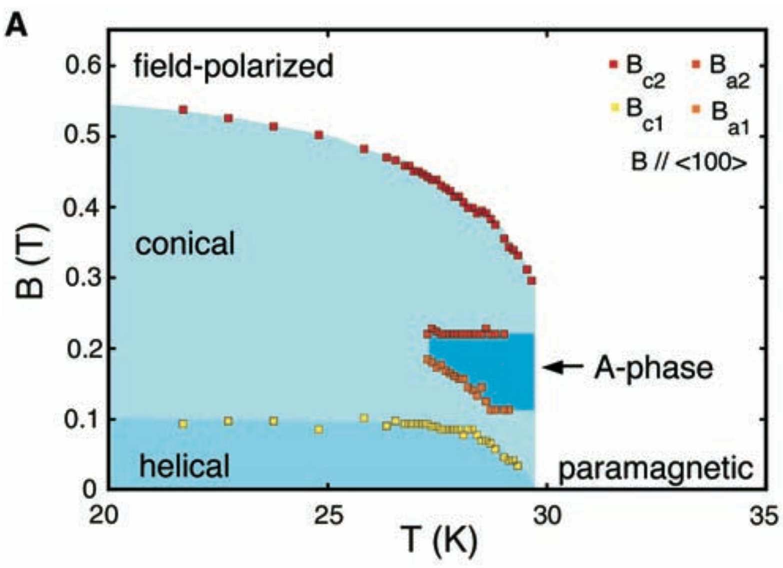


W. C. Koehler, in *Magnetic Properties of Rare Earth Metals*, ed. R. J. Elliot (Plenum Press, London, 1972) p. 81

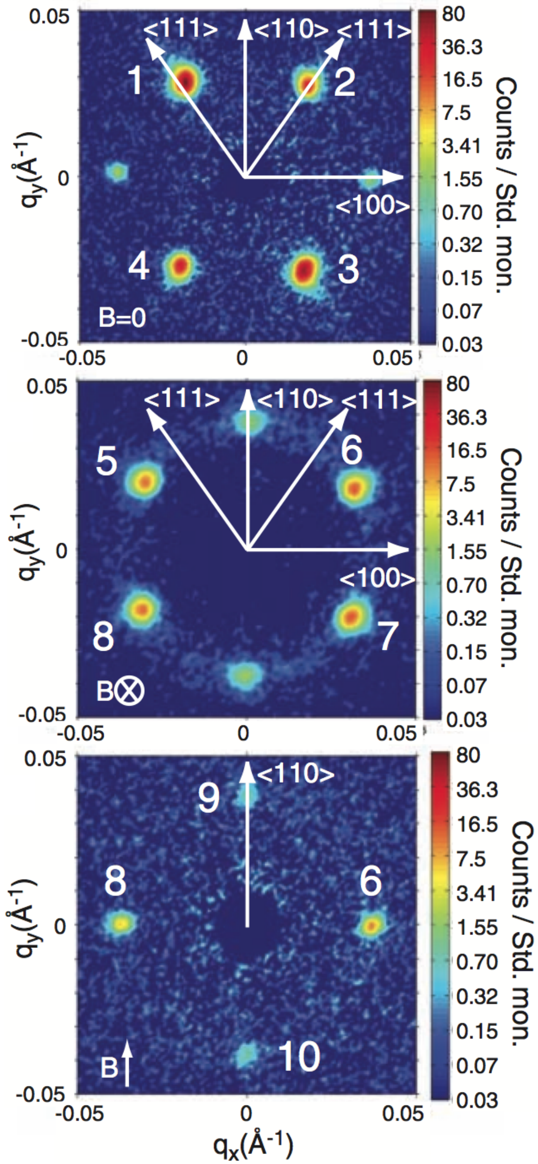
R. A. Cowley and S. Bates, J. Phys. C **21** (1988) 4113

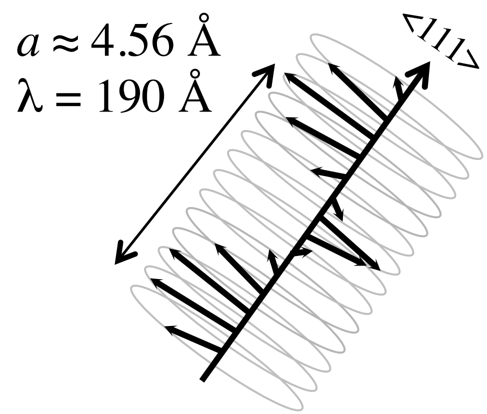
A. R. Mackintosh and J. Jensen, Physica B **180 & 181** (1992) 1

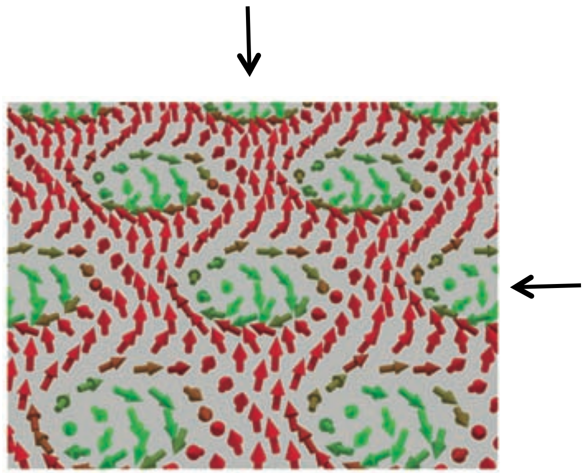
Skyrmions in MnSi



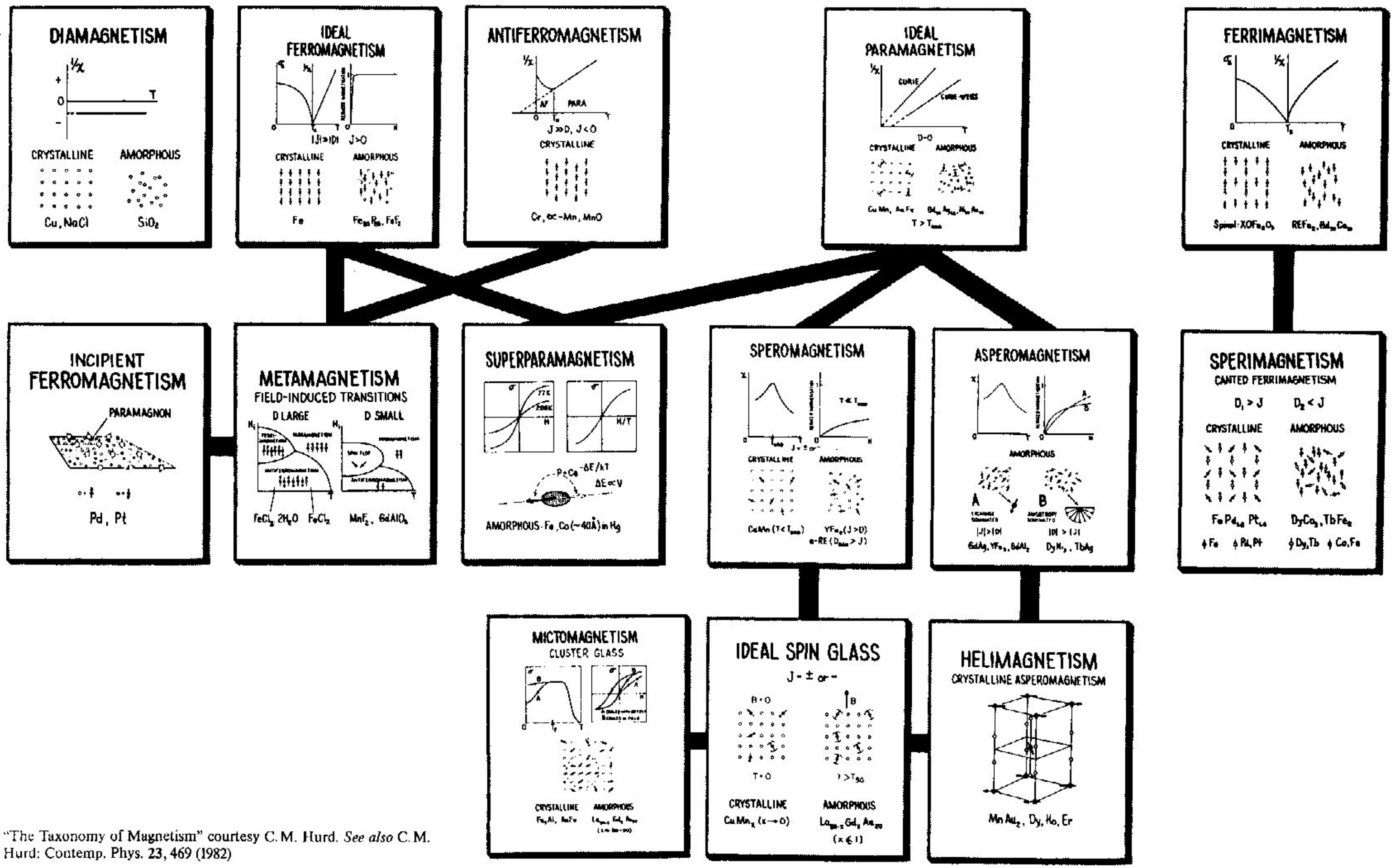
S. Mühlbauer et. al. Science **323** 915 (2009)







The 'Family Tree' of Magnetism

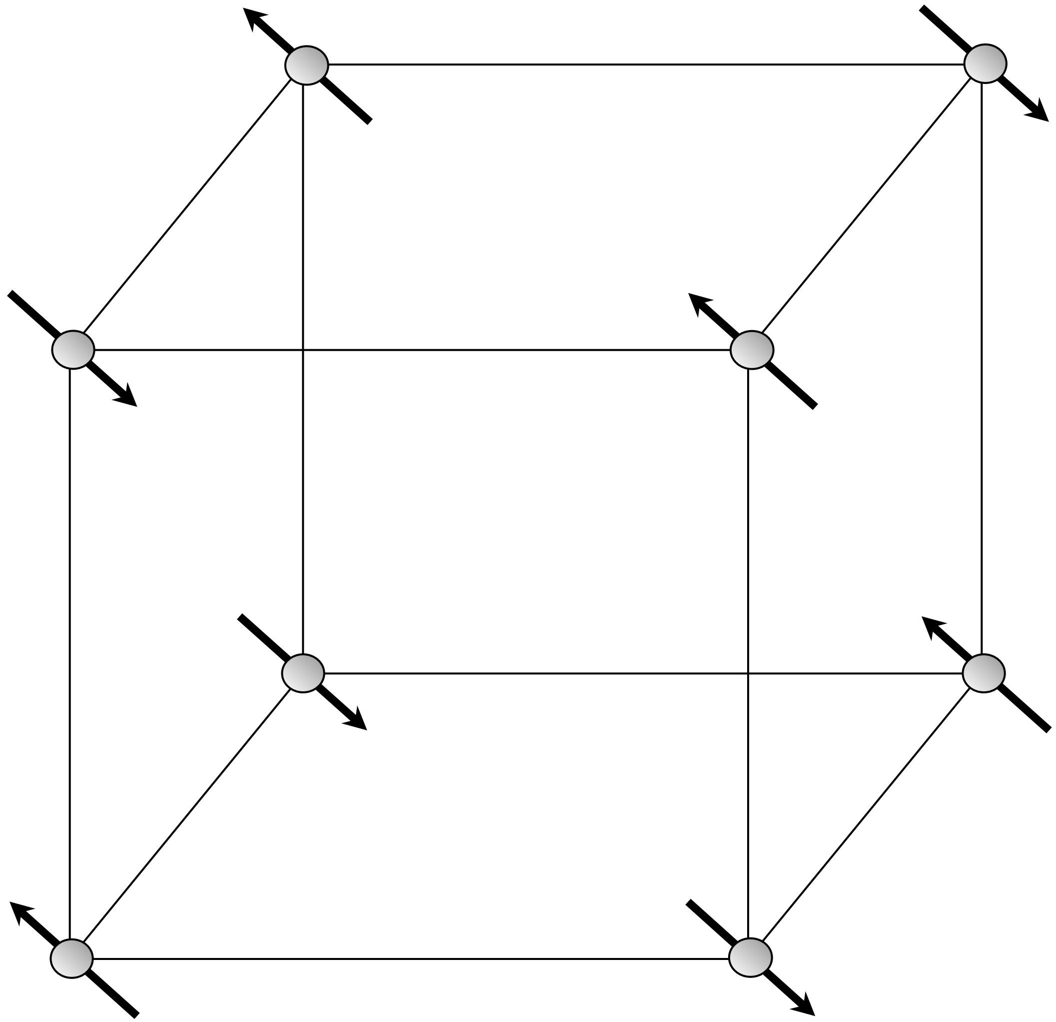


"The Taxonomy of Magnetism" courtesy C.M. Hurd. *See also* C.M. Hurd: Contemp. Phys. **23**, 469 (1982)

