Magnetic Scattering

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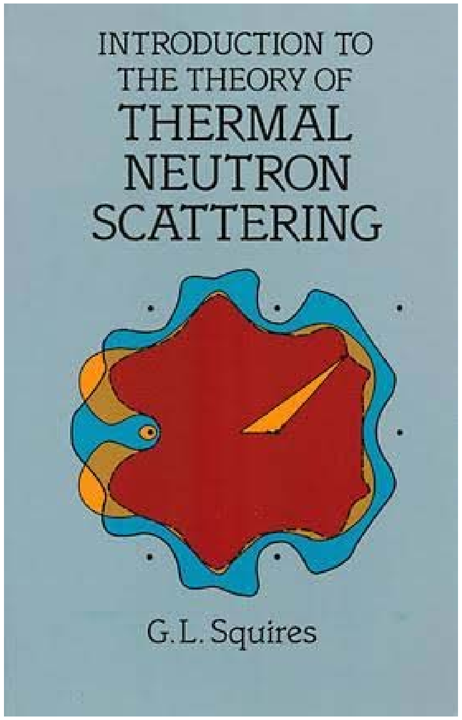
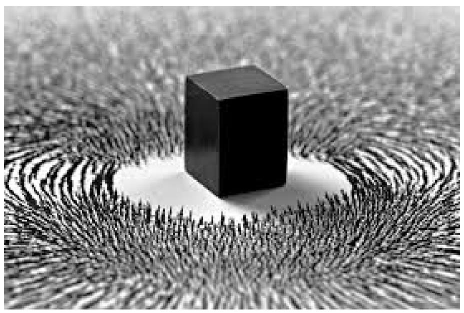


Ch 7 - 8

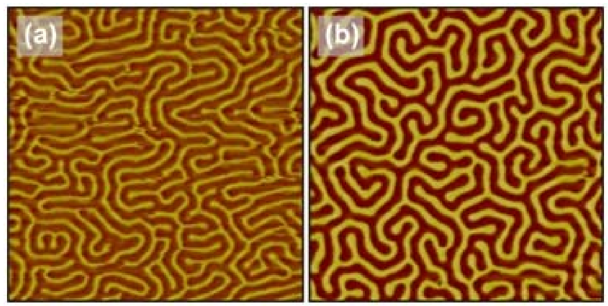
Magnetic Materials

Length Scale



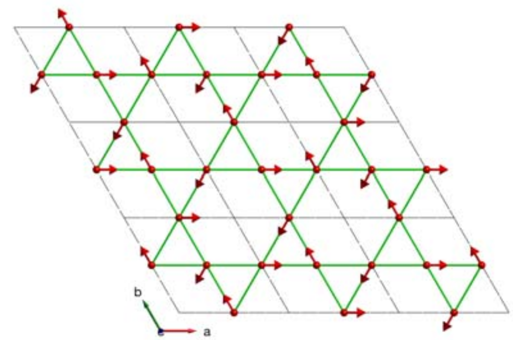
naked eye

Permanent magnet



magnetic force microscope

GdFe multilayer films



Magnetic neutron diffraction

Kagome antiferromagnet

Electron Configuration- Hund‘s Rules

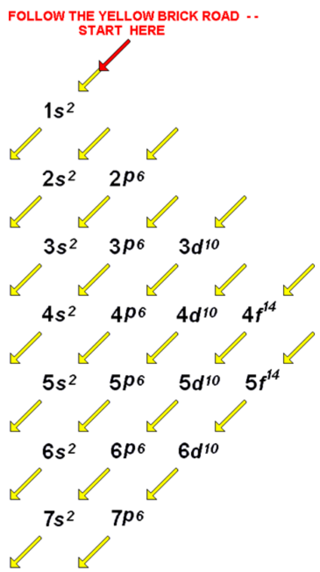
back to modern physics

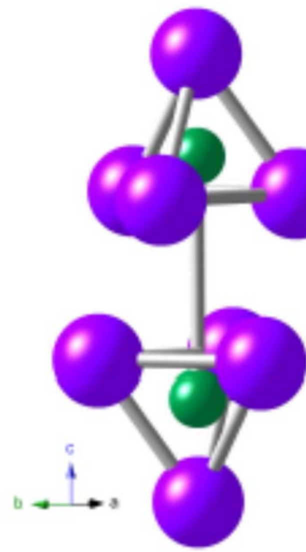
Group / Period	1	2		3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	1 **H** 1.008																		2 **He** 4.0026
2	3 **Li** 6.94	4 **Be** 9.0122												5 **B** 10.81	6 **C** 12.011	7 **N** 14.007	8 **O** 15.999	9 **F** 18.998	10 **Ne** 20.180
3	11 **Na** 22.990	12 **Mg** 24.305												13 **Al** 26.982	14 **Si** 28.085	15 **P** 30.974	16 **S** 32.06	17 **Cl** 35.45	18 **Ar** 39.948
4	19 **K** 39.098	20 **Ca** 40.078		21 **Sc** 44.956	22 **Ti** 47.867	23 **V** 50.942	24 **Cr** 51.996	25 **Mn** 54.938	26 **Fe** 55.845	27 **Co** 58.933	28 **Ni** 58.693	29 **Cu** 63.546	30 **Zn** 65.38	31 **Ga** 69.723	32 **Ge** 72.63	33 **As** 74.922	34 **Se** 78.96	35 **Br** 79.904	36 **Kr** 83.798
5	37 **Rb** 85.468	38 **Sr** 87.62		39 **Y** 88.906	40 **Zr** 91.224	41 **Nb** 92.906	42 **Mo** 95.96	43 **Tc** [97.91]	44 **Ru** 101.07	45 **Rh** 102.91	46 **Pd** 106.42	47 **Ag** 107.87	48 **Cd** 112.41	49 **In** 114.82	50 **Sn** 118.71	51 **Sb** 121.76	52 **Te** 127.60	53 **I** 126.90	54 **Xe** 131.29
6	55 **Cs** 132.91	56 **Ba** 137.33	*	71 **Lu** 174.97	72 **Hf** 178.49	73 **Ta** 180.95	74 **W** 183.84	75 **Re** 186.21	76 **Os** 190.23	77 **Ir** 192.22	78 **Pt** 195.08	79 **Au** 196.97	80 **Hg** 200.59	81 **Tl** 204.38	82 **Pb** 207.2	83 **Bi** 208.98	84 **Po** [208.98]	85 **At** [209.99]	86 **Rn** [222.02]
7	87 **Fr** [223.02]	88 **Ra** [226.03]	**	103 **Lr** [262.11]	104 **Rf** [265.12]	105 **Db** [268.13]	106 **Sg** [271.13]	107 **Bh** [270]	108 **Hs** [277.15]	109 **Mt** [276.15]	110 **Ds** [281.16]	111 **Rg** [280.16]	112 **Cn** [285.17]	113 **Uut** [284.18]	114 **Fl** [289.19]	115 **Uup** [288.19]	116 **Lv** [293]	117 **Uus** [294]	118 **Uuo** [294]

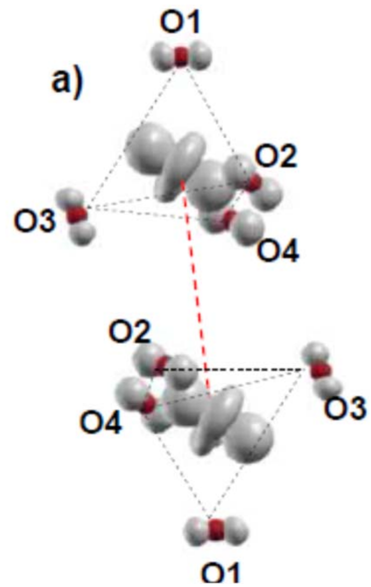
*Lanthanoids	*	57 **La** 138.91	58 **Ce** 140.12	59 **Pr** 140.91	60 **Nd** 144.24	61 **Pm** [144.91]	62 **Sm** 150.36	63 **Eu** 151.96	64 **Gd** 157.25	65 **Tb** 158.93	66 **Dy** 162.50	67 **Ho** 164.93	68 **Er** 167.26	69 **Tm** 168.93	70 **Yb** 173.05
**Actinoids	**	89 **Ac** [227.03]	90 **Th** 232.04	91 **Pa** 231.04	92 **U** 238.03	93 **Np** [237.05]	94 **Pu** [244.06]	95 **Am** [243.06]	96 **Cm** [247.07]	97 **Bk** [247.07]	98 **Cf** [251.08]	99 **Es** [252.08]	100 **Fm** [257.10]	101 **Md** [258.10]	102 **No** [259.10]