Magnetic form factors

A magnetic moment is spread out in space

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



Magnetic form factors

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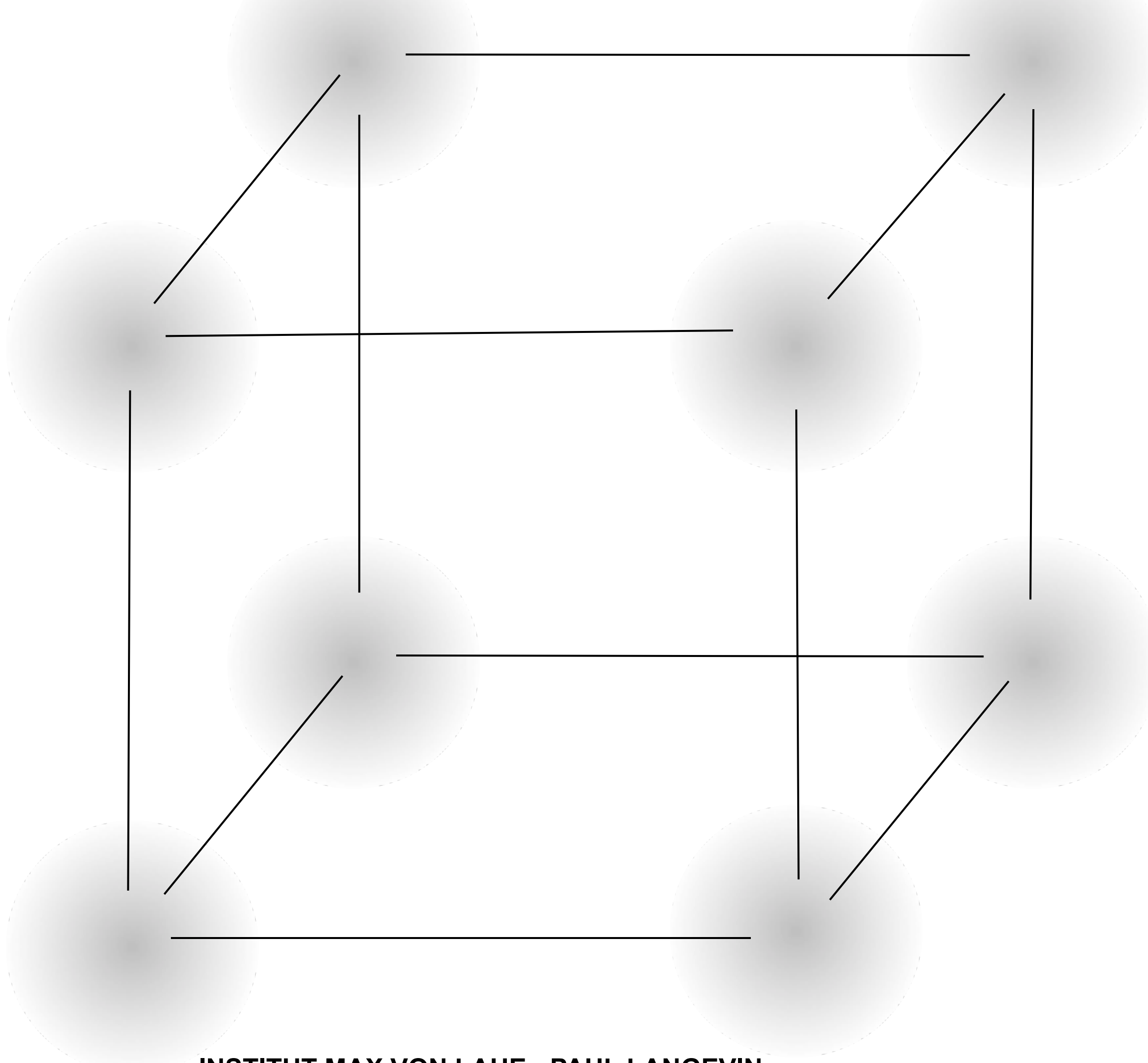
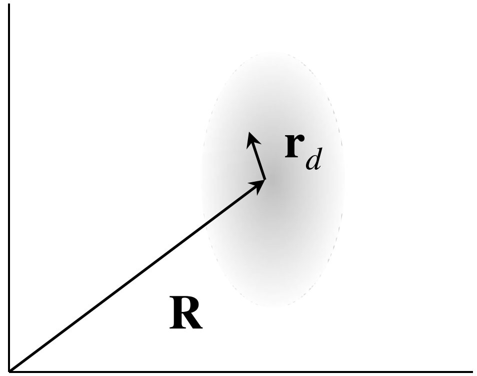


Magnetic form factors

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

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

$$\propto f^{2}(Q) \int S_{\perp}(\mathbf{R}_i) S_{\perp}^{*}\left(\mathbf{R}_j\right) e^{i\mathbf{Q}\cdot\left(\mathbf{R}_i - \mathbf{R}_j\right)} \cdot d\mathbf{R}$$

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

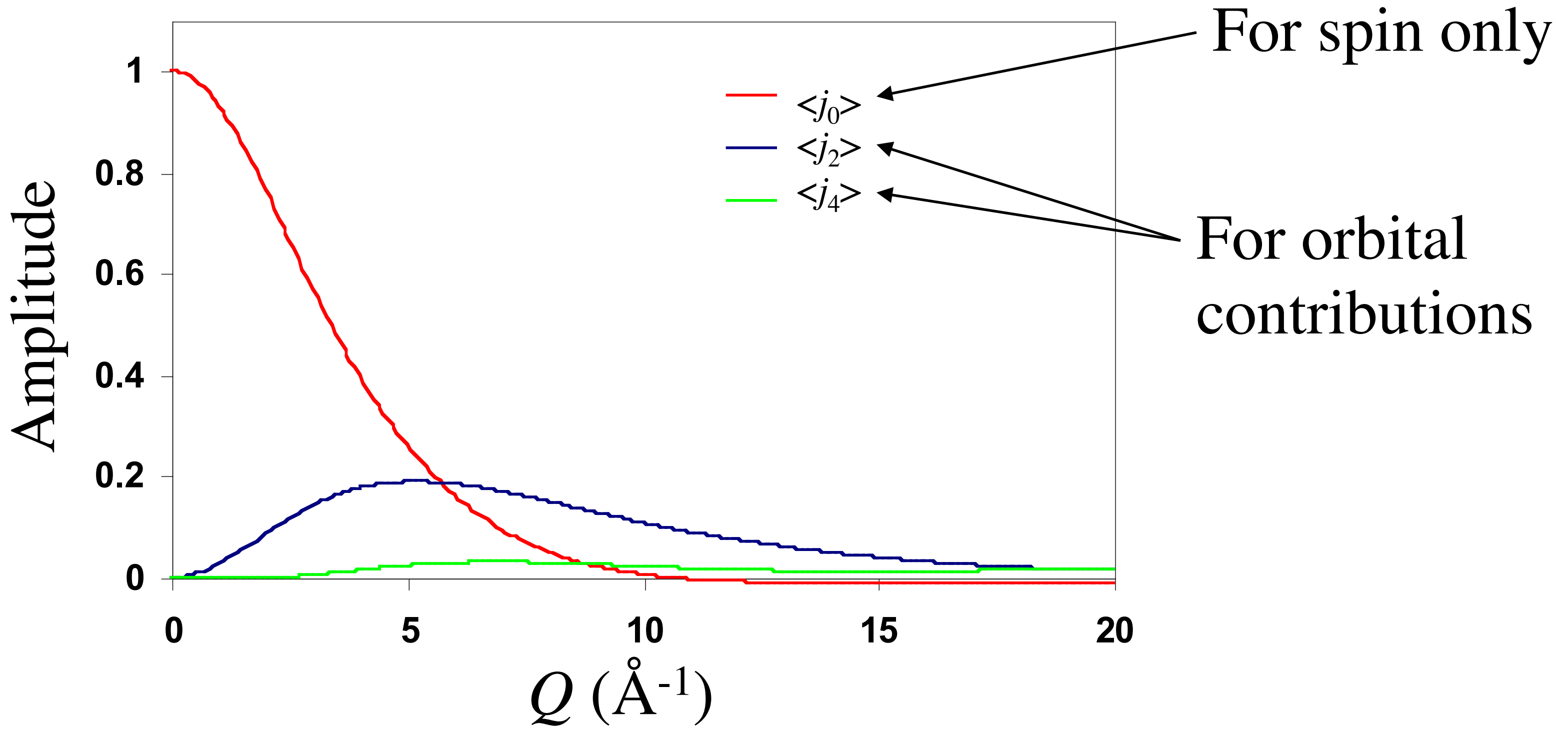
Magnetic form factors

Approximations for the form factors are tabulated

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

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

Form factors for iron



Magnetic electron density

Nickel

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

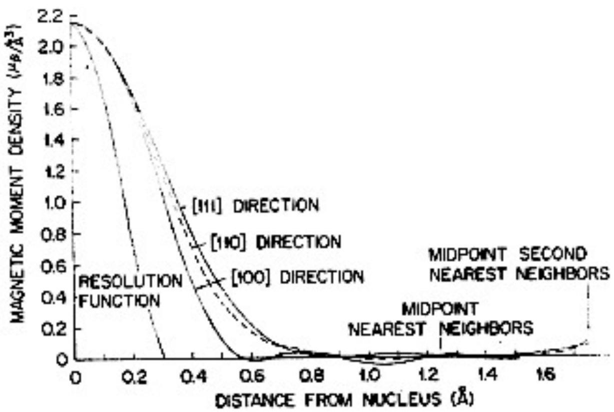


FIG. 1. Distribution of magnetic moment density along the three major crystallographic directions.

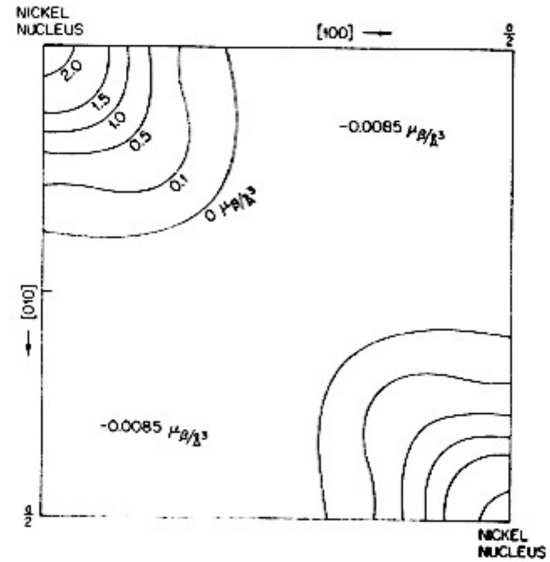


FIG. 4. The magnetic moment distribution in the [100] plane.

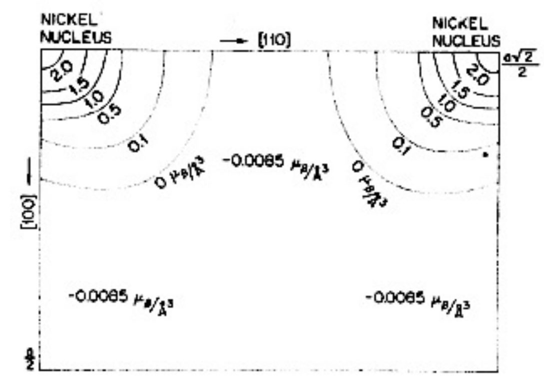
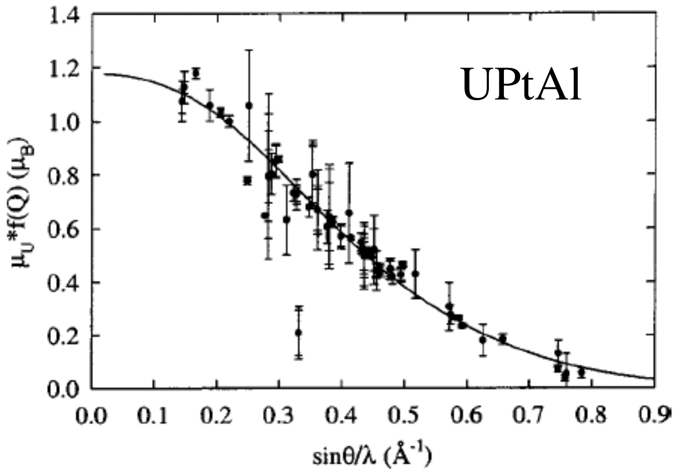


FIG. 5. The magnetic moment distribution in the [110] plane.

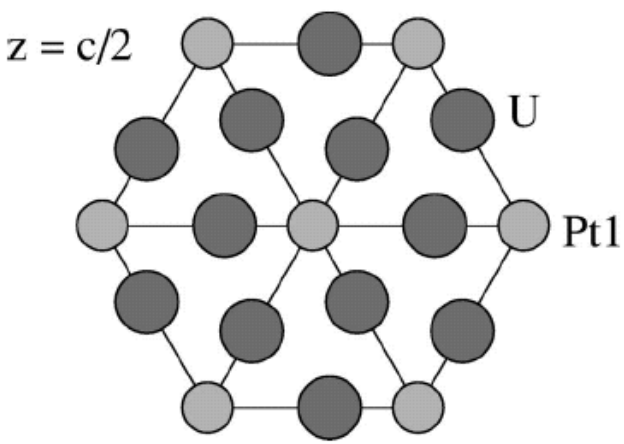
Magnetic electron density

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

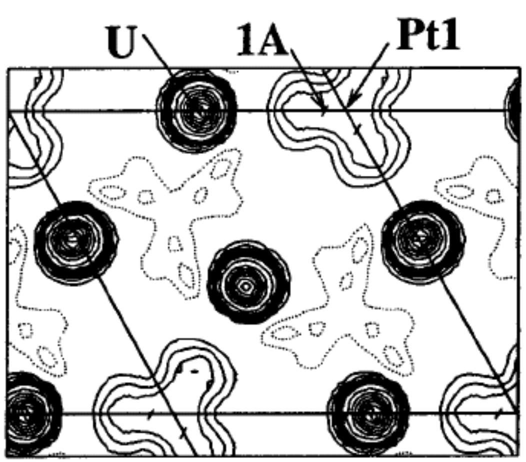


P. Javorsky *et al*., Phys. Rev. B **67** (2003) 224429

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



crystal structure



magnetic moment density

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

The crystal field is an electric field on an atom caused by neighbouring atoms in the sample.

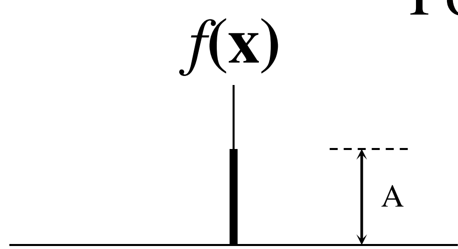
It may lift the degeneracy of the energy levels for the atomic electrons.

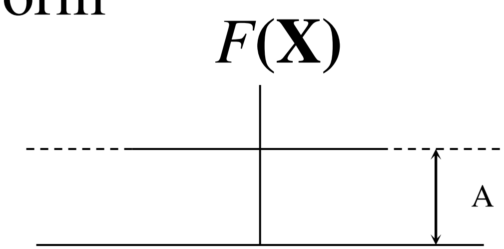
If the electrons are unpaired, neutrons can cause the electrons to jump between the energy levels.

Because the crystal field is at a single atomic site, the inelastic scattering is essentially independent of **Q**.

Fourier transform

A Delta function



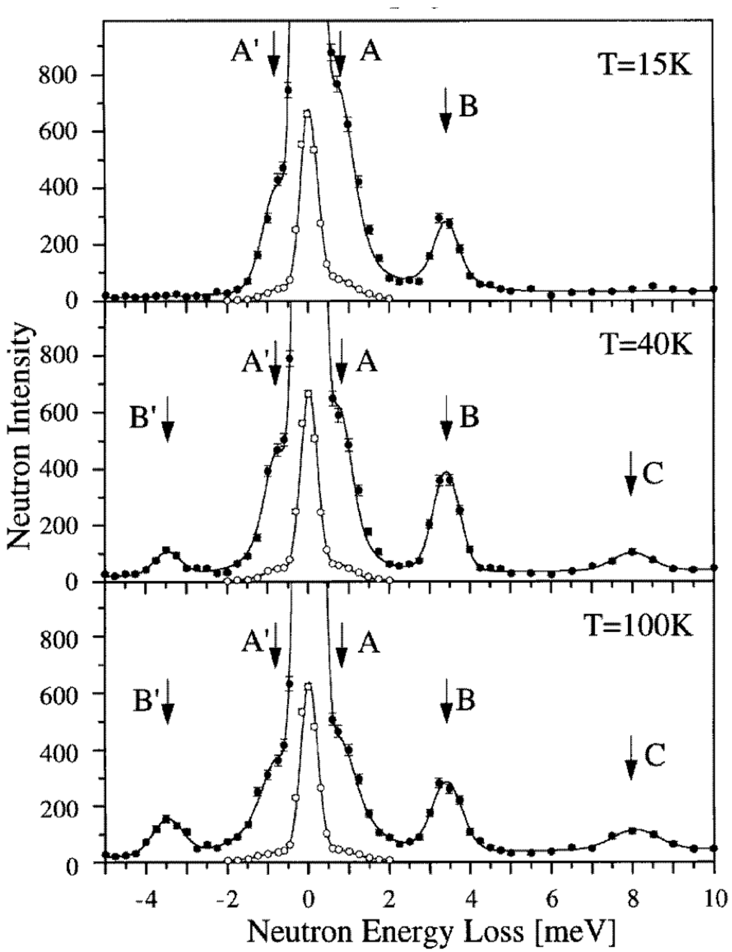


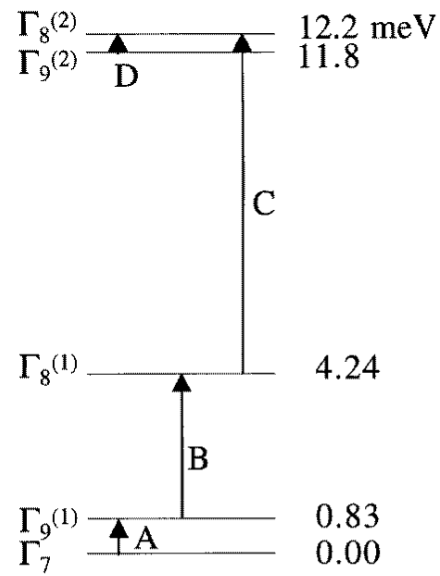
Crystal fields in $NdPd_2Al_3$

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

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

B = CF parameters, measured by neutrons

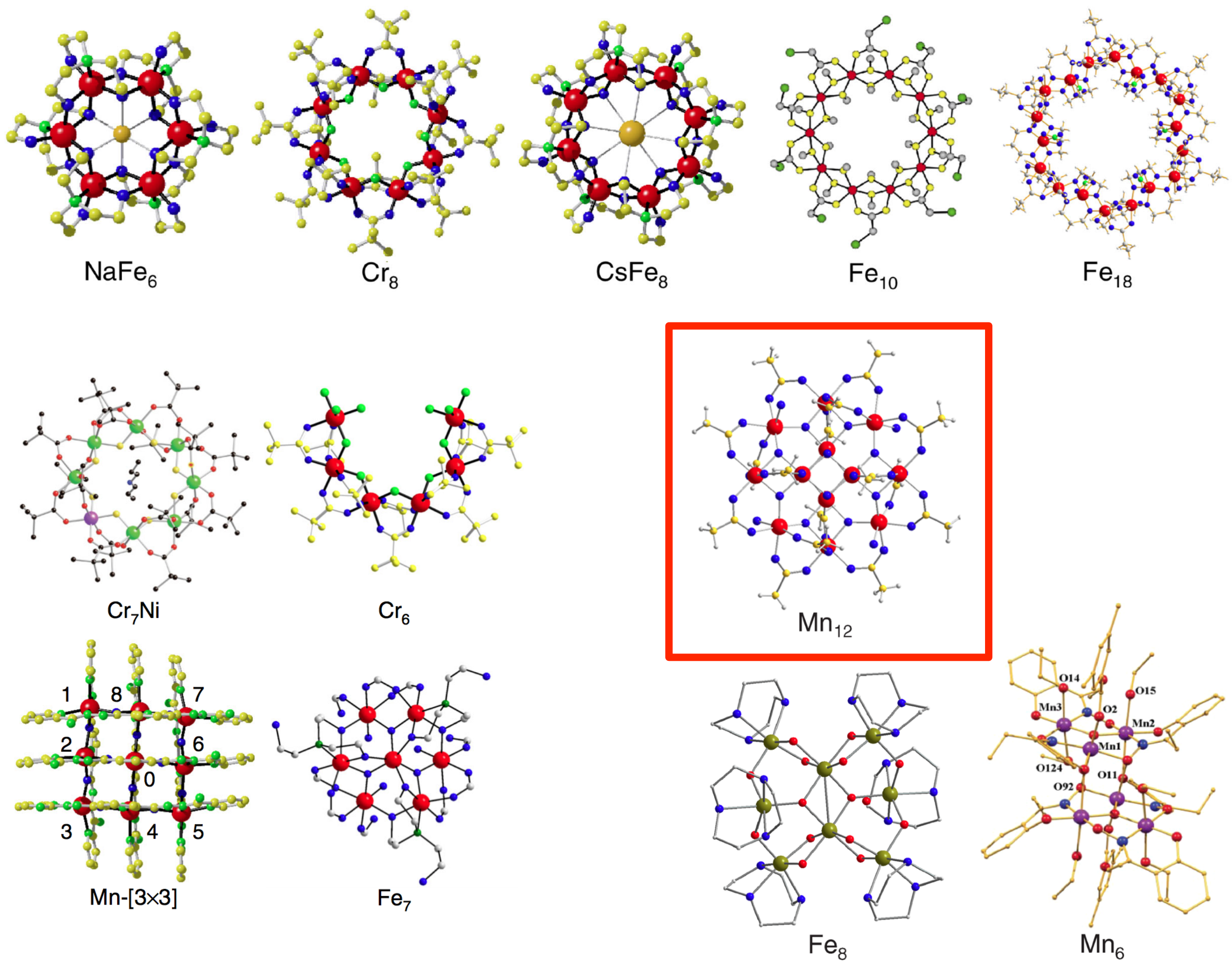




A. Dönni *et al*., J. Phys.: Condens. Matter **9** (1997) 5921

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

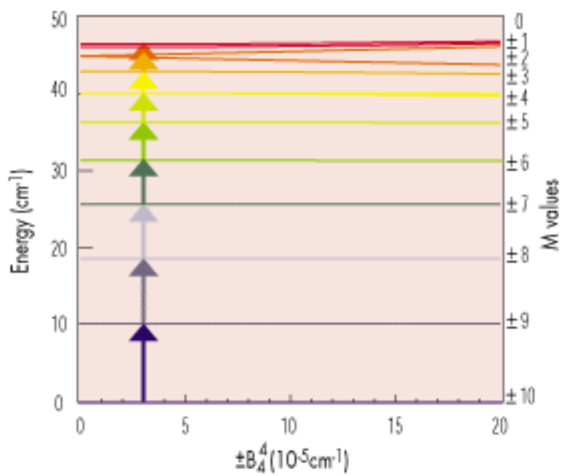
Molecular magnets



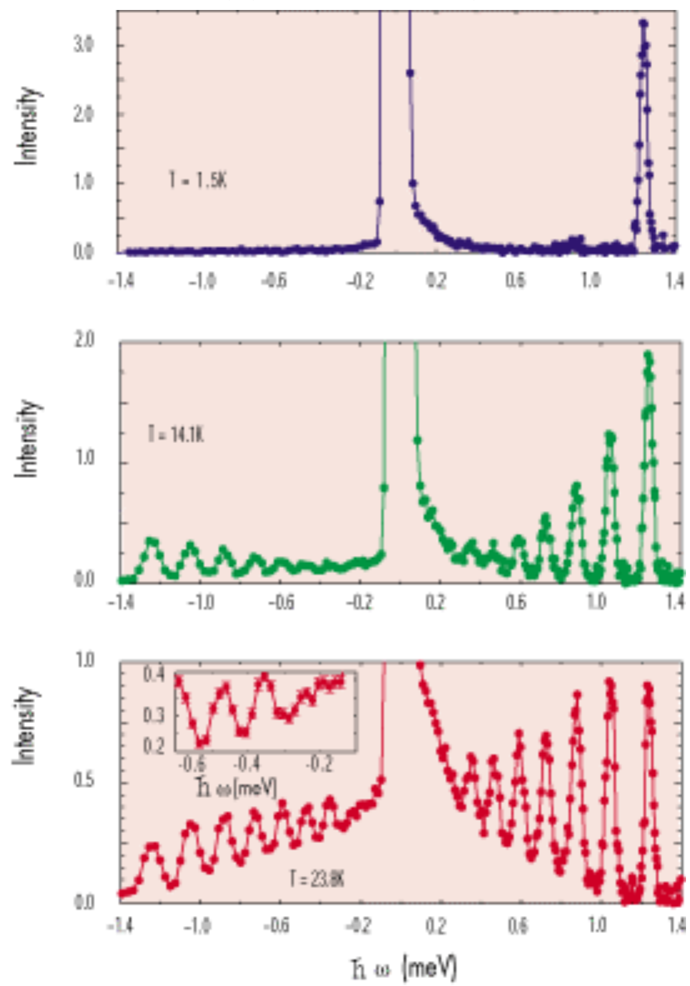
A. Furrer and O. Waldmann, Rev. Mod. Phys. **85** (2013) 367

Quantum tunneling in Mn_{12}-acetate

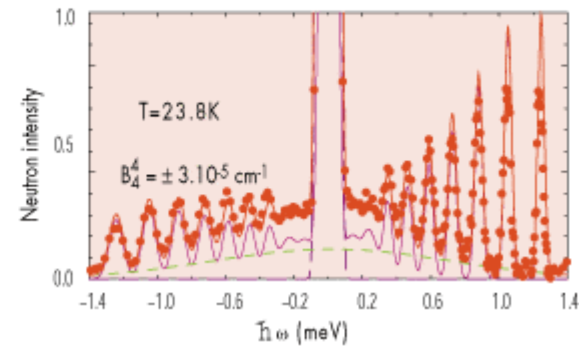
$$H = \sum_{l=2,4,6} B_l^0 O_l^0 + \sum_{l=2,4} B_l^4 O_l^4$$



Calculated energy terms



Neutron spectra



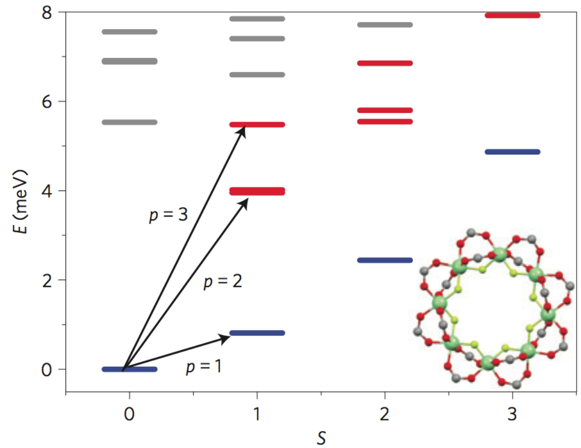
Fitted data with scattering from:

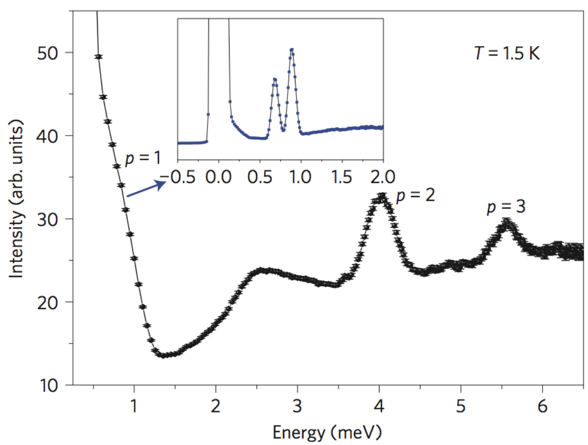
- energy levels
- elastic scattering
- incoherent background

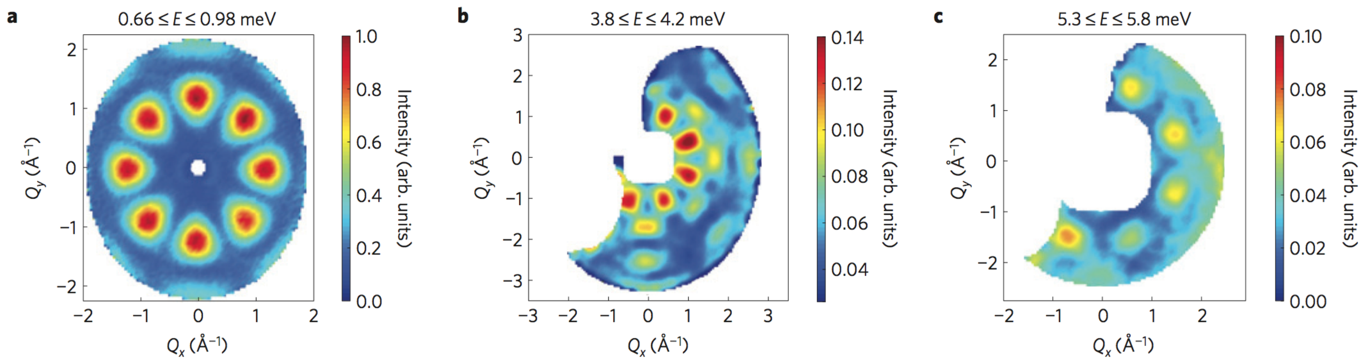
I. Mirebeau *et al*., Phys. Rev. Lett. **83** (1999) 628
R. Bircher *et al*., Phys. Rev. B **70** (2004) 212413