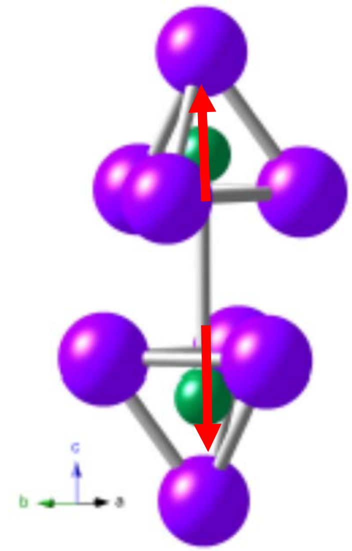
Magnetic Ions

back to modern physics









Orbital angular momentum:

$$L = \sum_i l_i$$

Spin quantum number:

$$S = \sum_i s_i$$

Total angular momentum:

$$J = L + S$$

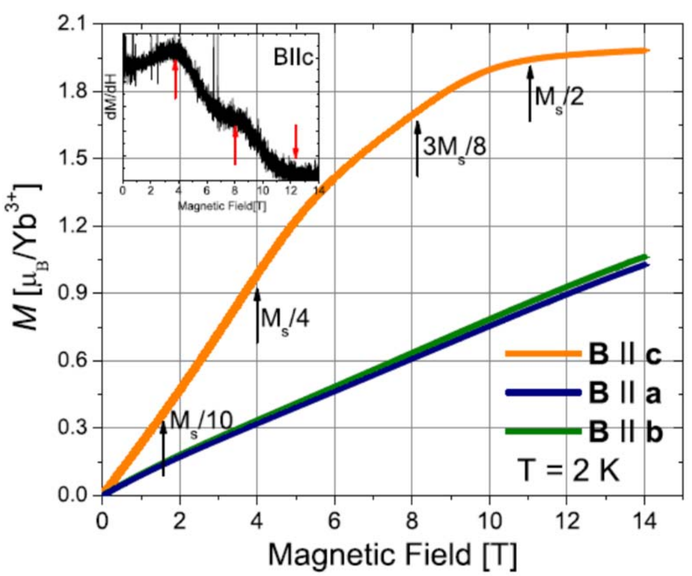
Total Magnetic moment

For an electron with l=1: Lz=h

$$\mu_B = \frac{e\,h}{2m_e} = 9.274 \times 10^{-24} J/T$$

Bohr Magneton – used as a Unit

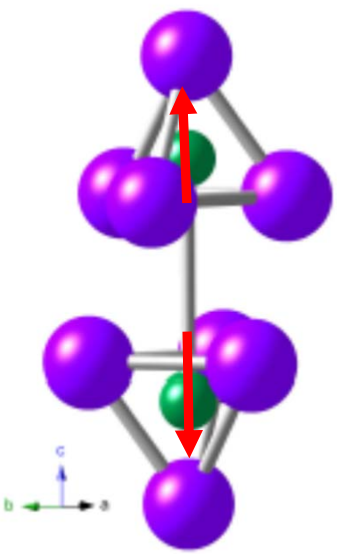
$$\mu_{eff} = g\mu_B\sqrt{J(J+1)}$$



Quintero, PRB 2010

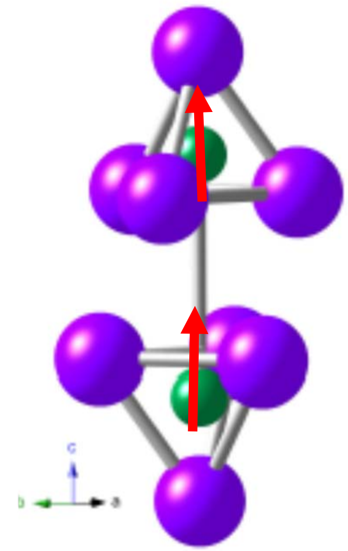
Magnetic Exchange Interaction

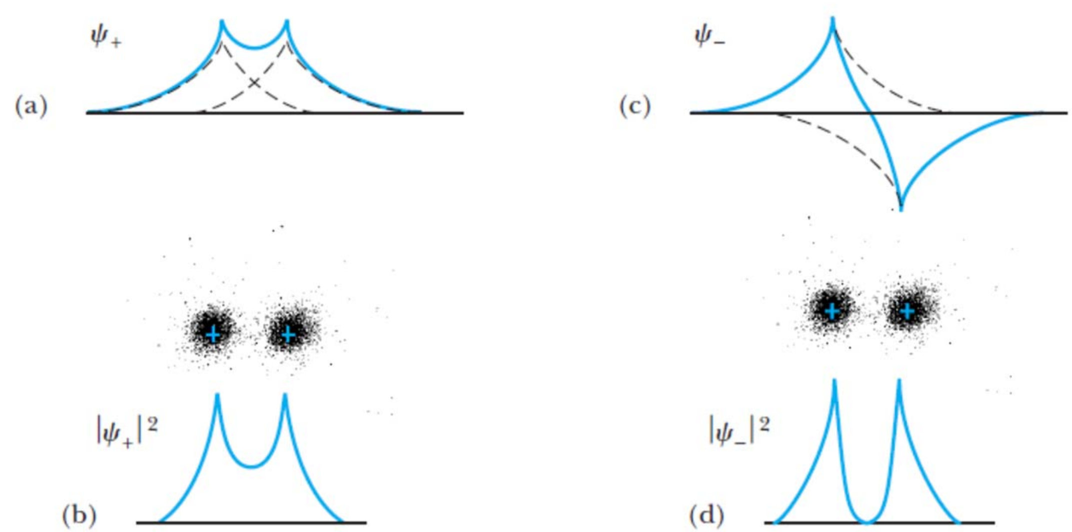