Space-time correlations in Cr_8

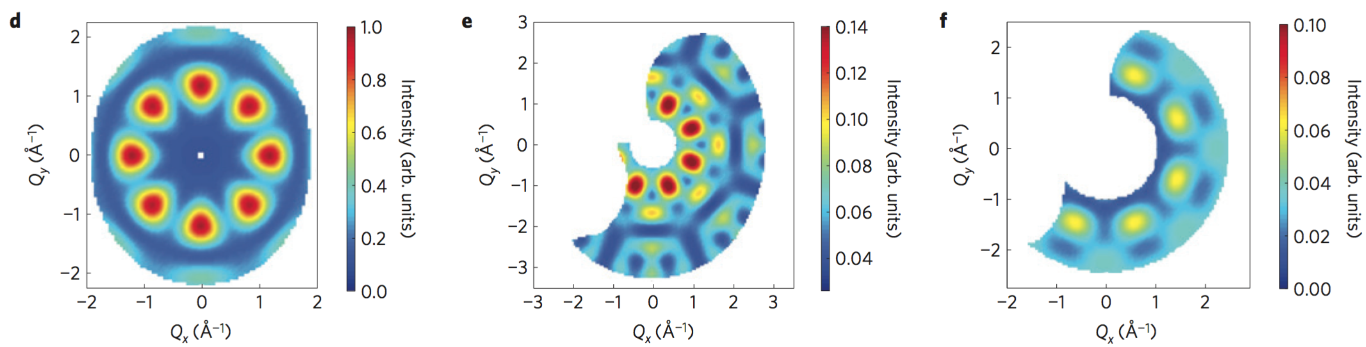
$$H = J\sum_{i=1}^{8} \mathbf{s}_i \cdot \mathbf{s}_{i+1}$$



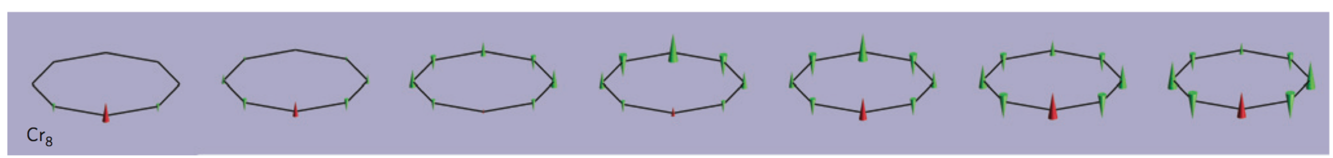




Data



Fit



M. Baker *et al*., Nature Phys. **8** (2012) 906

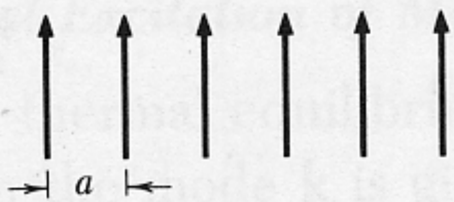
Spin waves and magnons

A simple Hamiltonian for spin waves is:

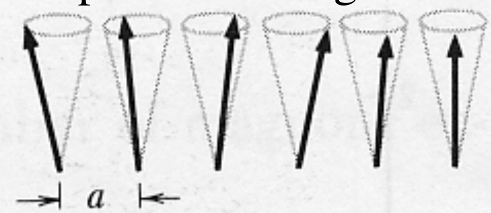
$$H = -J\sum_{i,j} \mathbf{s}_i \mathbf{s}_j$$

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

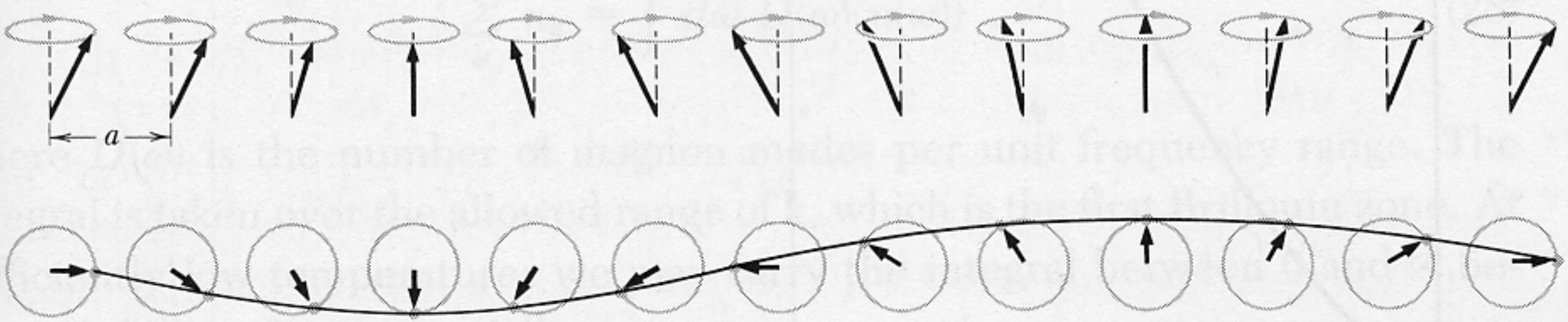
Take a simple ferromagnet:



The spin waves might look like this:

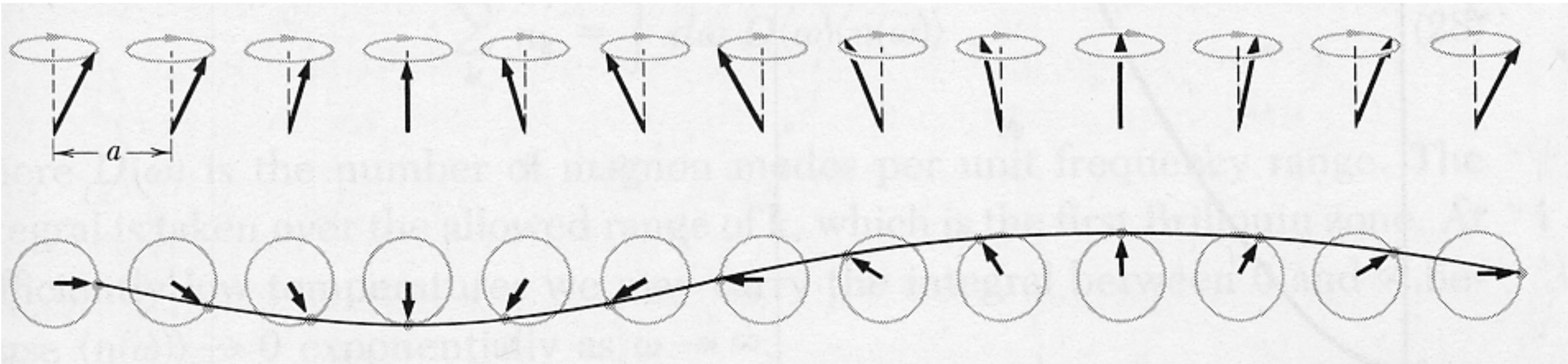


Spin waves have a frequency (ω) and a wavevector (**q**)

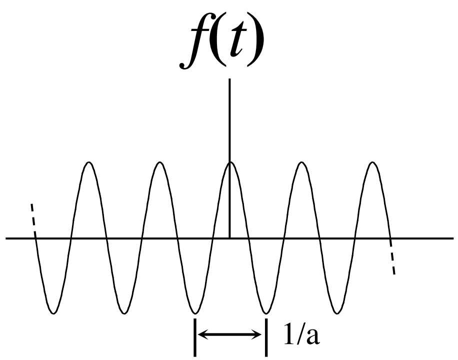


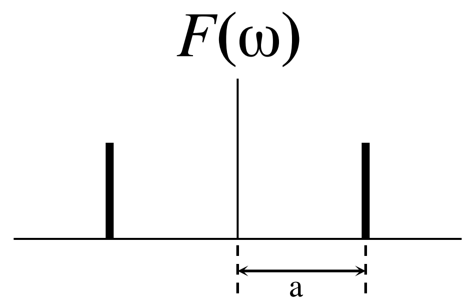
The frequency and wavevector of the waves are *directly measurable* with neutrons

Magnons



The Fourier Transform for a periodic function:

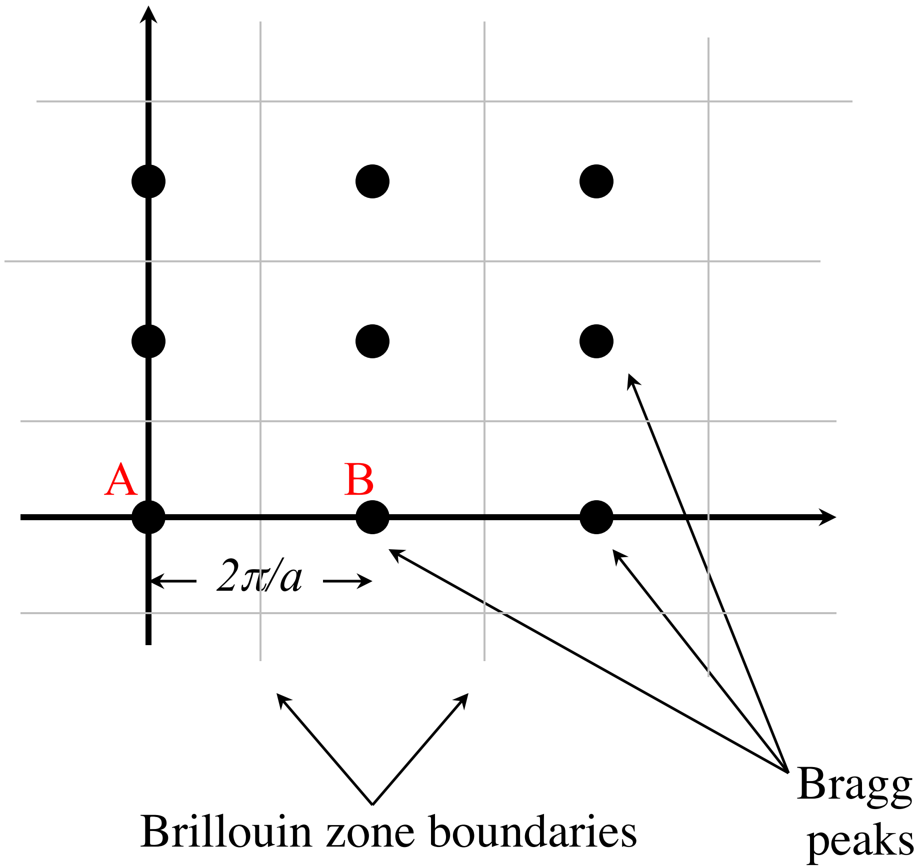




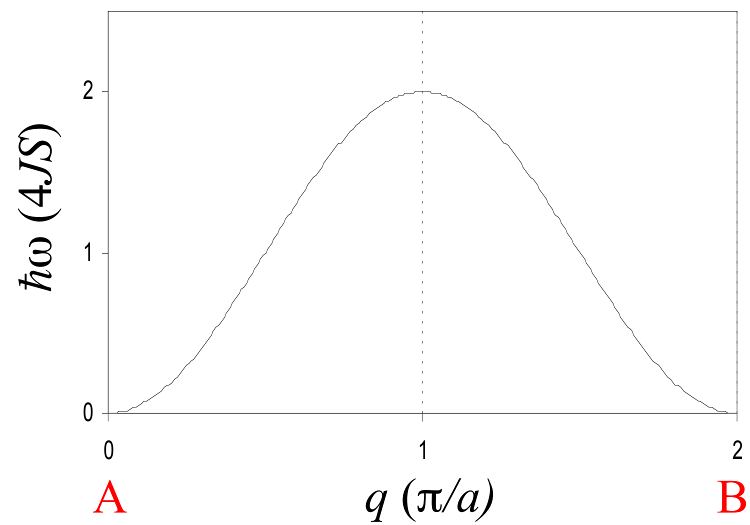
Each wavelength for the magnon has its own periodicity.
Each wavevector for the magnon has its own frequency (energy)

Magnons and reciprocal space

Reciprocal space



Spin wave dispersion

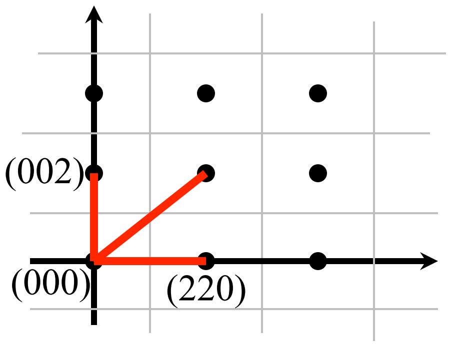


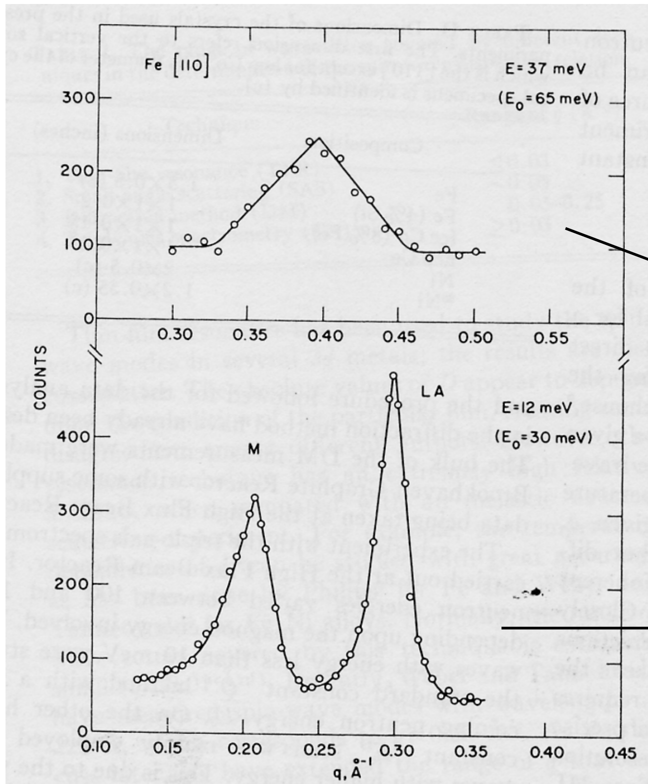
$$\hbar\omega = 4JS(1 - \cos qa)$$
$$= Dq^2 \quad (\text{for } qa << 1)$$
$$D = 2JSa^2$$

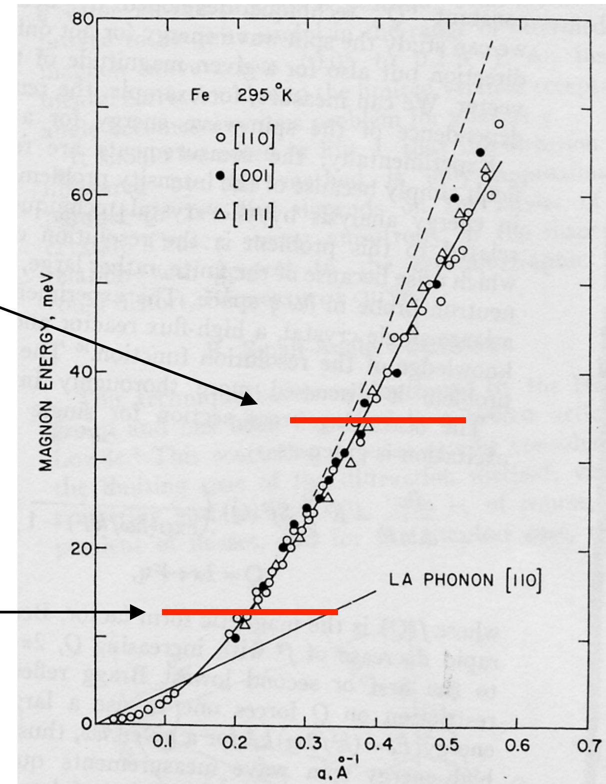
C. Kittel, *Introduction to Solid State Physics*, 1996, Wiley, New York

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

Magnons in crystalline iron

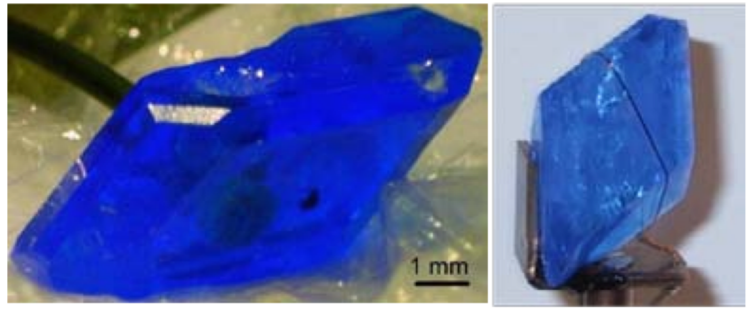


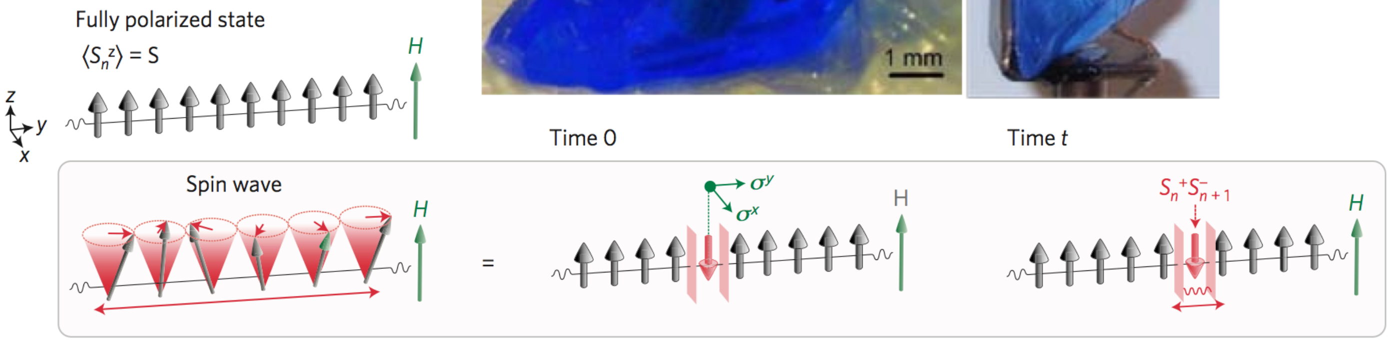


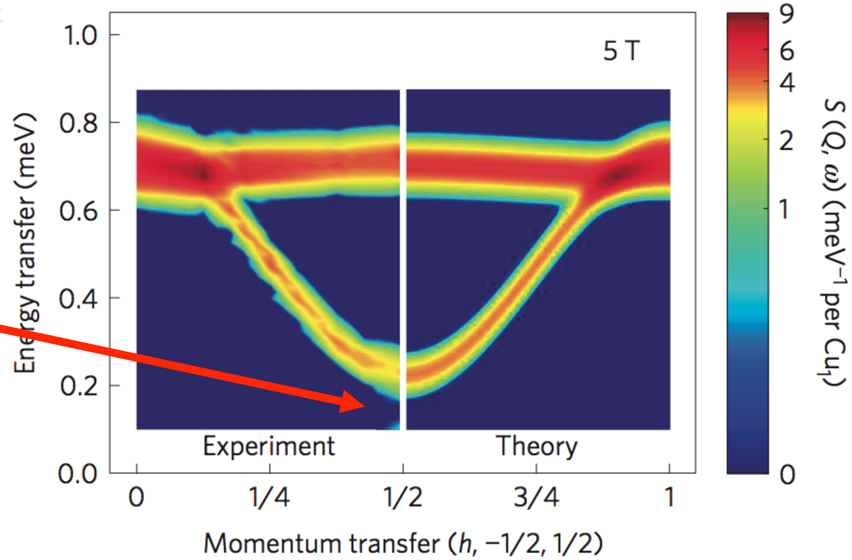


G. Shirane *et al*., J. Appl. Phys. **39** (1968) 383

Magnetic excitations in $CuSO_4$





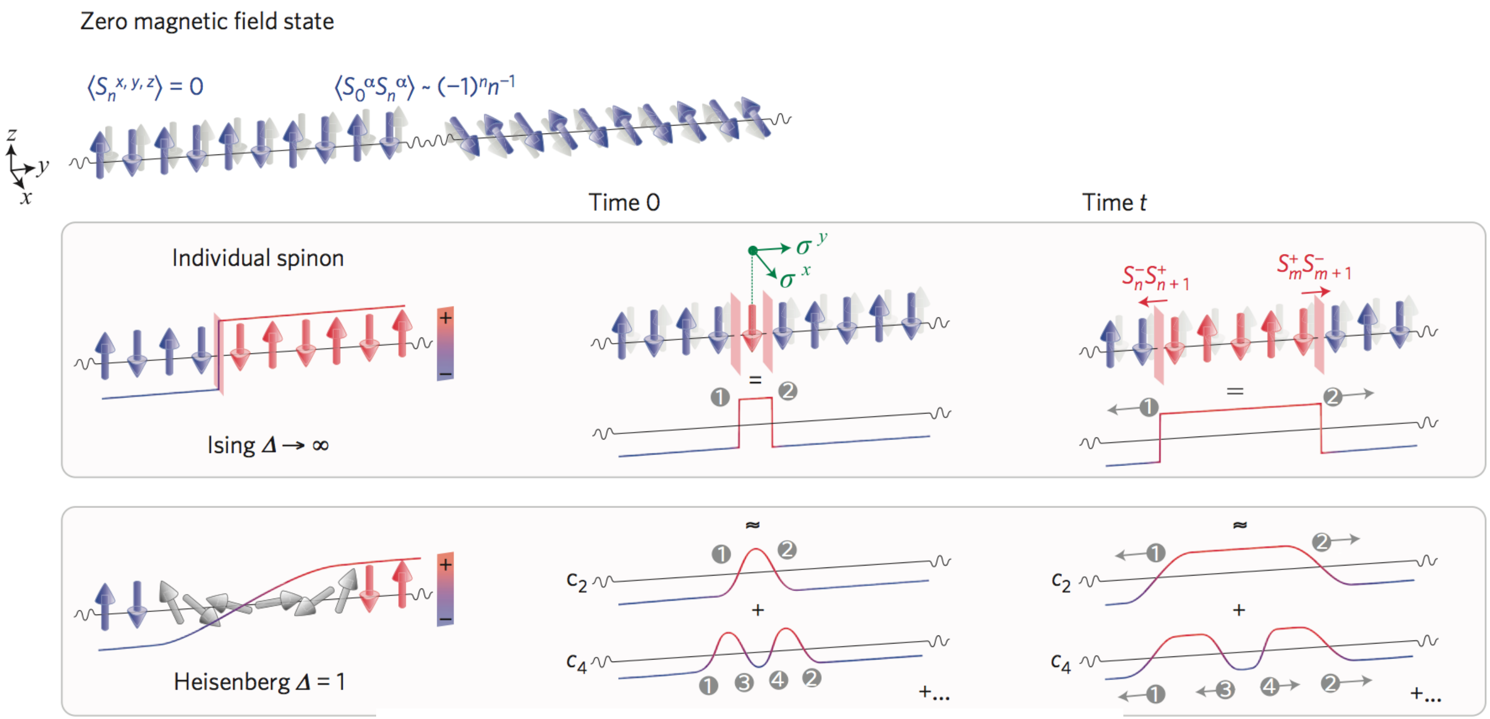


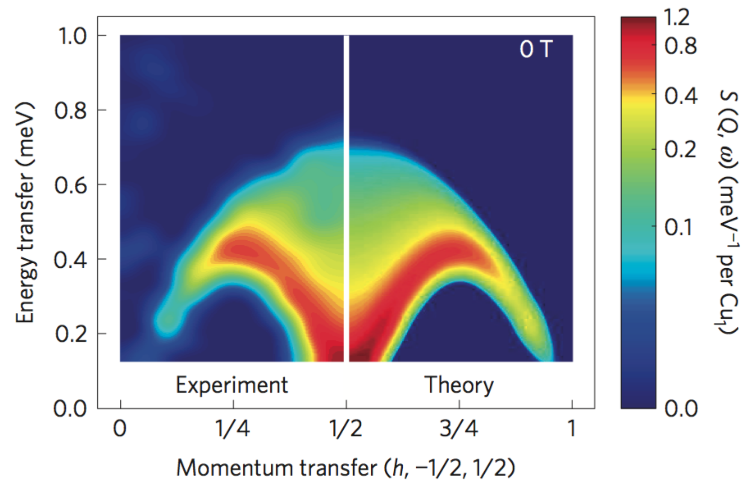
Gap in dispersion due to magnetic anisotropy

M. Mourigal *et al*.,

Nature Phys. **9** (2013) 435

Magnetic excitations in $CuSO_4$





M. Mourigal *et al*.,

Nature Phys. **9** (2013) 435

Neutron scattering and magnetic susceptibility

Magnetic susceptibility is a fundamental property of a material. It is defined as:

$$\chi = \frac{M}{H}$$

In a magnetic system, **M** is a vector which varies as a function of space, **r**, and (due to fluctuations) as a function of time, *t*.

The time is related to the susceptibility by:

$$M_\alpha(t) \propto \chi_{\alpha\alpha}(\omega) H_{0\alpha} e^{-i\omega t} + \chi^*_{\alpha\alpha}(\omega) H^*_{0\alpha} e^{i\omega t}$$

The susceptibility is a complex tensor:

$$\chi_{\alpha\alpha}(\omega) = \chi'_{\alpha\alpha}(\omega) + i\chi''_{\alpha\alpha}(\omega)$$

The rate of energy gain is given by:

$$\frac{d\bar{E}}{dt} = -M_\alpha \frac{dH}{dt} \propto \chi''_{\alpha\alpha}(\omega)$$

and the inelastic cross-section is then related to a *generalized* susceptibility:

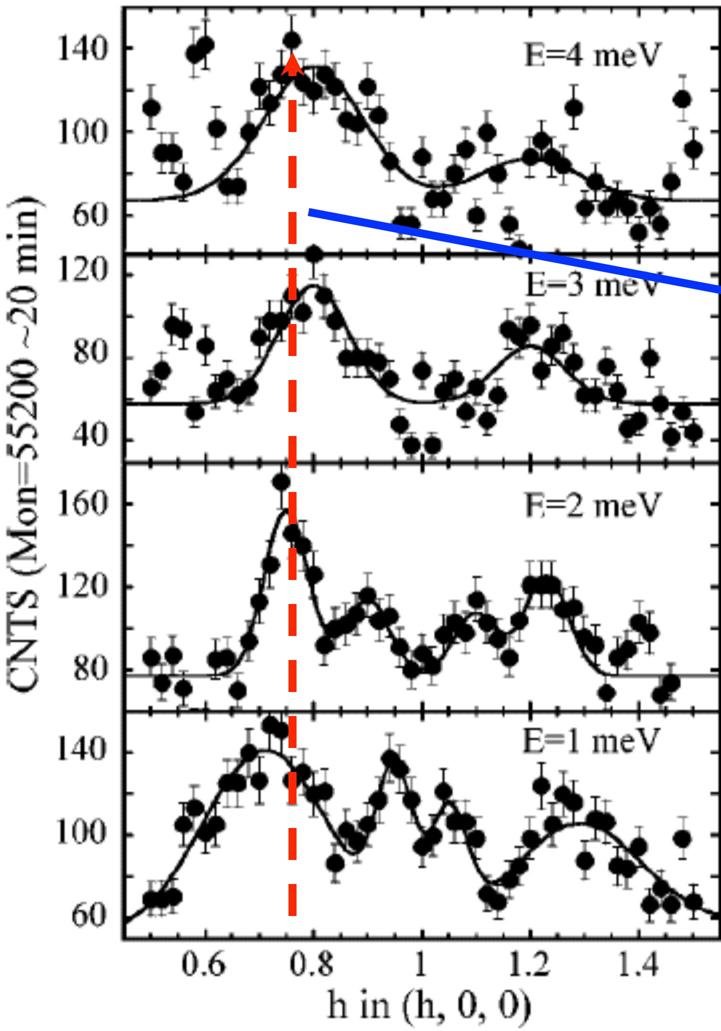
$$\frac{d^2\sigma}{d\Omega dE} \propto \frac{k'}{k} \sum_\alpha \frac{\chi''_{\alpha\alpha}(\mathbf{Q},\omega)}{\left(1 - e^{-\beta\hbar\omega}\right)}$$