AFM interaction



$$H_{ij} = -J_{ij}\boldsymbol{S}_i.\boldsymbol{S}_j$$

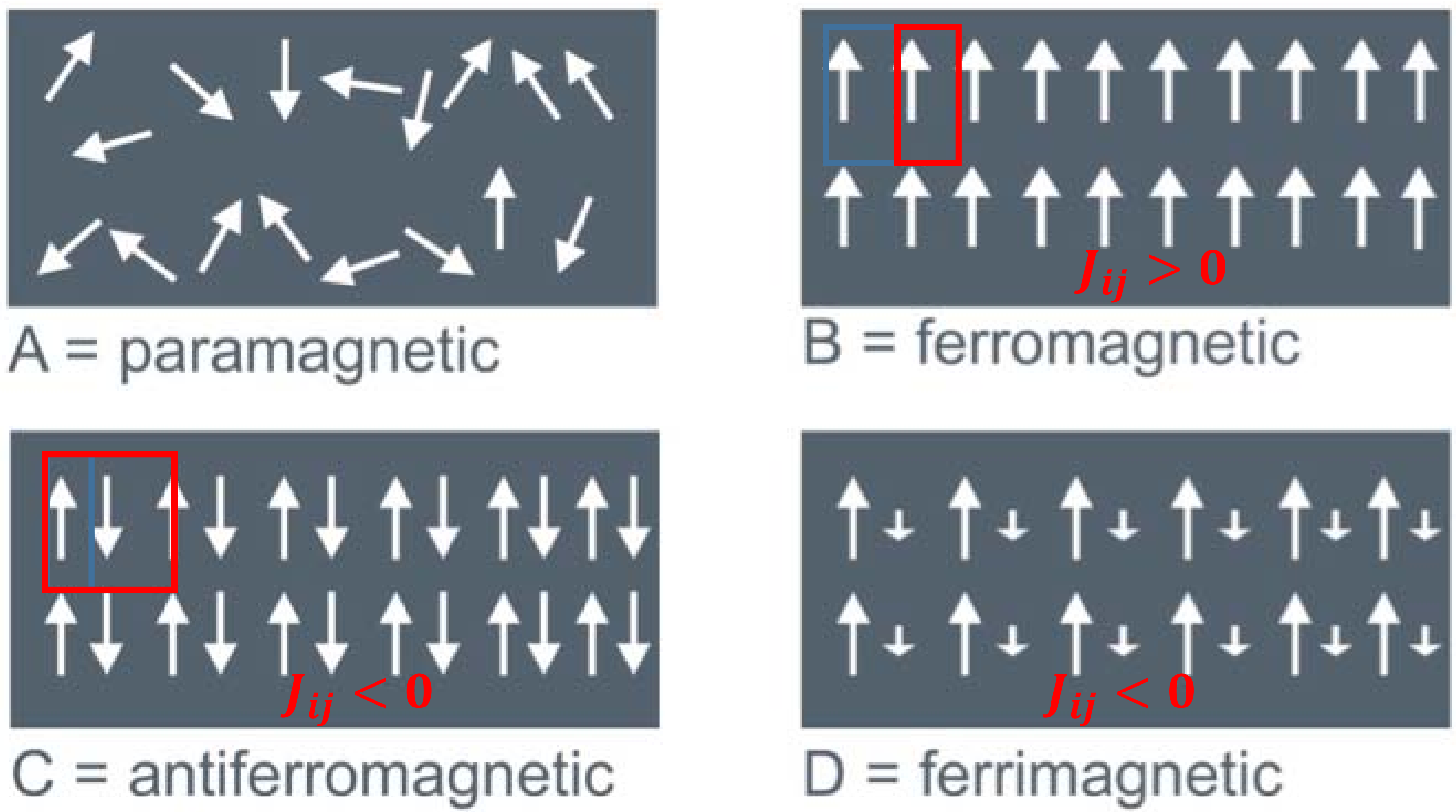
FM interaction





Static Magnetic Ordering

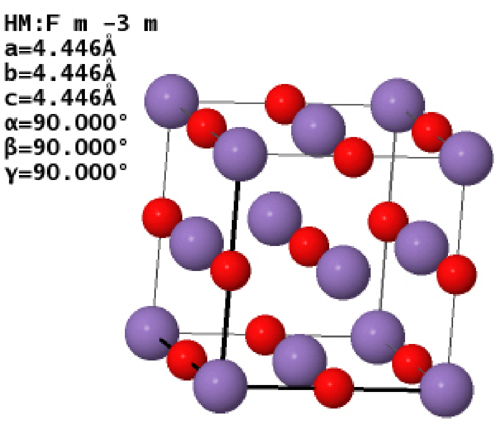
$$H_{ij} = -J_{ij}\boldsymbol{S}_i . \boldsymbol{S}_j$$

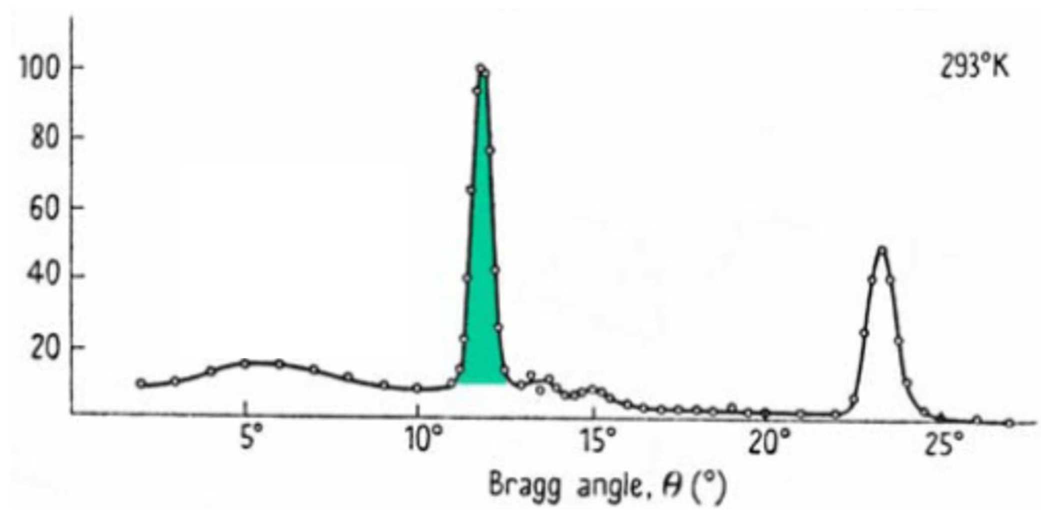


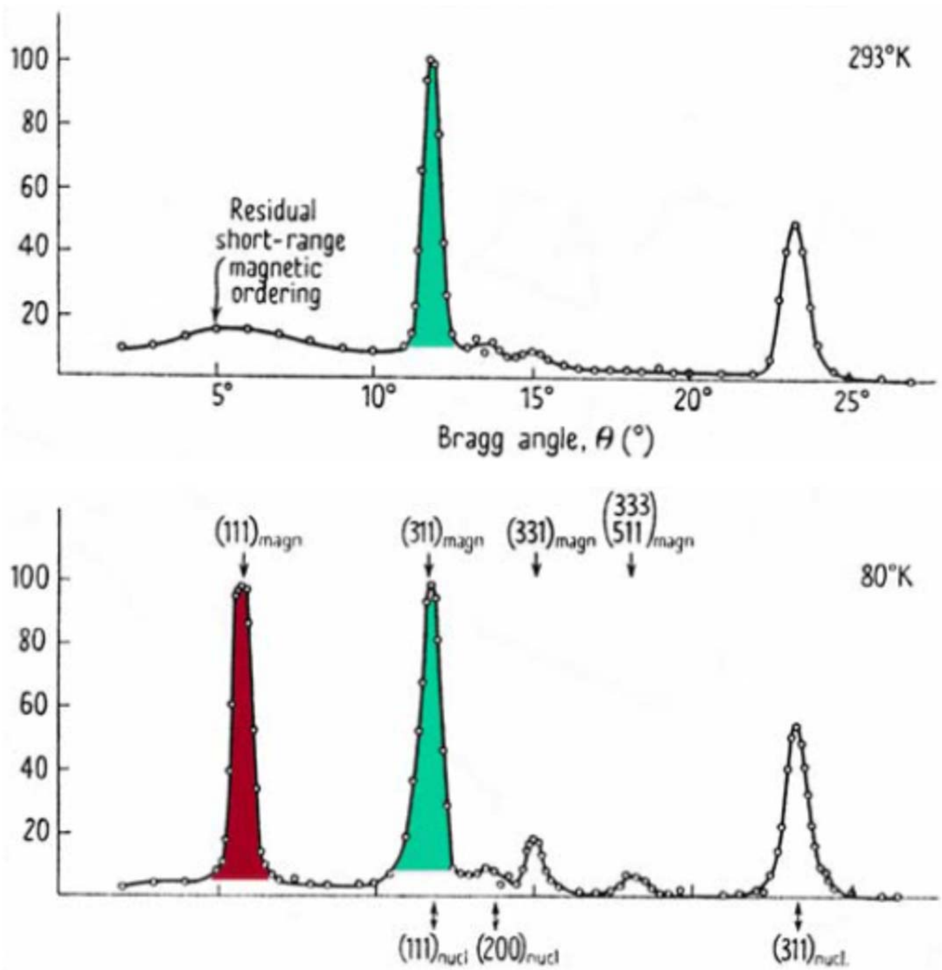
Example: Manganosite (MnO)

Space Group	F m -3 m(225)	Pearson Symbol	cF8	Meas. Dens.	5.36
Crystal System	cubic	Crystal Class	m-3m	Laue Class	m-3m
Wyckoff Sequence	b a	Structure Type	NaCl		
Axis Ratios	a/b 1.0000	b/c 1.0000	c/a 1.0000		
Remark					