T. J. Hicks, *Magnetism in disorder*, Oxford Unversity Press, Oxford, 1995

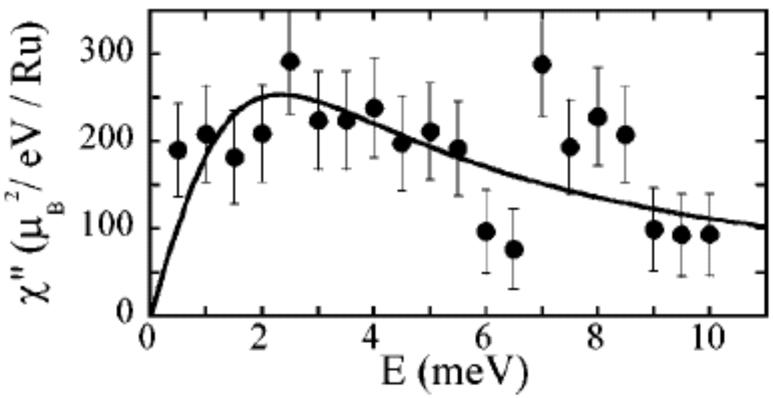
S. W. Lovesey, *Theory of neutron scattering from condensed matter*, Oxford University Press, Oxford, 1986

Spin excitations in $Sr_3Ru_2O_7$

$Sr_3Ru_2O_7$ is from a family of materials that are low-dimensional magnetic, and superconductors



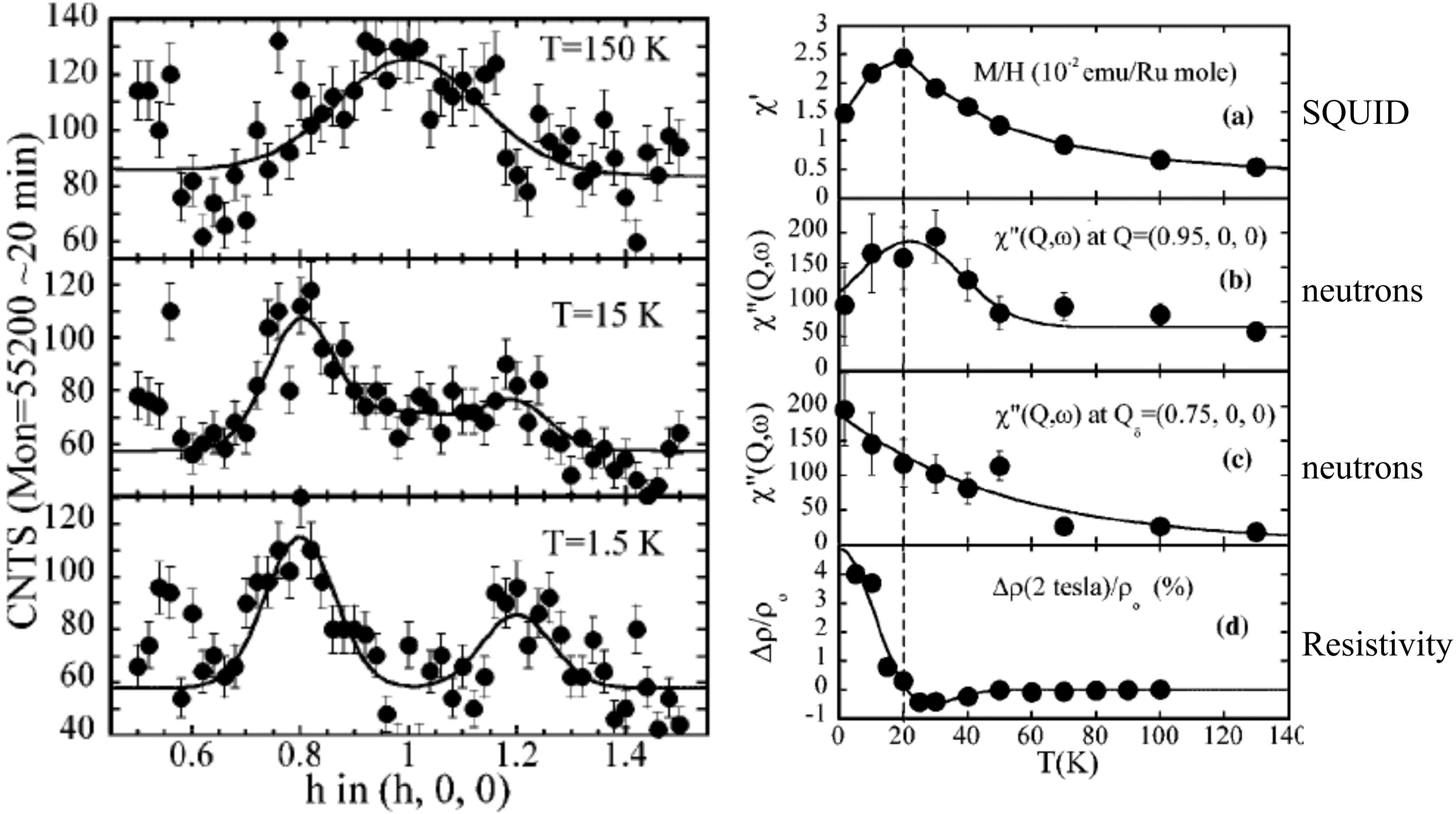
Inelastic neutron scattering at 1.5K



Susceptibility

L. Capogna *et al*., Phys. Rev. B. **87** (1998) 143

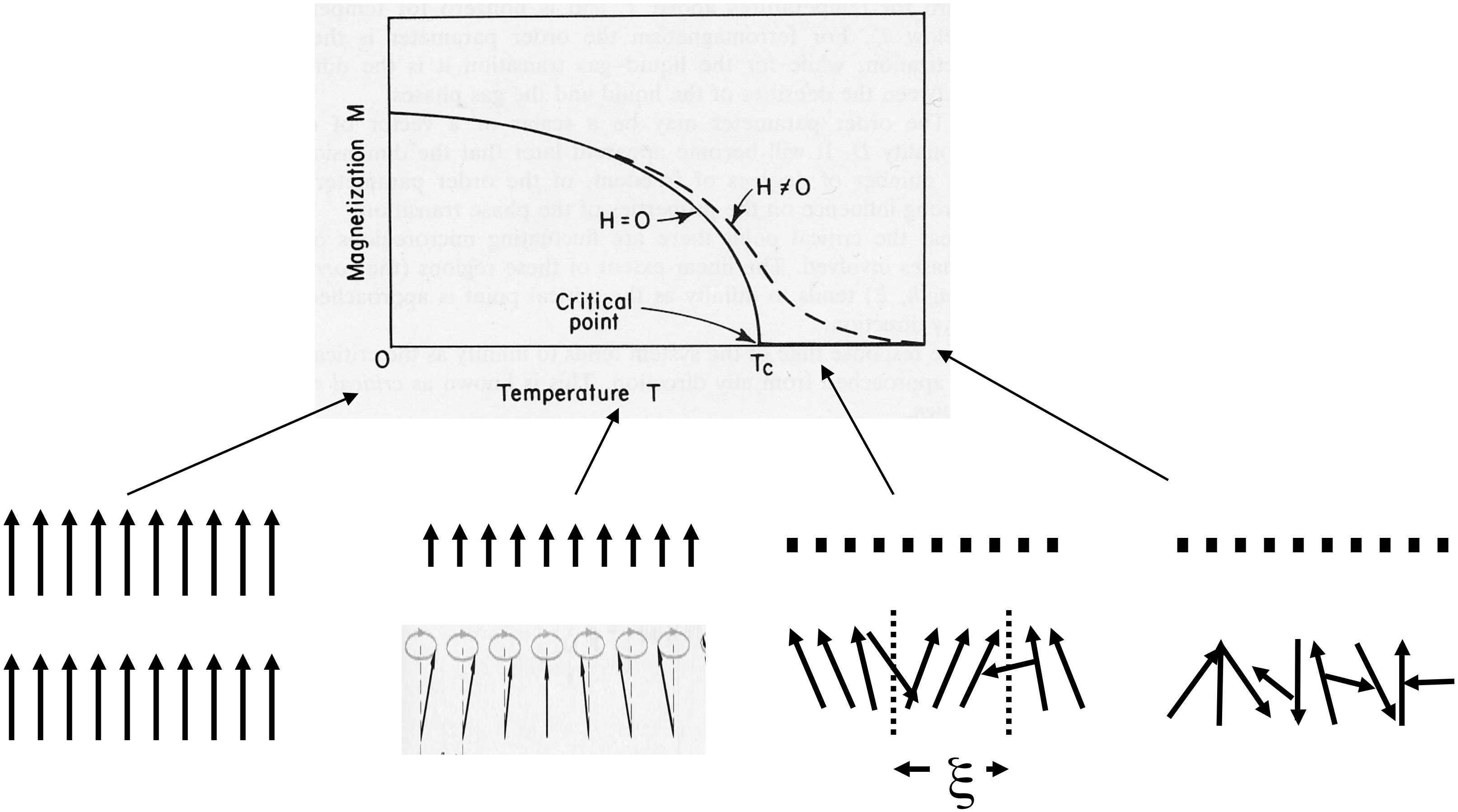
Temperature dependence of the spin excitations in $Sr_3Ru_2O_7$



L. Capogna *et al*., Phys. Rev. B **87** (1998) 143

Magnetic phase transitions

The magnetic structure of a simple ferromagnet as a function of temperature



Time-average
$(\hbar\omega = 0)$

Snapshot

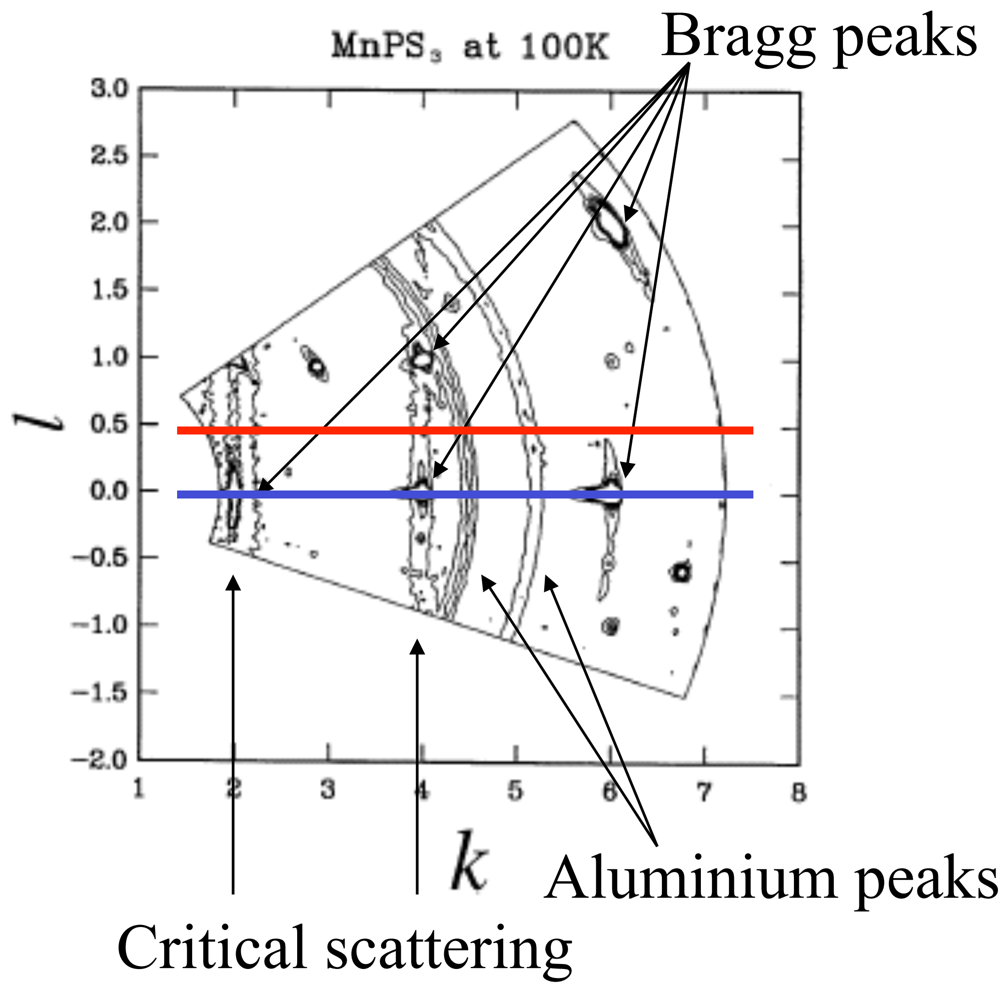
$(\int_{-\infty}^{\infty} \hbar\omega)$

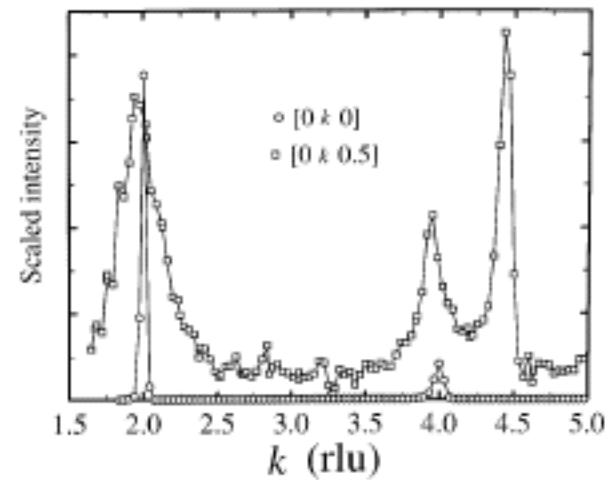
Renormalization theory and universality:

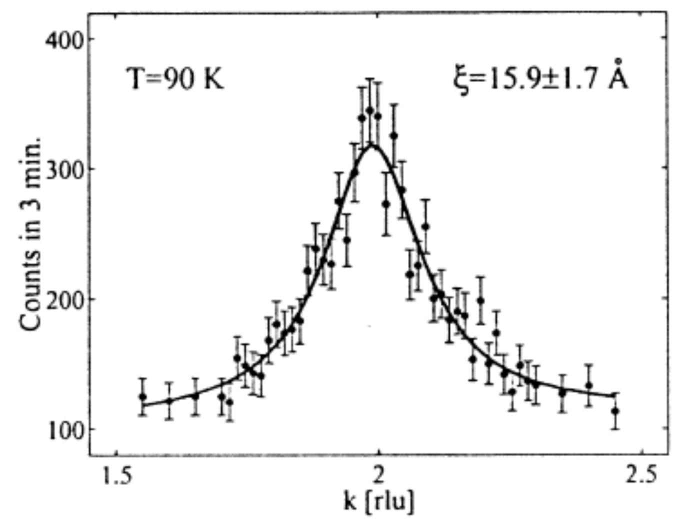
$$M(T) \propto (T-T_N)^{-\beta} \quad \xi(T) \propto (T-T_N)^{-\nu}$$