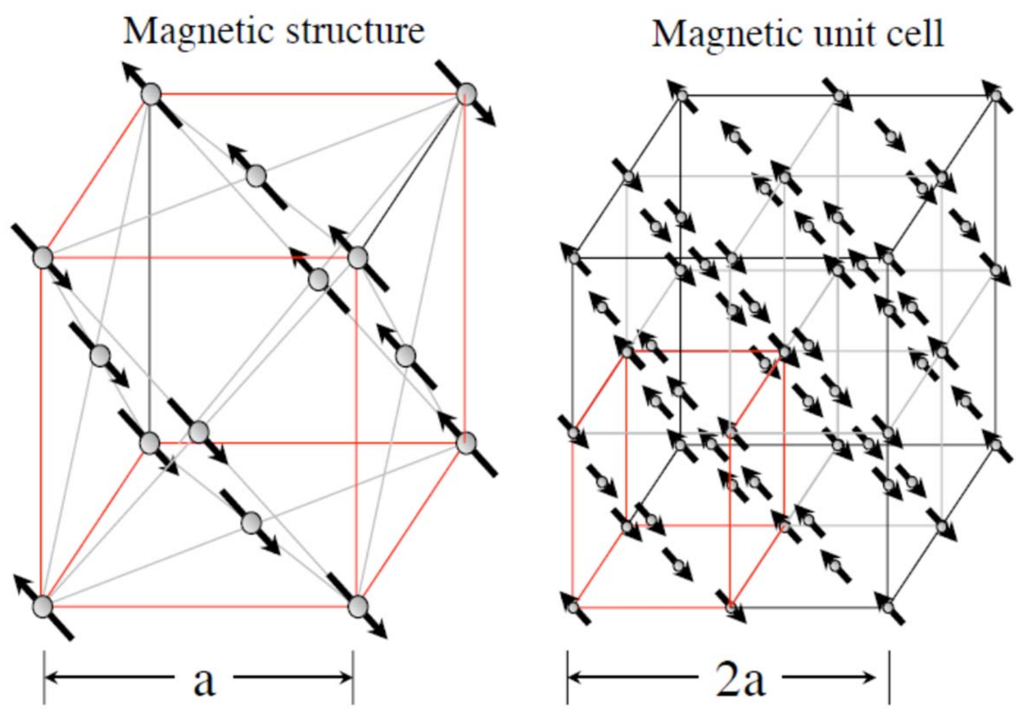
EL	Lbl	OxState	WyckSymb	X	Y	Z	B	SOF	H
Mn	1	+2.00	4a	0	0	0	0.617(5)		
O	1	-2.00	4b	0.5	0.5	0.5	0.72(1)		





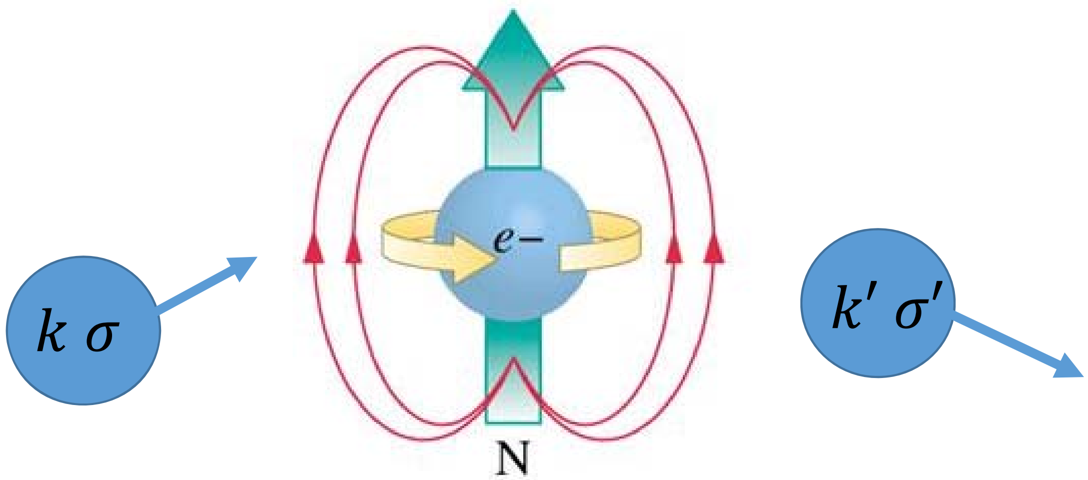


Mn2+
Electronic configuration:
(3d5) S = 5/2, l=0,



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

Partial differential cross section



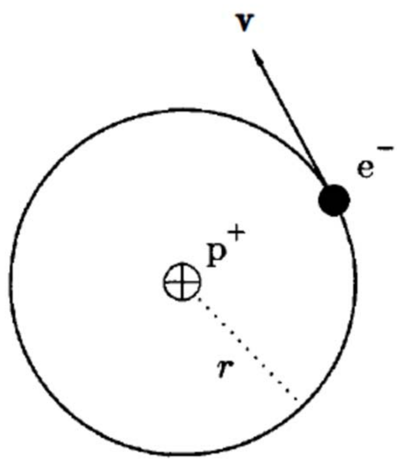
$\lambda \quad to \quad \lambda'$

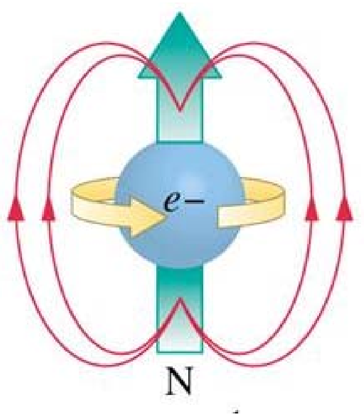
$$\frac{d^2\sigma}{d\Omega dE_f} = \frac{k_f}{k_i}\left(\frac{m_n}{2\pi\hbar^2}\right)^2 \left|\langle \lambda' k' \sigma' | \hat{V} | \lambda k \sigma \rangle\right|^2 \delta(E_\lambda - E_{\lambda'} + \hbar\omega)$$

Dipole-dipole interaction

Magnetic Moment of Electron Systems

back to electrodynamics





Orbital contribution:

$$\boldsymbol{\mu}_l = \mu_B \boldsymbol{l}$$

Spin contribution:

$$\boldsymbol{\mu}_s = g\mu_B \boldsymbol{s}$$

$$g = 2.0023$$

By now—
Only spin contribution

$$\boldsymbol{\mu}_e = g\mu_B \boldsymbol{s}$$

Bohr magneton:

$$\mu_B = -\pi r^2 I = \frac{rev}{2} = -\frac{e\hbar}{2m_e}$$

$$\mu_B = 5.788.10^{-5} eV/T$$

Neutron‘s magnetic properties

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

$$\boldsymbol{\mu_n} = -\gamma \mu_B \frac{m_e}{m} \hat{\boldsymbol{\sigma}}$$

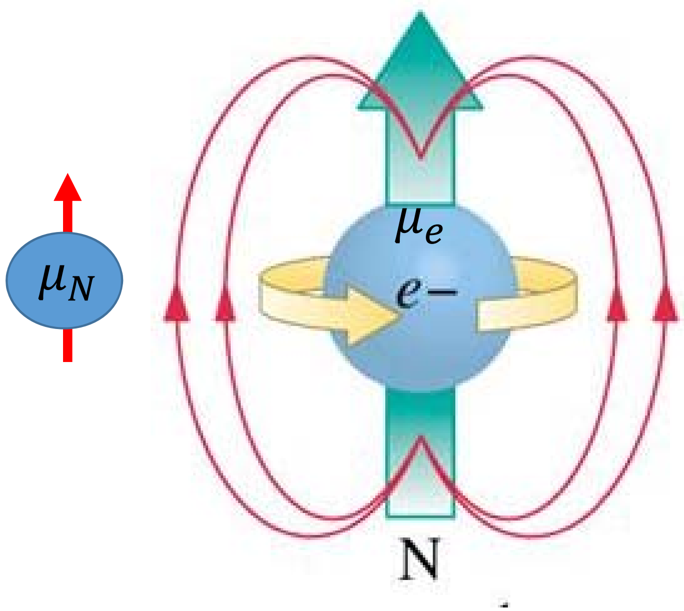
Gyromagnetic ratio, $\gamma = 1.97$

$\hat{\sigma}$: Pauli spin operator, eigenvalues ± 1

And for the electron: $\boldsymbol{\mu_e} = g\mu_B \boldsymbol{s}$

$$\mu_n \ll \mu_e, \qquad \frac{\mu_e}{\mu_n} = \frac{m}{m_e \gamma} = \frac{1836}{1.913} = 960$$

Potential energy of a dipole in a field



Potential:

$$V(\vec{r}) = -\vec{\mu}.\vec{B}(\vec{r})$$

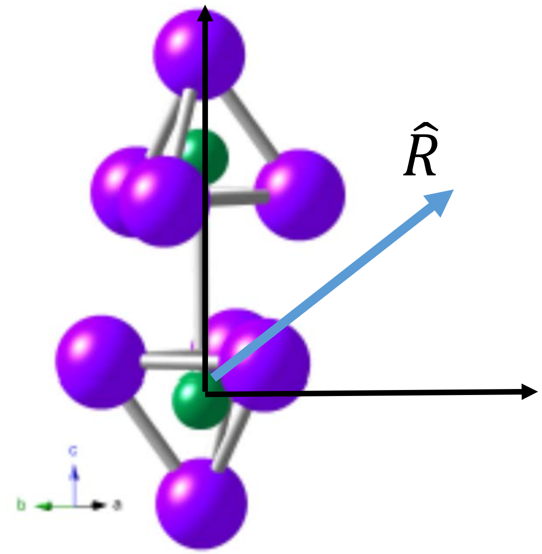
Torque:

$$\vec{\tau} = \vec{\mu} \times \vec{B}$$

Force:

$$\vec{F} = \nabla(\vec{\mu}.\vec{B})$$

Generated Magnetic Field by one electron



$$\vec{B} = \frac{\mu_0}{4\pi}\vec{\nabla}\times\left(\frac{\vec{\mu}_e\times\hat{R}}{R^2}\right) = \frac{\mu_0}{4\pi}\vec{\nabla}\times\left(g\mu_B\frac{\vec{s}\times\vec{R}}{R^3}\right)$$

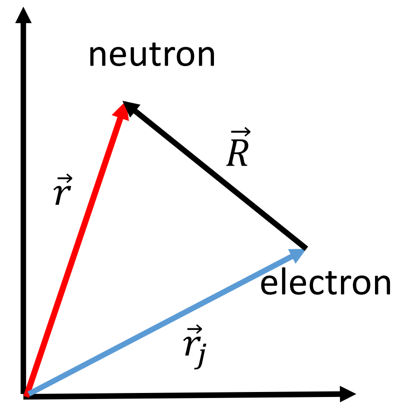
$$V(\vec{r}) = -\overrightarrow{\mu_n}.\left(\vec{\nabla}\times\left(\frac{\mu_0}{4\pi}g\mu_B\frac{\vec{s}\times\vec{R}}{R^3}\right)\right)$$

$$V(\vec{r}) = \gamma\mu_B\frac{m_e}{m}\hat{\boldsymbol{\sigma}}.\left(\vec{\nabla}\times\left(\frac{\mu_0}{4\pi}g\mu_B\frac{\vec{s}\times\vec{R}}{R^3}\right)\right)$$

$$V(\vec{r}) = \frac{\mu_0}{4\pi}g\mu_B^2\gamma\frac{m_e}{m}\hat{\boldsymbol{\sigma}}.\left(\vec{\nabla}\times\left(\frac{\vec{s}\times\vec{R}}{R^3}\right)\right)$$

Generated magnetic field by multiple electrons

$$\sum_j V(\vec{r}_j) = \sum_j \frac{\mu_0}{4\pi} g\mu_B^2 \gamma \frac{m_e}{m} \hat{\boldsymbol{\sigma}}. \left(\vec{\nabla} \times \left(\frac{\vec{s_j} \times (\vec{r} - \vec{r}_j)}{\left|\vec{r} - \vec{r}_j\right|^3} \right) \right)$$



Back to the partial differential cross section

$$\frac{d^2\sigma}{d\Omega dE_f} = \frac{k_f}{k_i} \left(\frac{m_n}{2\pi\hbar^2} \right)^2 \left| \langle \lambda' k' \sigma' | \hat{V} | \lambda' k \sigma \rangle \right|^2 \delta(E_\lambda - E_{\lambda'} + \hbar\omega)$$

$$\frac{d^2\sigma}{d\Omega dE_f} = \frac{k_f}{k_i} \left(\frac{m_n}{2\pi\hbar^2} \right)^2 \left| \left\langle \lambda' k' \sigma' \left| \frac{\mu_0}{4\pi} g\mu_B^2 \gamma \frac{m_e}{m} \hat{\boldsymbol{\sigma}}. \left(\vec{\nabla} \times \left(\frac{\vec{s_j} \times (\vec{r} - \vec{r}_j)}{\left|\vec{r} - \vec{r}_j\right|^3} \right) \right) \right| \lambda k \sigma \right\rangle \right|^2 \delta(E_\lambda - E_{\lambda'} + \hbar\omega)$$

The magnetic matrix element

$$\vec{\nabla} \times \left(\frac{\vec{s}\times\vec{r})}{|\vec{r}|^3}\right) = \frac{1}{2\pi^2}\int \hat{q}' \times (\vec{s} \times \hat{q}')e^{(i\vec{q}'.\vec{r})}d^3\vec{q}'$$

$$\frac{1}{2\pi^2}\left\langle \lambda' k' \sigma' \middle| \sum_j \int \hat{\boldsymbol{\sigma}}.(\hat{q}' \times (\vec{s_j} \times \hat{q}')e^{(i\vec{q}'.\vec{r_j})})d^3\vec{q}' \middle| \lambda k \sigma \right\rangle = 4\pi \left\langle \lambda'\sigma' \middle| \sum_j e^{(i\vec{q}.\vec{r_j})}\, \hat{\boldsymbol{\sigma}}.\hat{q} \times (\vec{s_j} \times \hat{q}) \middle| \lambda\sigma \right\rangle$$

$s_{j\perp}$

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

$$\mathrm{r}_0 \frac{g}{2} F(\vec{q})\langle \lambda'\sigma' | \hat{\boldsymbol{\sigma}}.\vec{s}_\perp | \lambda\sigma \rangle$$

Magnetic form factor:

$$F(\vec{q}) = \int s(\vec{r})e^{(i\vec{q}.\vec{r})}d\vec{r}$$

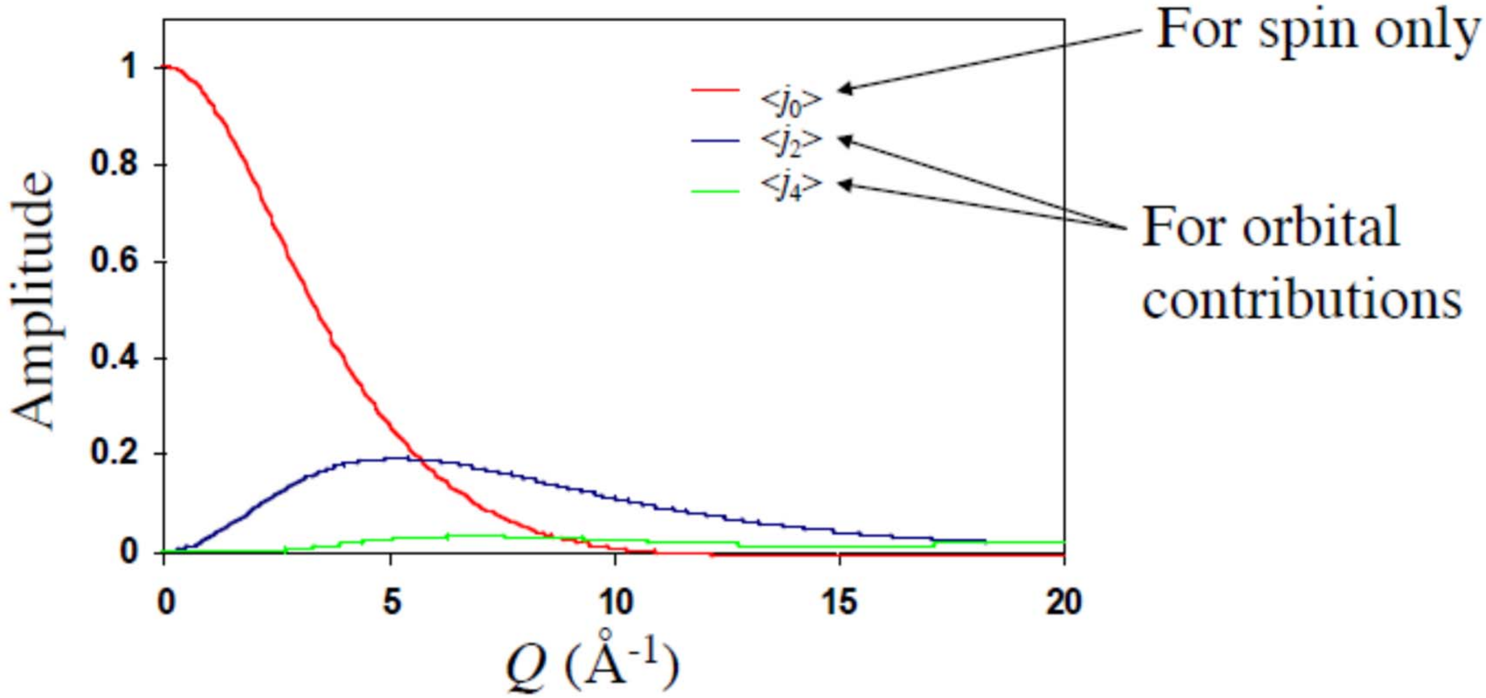
Spatial extend of the spin density

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



https://www.ill.eu/sites/ccsl/ffacts/ffachtml.html

Scattering cross section

$$\mathrm{r}_0 \frac{g}{2} F(\vec{q}) \langle \lambda' \sigma' | \hat{\boldsymbol{\sigma}} . \vec{s}_\perp | \lambda \sigma \rangle$$

Where, r_0 is the classical electron radius:

$$\mathrm{r}_0 = \gamma \frac{\mu_0}{4\pi} \frac{e^2}{m_e} = 0.54 \times 10^{-12}\ \mathrm{cm}$$

Similar to the bound coherence scattering length for many nuclei

- **We can only measure spin components perpendicular to the transfered momentum**
- **The strenght of the magnetic scattering is close to the nuclear scattering**
- **The magnetic scattering depends on the spatial distribution of the spin density of the sample**
- **The magnetic scattering strength falls off at high wave vector transfers**

Generalization

$$r_0 \frac{g}{2} F(\vec{q}) \langle \lambda' \sigma' | \hat{\boldsymbol{\sigma}} . \vec{s}_{\perp} | \lambda \sigma \rangle$$

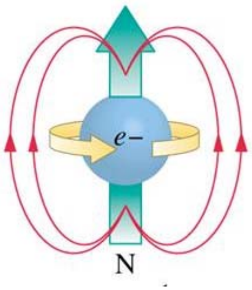
$$4\pi \vec{Q}_{\perp} = \sum_i \langle k' | W_{si} + W_{Li} | k \rangle$$

Spin

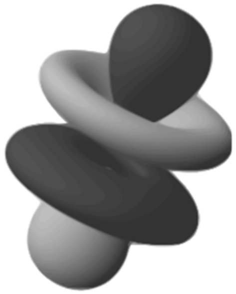
$$\vec{Q}_S = -\frac{1}{2\mu_B} \vec{M}_S(k)$$

Orbital

$$\overrightarrow{Q_{\perp L}} = -\frac{1}{2\mu_B} \hat{k} \times \{\vec{M}_L(k) \times \hat{k}\}$$



$$\vec{Q} = \vec{Q}_S + \vec{Q}_L = -\frac{1}{2\mu_B} \vec{M}(k)$$



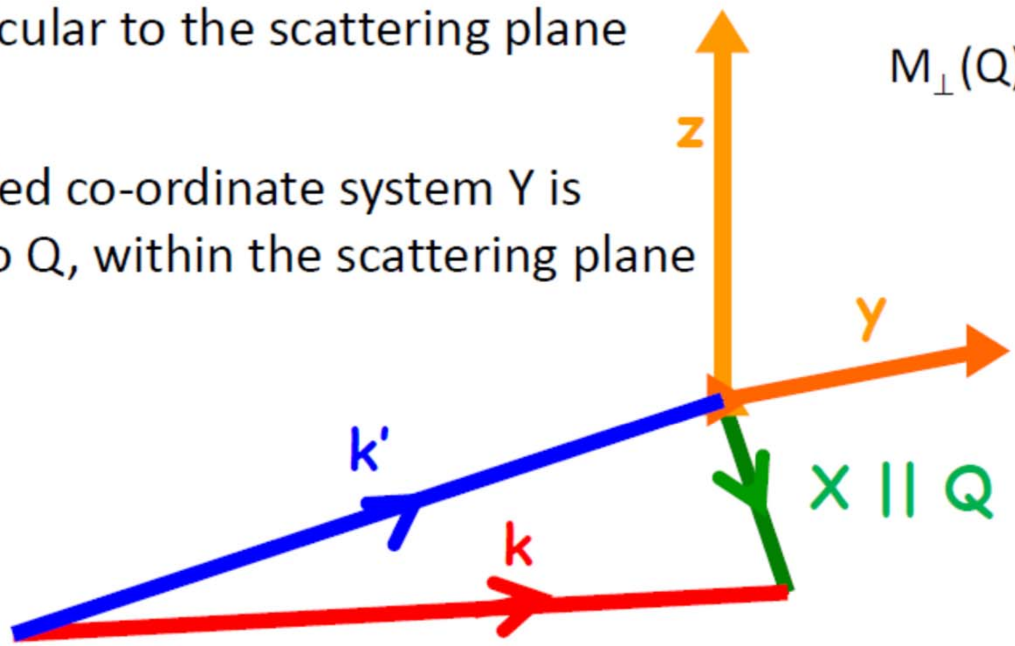
Fourier transform of the sample's total magnetization

Axes

X is parallel to Q

Z is perpendicular to the scattering plane

Right handed co-ordinate system Y is perpendicular to Q, within the scattering plane



Define the magnetic interaction vector:

$$M_{\perp}(Q) = \hat{Q} \times \left(-\frac{1}{2\mu_B} M(Q) \times \hat{Q} \right)$$

$$= \frac{1}{2\mu_B} \begin{pmatrix} 0 \\ M_y(Q) \\ M_z(Q) \end{pmatrix}$$

Scattering cross section – time dependence

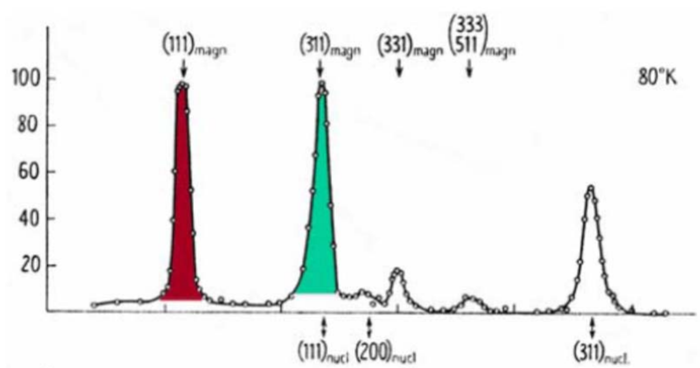
$$\frac{d^2\sigma}{d\Omega dE_f} = \frac{k_f}{k_i} r_0^2 \left|\frac{g}{2} F(\vec{q})\right|^2 e^{-2W(k)} \frac{1}{2\pi\hbar} \int dt\, e^{-i\omega t} \sum_j e^{i\vec{q}.(\vec{r}-\vec{r}_j)} \times \langle\langle\sigma|\vec{\sigma}.s_\perp(0)|\sigma'\rangle\langle\sigma'|\vec{\sigma}.s_\perp(t)|\sigma\rangle\rangle$$