M. F. Collins, *Magnetic critical scattering*, 1989, Oxford University, Oxford

Magnetic critical scattering in $MnPS_3$





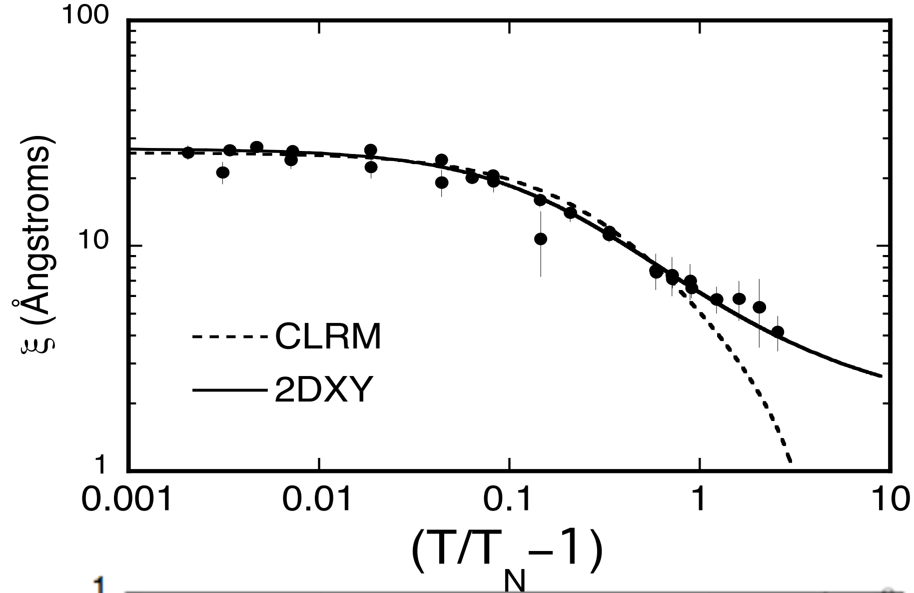


A.R. Wildes *et al*., J. Magn. Magn. Mater. **87** (1998) 143

Magnetic critical scattering in $MnPS_3$

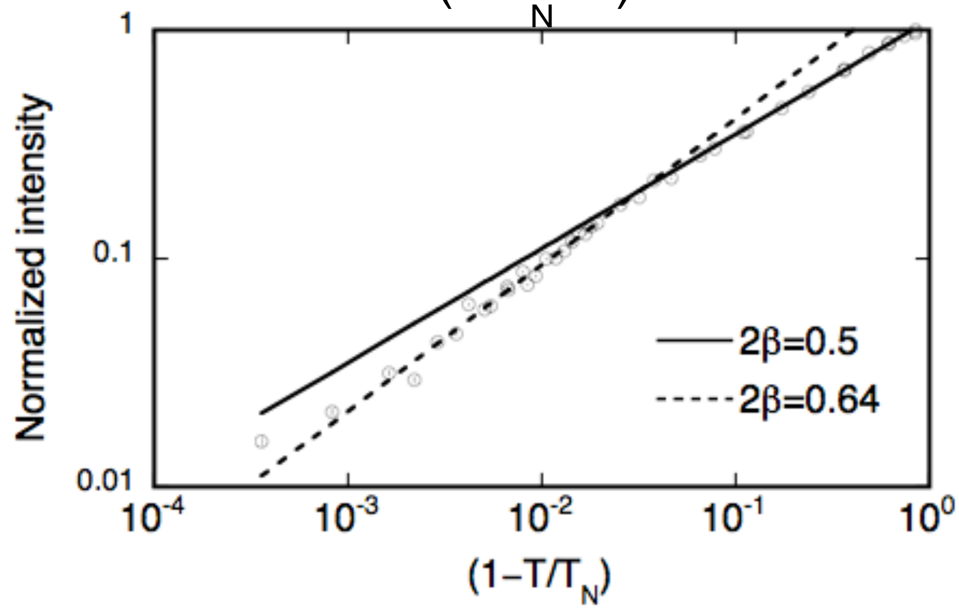
Correlation length
(from the widths of the rods, *energy integrated*)

H.M. Rønnow *et al.*, Physica B **276-278** (2000) 676



Sublattice magnetization
(from the intensities of the Bragg peaks, *zero energy transfer*)

A. R. Wildes *et al.*, PRB **74** (2006) 094422



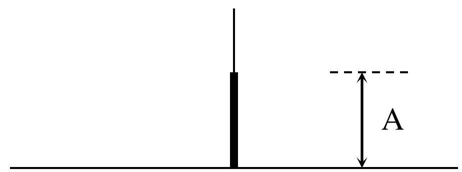
Diffuse scattering from a paramagnet

An ideal paramagnet has no correlation in space *or* time

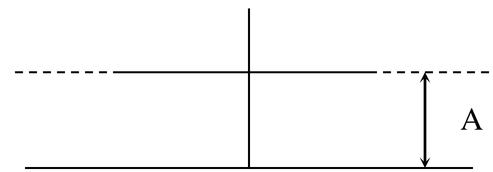
Fourier transforms

A Delta function

$f(\mathbf{x})$



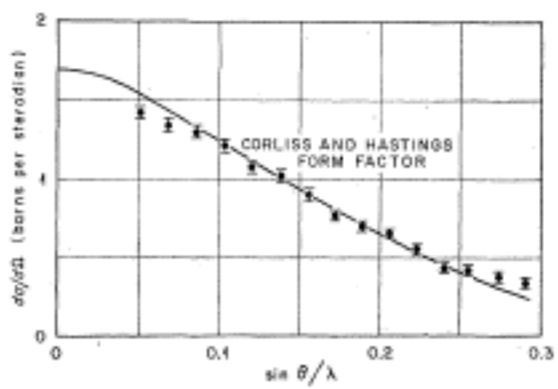
$F(\mathbf{X})$



For a paramagnet, $z(\mathbf{r}) = \delta(r)$, and must *integrate* over energy

$$\frac{d\sigma^{\pm\mp}}{d\Omega} \propto \frac{2}{3} f^2(Q) S(S+1)$$

Paramagnetic scattering from MnF_2



R. M. Moon, T. Riste and W. K. Koehler, Phys. Rev. **181** (1969) 920

Neutrons and bulk susceptibility

If neutrons measure the generalized susceptibility,
it must be possible to convert between bulk susceptibility measurements and neutron cross-sections.
This can be done using the Kramers-Krönig relation:

$$\int d\omega \frac{\chi''(\mathbf{Q},\omega)}{\omega} = \pi\chi'(\mathbf{Q},\omega)$$

Integrate the neutron scattering over all energies:

$$\frac{d\sigma}{d\Omega} = \int \hbar\, d\omega \left(\frac{d^2\sigma}{d\Omega d\omega}\right)$$

$$\propto k_B T \sum_\alpha \chi'_{\alpha\alpha}(\mathbf{Q},0)$$

Bulk susceptibility measures the real part of the susceptibility.
Bulk susceptibility averages over all the sample, which is equivalent to $\mathbf{Q} = 0$.

$$i.e. \frac{d\sigma}{d\Omega}(\mathbf{Q}=0) \propto k_B T \chi'$$

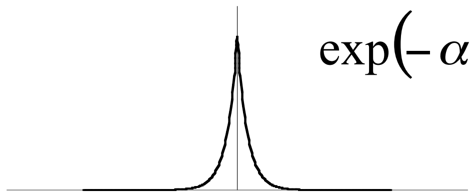
Bulk susceptibility can be put as a point on a neutron scattering plot!

Diffuse scattering from a paramagnet

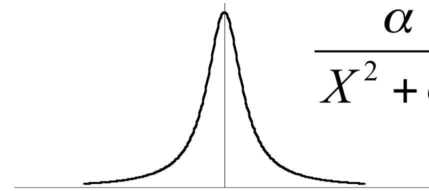
Paramagnets/spin glasses always have some correlations, particularly in time

$f(\mathbf{x})$ $F(\mathbf{X})$

An exponential

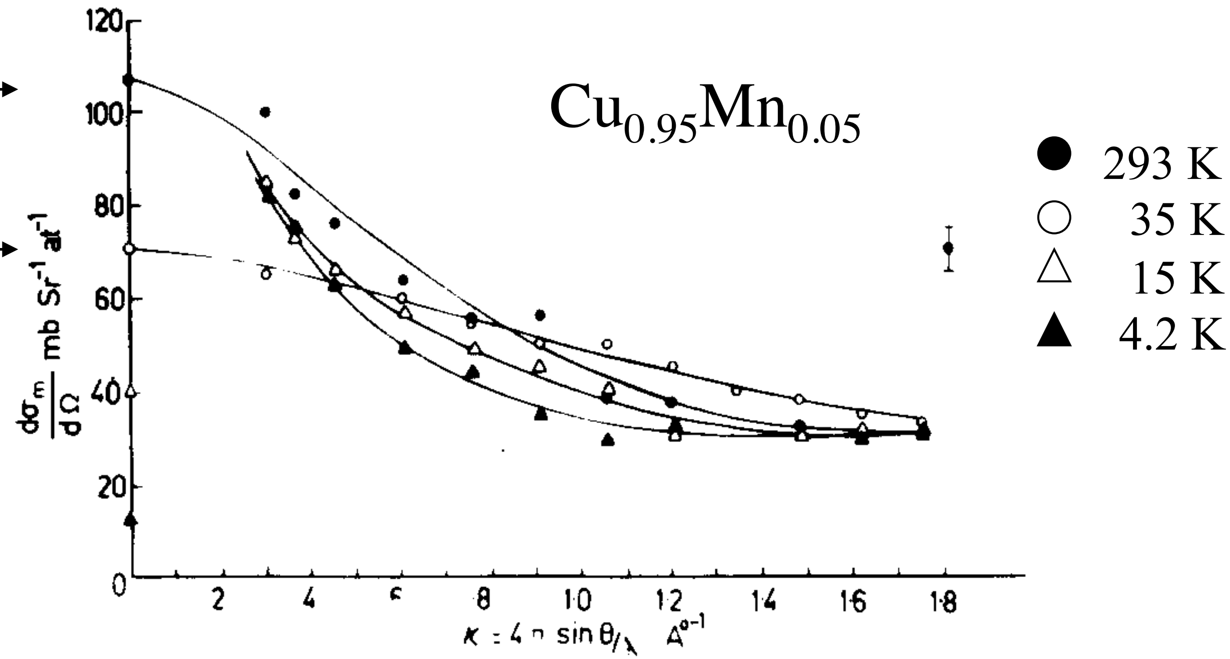


$\exp(-\alpha|x|)$



$$\frac{\alpha}{X^2+\alpha^2}$$

Points taken from bulk susceptibility



N. Ahmed and T. J. Hicks, Solid State Comm. **15** (1974) 415

T. J. Hicks, *Magnetism in disorder*, 1995, Clarendon, Oxford

Diffuse scattering and short-ranged order

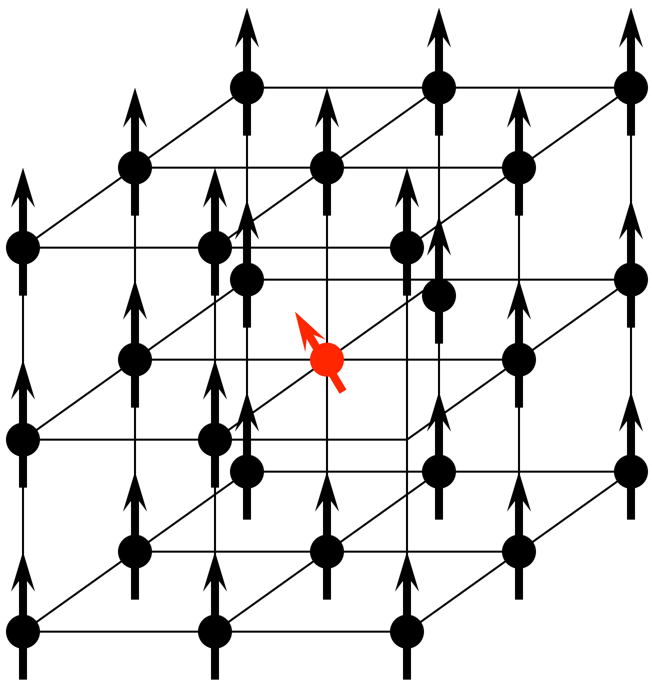
$$\left(\left|\left\langle \hat{V}^2 \right\rangle\right| - \left|\left\langle \hat{V} \right\rangle\right|^2\right) \int z(\mathbf{r}) e^{i\mathbf{Q}\cdot\mathbf{r}} \cdot d\mathbf{r}$$

Take a magnetic moment at the origin.

$z(\mathbf{r})$ describes the probability of finding the same moment at position $\mathbf{r}$.