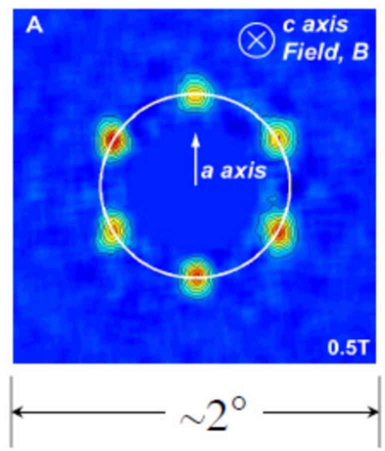
For unpolarized neutrons, $\sigma \leftrightarrow \sigma'$

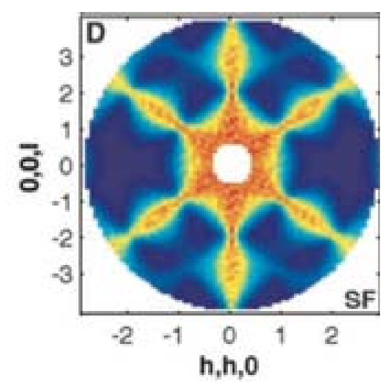
$$\frac{d^2\sigma}{d\Omega dE_f} = \frac{k_f}{k_i} r_0^2 \underbrace{\left|\frac{g}{2} F(\vec{q})\right|^2}_{\text{Squared form factor}} \underbrace{e^{-2W(k)}}_{\text{DW factor}} \underbrace{\sum_{\alpha\beta} (\delta_{\alpha\beta} - \hat{q}_\alpha \hat{q}_\beta)}_{\text{Polarization factor}} \frac{1}{2\pi\hbar} \underbrace{\int dt\, e^{-i\omega t} \sum_{ll\prime}}_{\text{Fourier transform}} e^{i\vec{q}.(\vec{r_l} - \vec{r}_{l\prime})} \underbrace{\left\langle S_l^\alpha(0) S_{l'}^\beta(t) \right\rangle}_{\text{Spin correlation function}}$$

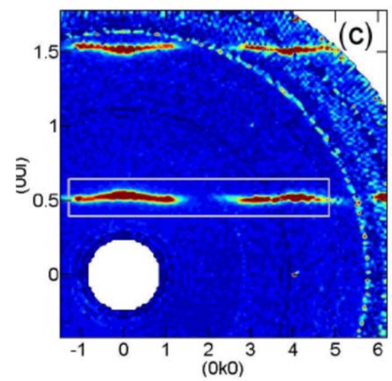
Scattering cross section – Static

$$\frac{d\sigma}{d\Omega} = \cancelto{1}{\frac{k_f}{k_i}} r_0^2 \left|\frac{g}{2}F(\vec{q})\right|^2 e^{-2W(k)} \sum_{\alpha\beta}(\delta_{\alpha\beta} - \hat{q}_\alpha\hat{q}_\beta)\frac{1}{2\pi\hbar}\sum_{ll'} e^{i\vec{q}.(\vec{r}_{ld} - \vec{r}_{ld'})}\langle S_l^\alpha\rangle\left\langle S_{l'}^\beta\right\rangle$$









Magnetic Scattering II

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Contents- Second part

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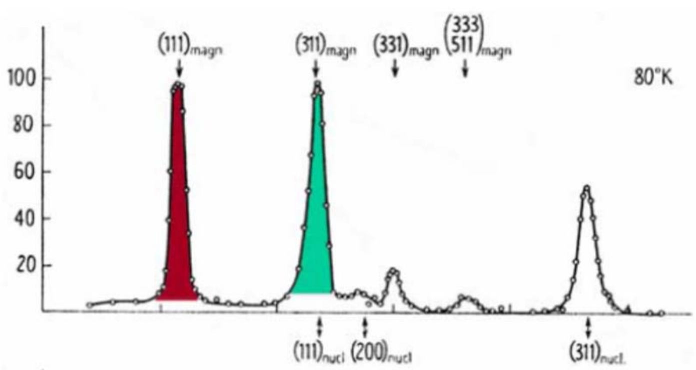
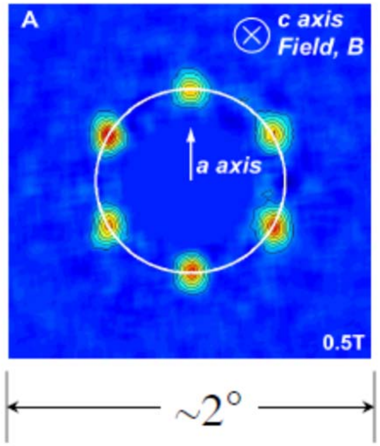
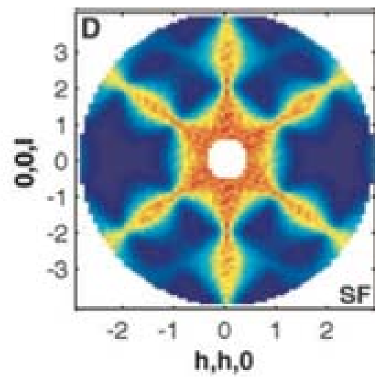
- *Parametric studies*
- *Experimental methods*

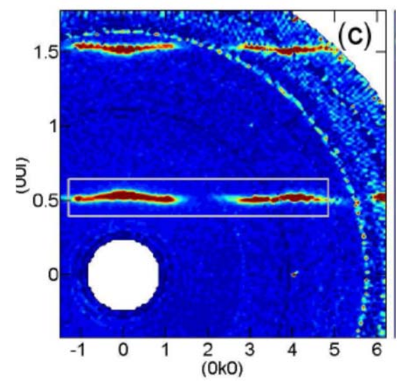
Scattering cross section

$$\frac{d^2\sigma}{d\Omega dE_f} = \frac{k_f}{k_i} r_0^2 \left| \frac{g}{2} F(\vec{q}) \right|^2 e^{-2W(k)} \sum_{\alpha\beta} (\delta_{\alpha\beta} - \hat{q}_\alpha \hat{q}_\beta) \frac{1}{2\pi\hbar} \int dt\, e^{-i\omega t} \sum_{ll'} e^{i\vec{q}.(\vec{r_{ld}} - \vec{r}_{ld'})} \left\langle S_l^\alpha(0) S_{l'}^\beta(t) \right\rangle$$



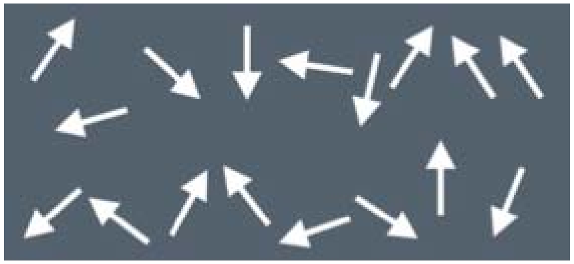






Diffraction from a Paramagnet

$$\frac{d^2\sigma}{d\Omega dE_f} = \frac{k_f}{k_i} r_0^2 \left|\frac{g}{2} F(\vec{q})\right|^2 e^{-2W(k)} \sum_{\alpha\beta} (\delta_{\alpha\beta} - \hat{q}_\alpha \hat{q}_\beta) \frac{1}{2\pi\hbar} \int dt\, e^{-i\omega t} \sum_{ll'} e^{i\vec{q}.(\vec{r_{ld}} - \vec{r}_{l'd'})} \left\langle S_l^\alpha(0) S_{l'}^\beta(t) \right\rangle$$