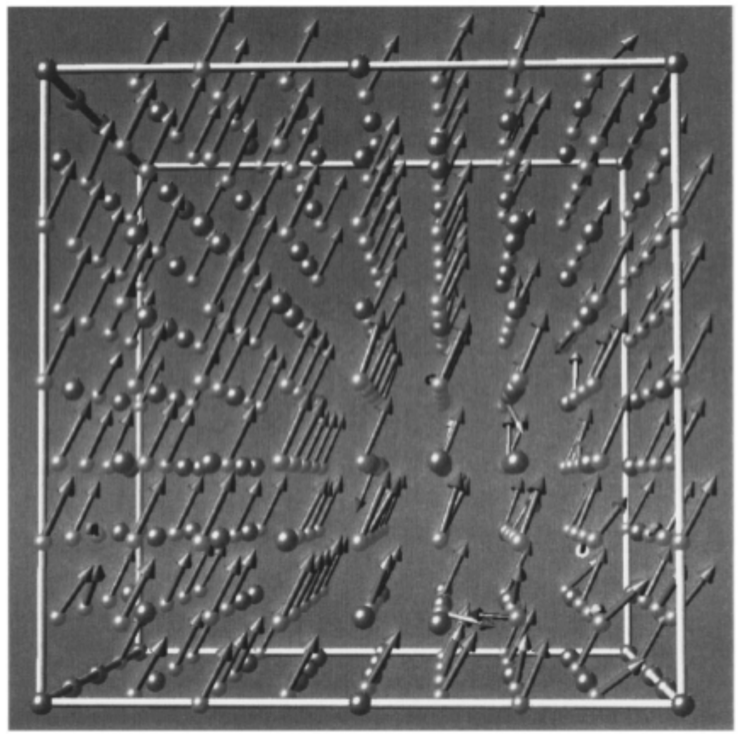
In a crystalline material the integral becomes a sum over neighbours

$$\propto S(S+1) + \sum_{R_n} \left\langle \mathbf{S}_0 \cdot \mathbf{S}_{R_n} \right\rangle \frac{\sin(QR_n)}{QR_n}$$



"Short-ranged" order can still extend over many nanometres

Calculation of the magnetic structure of $Ni_{0.65}Fe_{0.35}$

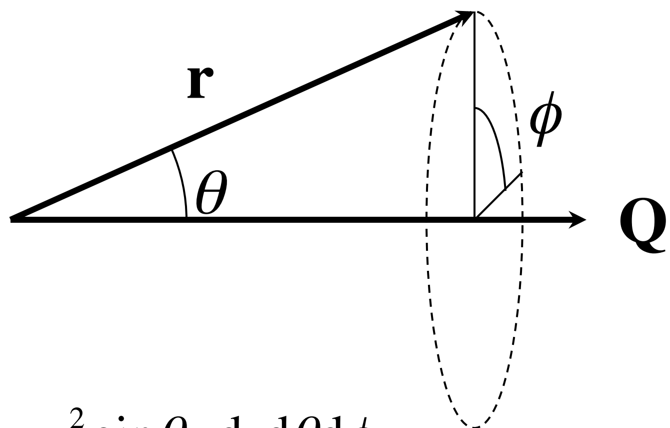


256 atoms, Yang *et al*. J. Appl. Phys. **81** (1997) 3973

Isotropic Fourier Transforms

Most magnetic diffuse scattering experiments are done on powders

In the case of scattering that is isotropic in three dimensions:



$$\mathrm{d}\mathbf{r} = r^2 \sin\theta \cdot \mathrm{d}r\mathrm{d}\theta\mathrm{d}\phi$$

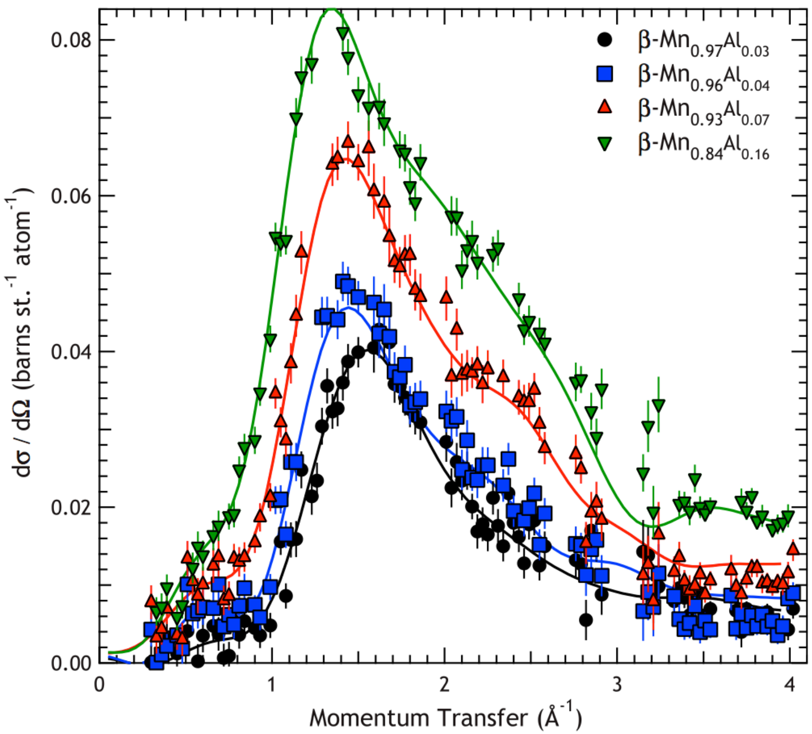
$$\mathbf{Q}\cdot\mathbf{r} = Qr\cos\theta$$

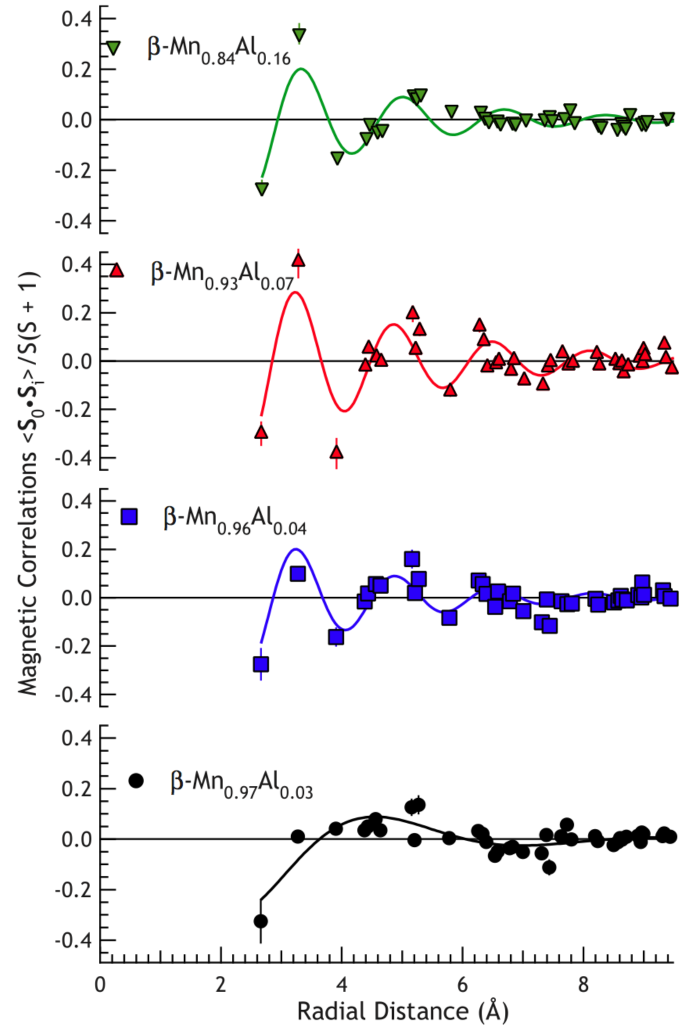
$$\int_{-\infty}^{\infty} f(\mathbf{Q})\exp(i\mathbf{Q}\cdot\mathbf{r})\cdot \mathrm{d}\mathbf{r} = 4\pi\int_0^{\infty} r^2 f(r)\frac{\sin Qr}{Qr}\cdot \mathrm{d}r$$

Short-range order in β-MnAl

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

$$\propto S(S+1) + \sum_{R_n} \left\langle \mathbf{S}_0 \cdot \mathbf{S}_{R_n} \right\rangle \frac{\sin(QR_n)}{QR_n}$$

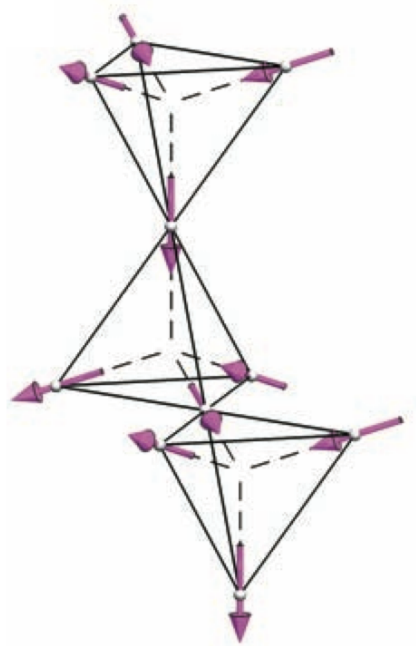




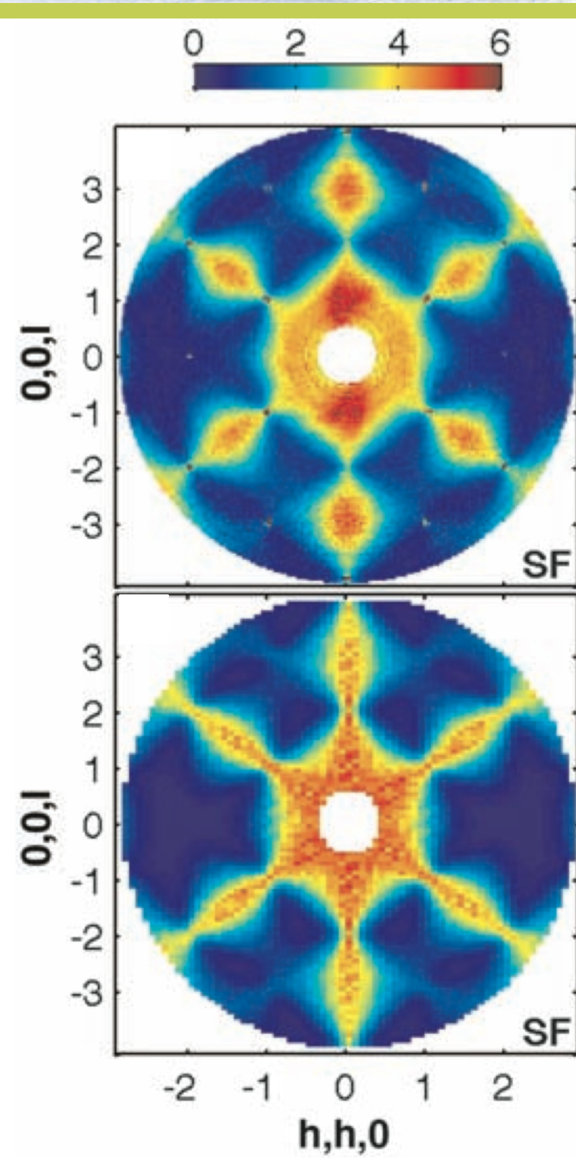
J. R. Stewart *et al*., Phys. Rev. B **78** (2008) 014428

Diffuse scattering from $Ho_2Ti_2O_7$

$Ho_2Ti_2O_7$ is a 'spin-ice' compound



T. Fennell *et al*., Science **326** (2009) 1177582

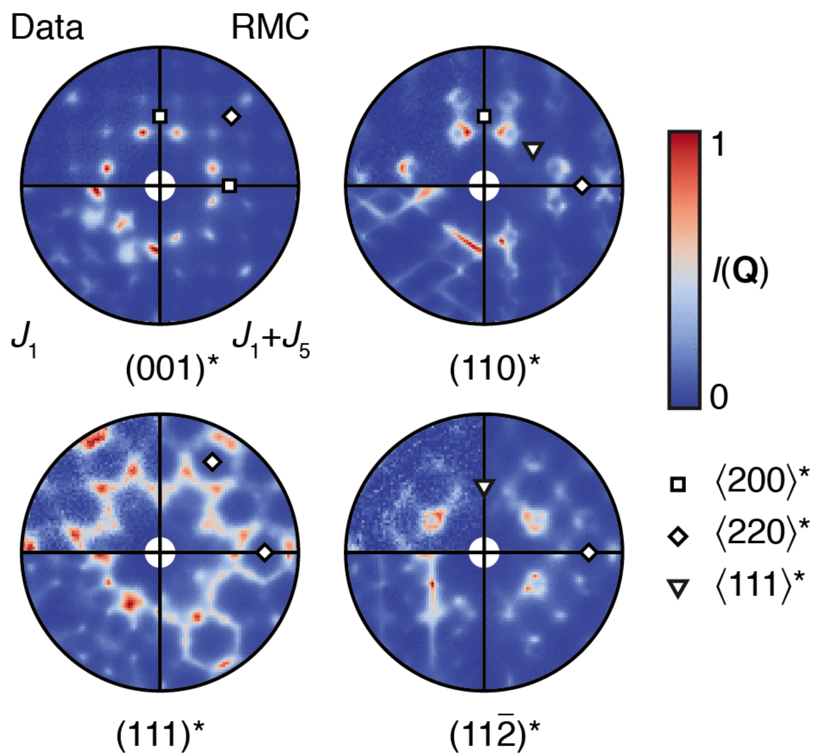


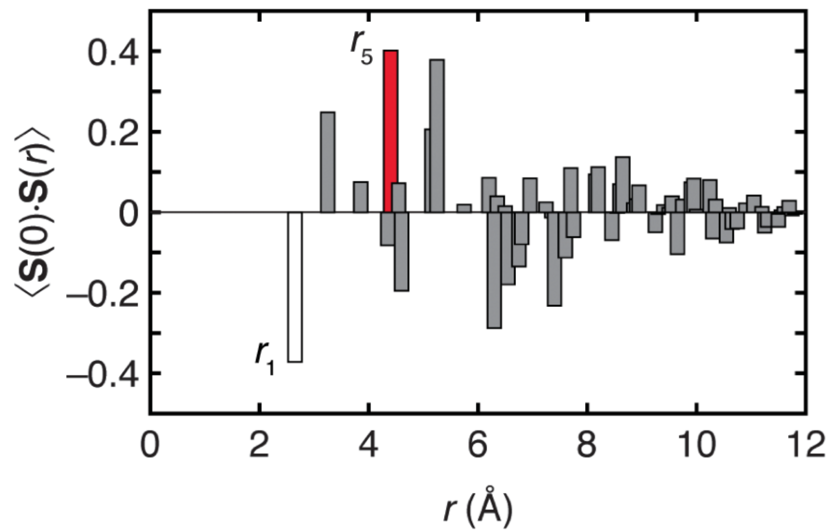
Data

Calculation

Diffuse scattering in $Mn_{0.8}Co_{0.2}$

Use of "Reverse Monte-Carlo" to fit data





J. A. M. Paddison *et al.*, PRL **110** (2013) 267207

Conclusions:

- Learn your Fourier transforms
- Get used to using vectors
- 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*
- Neutron scattering can measure a susceptibility
- Be conscious of the relationship between time and energy, particularly for diffuse scattering
- Analysing diffuse scattering is non-trivial