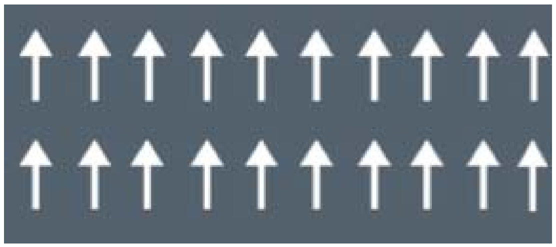


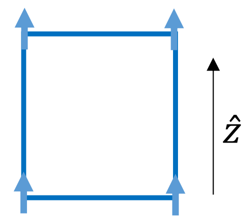
$$\left\langle S_l^\alpha(0) S_{l'}^\beta(t) \right\rangle = \left\langle S_l^\alpha S_{l'}^\beta \right\rangle = \delta_{\alpha\beta} \langle (S_0^\alpha)^2 \rangle = \frac{1}{3} \delta_{\alpha\beta} S(S+1)$$

$$\frac{d\sigma}{d\Omega} = \frac{2}{3} r_0^2 N \left|\frac{g}{2} F(\vec{q})\right|^2 e^{-2W(k)} S(S+1)$$

Diffuse scattering (continuosly distributed over all scattering directions)

Diffraction from a Ferromagnet





$\langle S_l^x \rangle = \langle S_l^y \rangle = 0$

$\langle S_l^z \rangle = \langle S^z \rangle$ Proportional to the domain's magnetisation

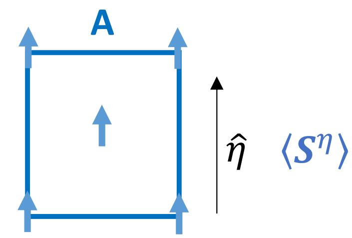
$$\frac{d\sigma}{d\Omega} = r_0^2 N \left| \frac{g}{2} F(\vec{q}) \right|^2 e^{-2W(k)} \left(1 - \widehat{q_z}^2\right) \langle S^z \rangle^2 \sum_l e^{i\vec{q}.(\overrightarrow{r_{ld}})}$$

$$\sum_l e^{i\vec{q}.(\overrightarrow{r_l})} = \frac{(2\pi)^3}{v_0} \sum_{\tau_m} \delta(\vec{q}.\overrightarrow{\tau_m})$$

Reciprocal lattice vector (magnetic)

Diffraction from a Ferromagnet

$$\frac{d\sigma}{d\Omega} = r_0^2 N_m \frac{(2\pi)^3}{v_m} \sum_{\vec{\tau}_m} \left(\left|\vec{\boldsymbol{F}}(q)\right|^2 - \left|\hat{q}.\vec{\boldsymbol{F}}(q)\right|^2 \right) \delta(q - \vec{\tau}_m)$$



Structure factor:

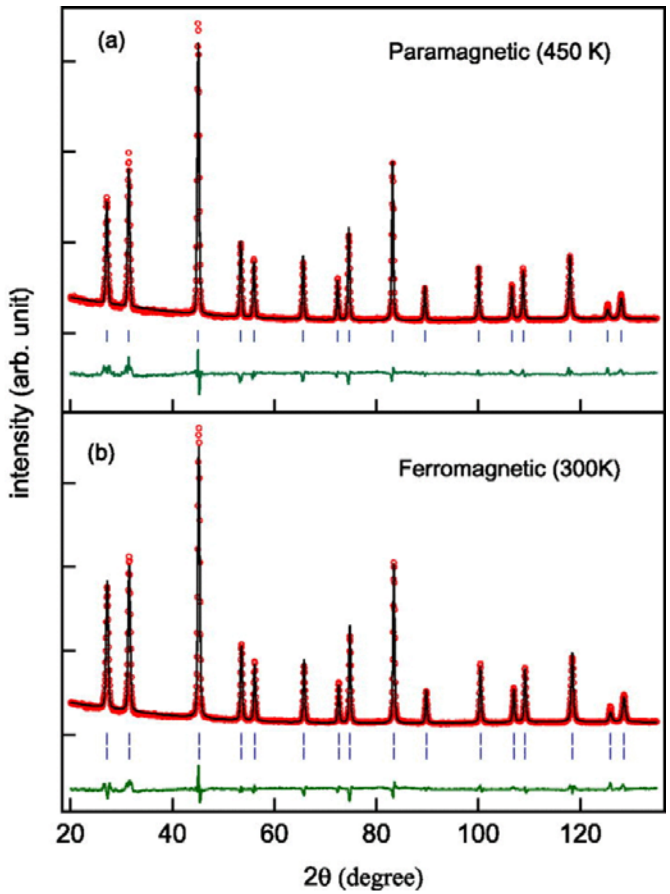
$$\left|\vec{\boldsymbol{F}}\right|^2 = \left| \sum_{\boldsymbol{d}} (b_{\boldsymbol{d}} + \boldsymbol{\sigma} r_0 S_{\perp \boldsymbol{d}})\, e^{i\boldsymbol{\tau}.\boldsymbol{d}} \right|^2 = \underbrace{\left| \sum_{\boldsymbol{d}} b_{\boldsymbol{d}}\, e^{i\boldsymbol{\tau}.\boldsymbol{d}} \right|^2}_{\text{Nuclear}} + \underbrace{\left| \sum_{\boldsymbol{d}} \boldsymbol{\sigma} r_0 S_{\perp \boldsymbol{d}}\, e^{i\boldsymbol{\tau}.\boldsymbol{d}} \right|^2}_{\text{Magnetic}} + \underbrace{2\sigma \sum_{\boldsymbol{dd'}} \boldsymbol{b_d} r_0 S_{\perp \boldsymbol{d}}\, e^{i\boldsymbol{\tau}.(\boldsymbol{d}-\boldsymbol{d'})}}_{\text{Nuclear-Magnetic}}$$

If:

$$b_{\boldsymbol{d}} \approx r_0 S_{\perp \boldsymbol{d}} \qquad \left|\vec{\boldsymbol{F}}\right|^2 \approx \begin{cases} 4|b_d|^2 \;\; for\ \sigma = 1 \\ 0 \;\; for\ \sigma = -1 \end{cases}$$

Polarized Beam!

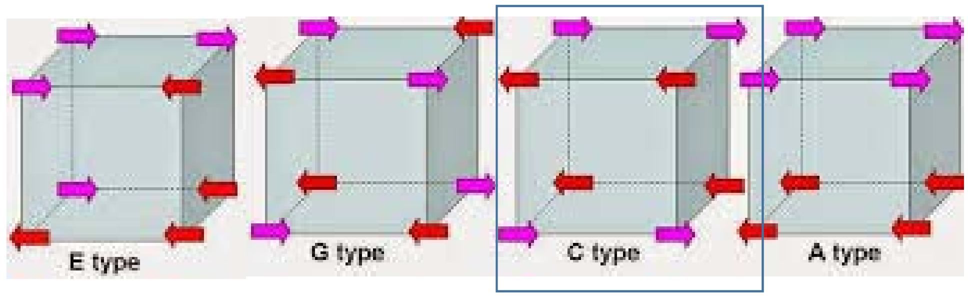
Diffraction from a Ferromagnet II



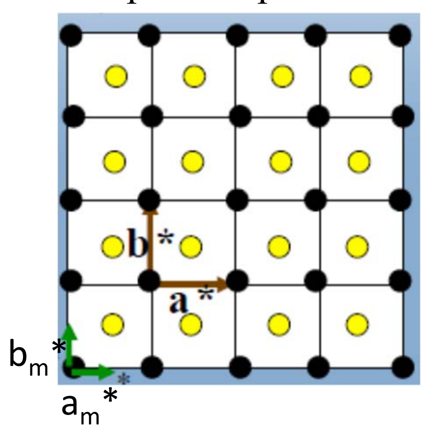
$Ni_{1.8}Pt_{0.2}MnGa$

Singh, Sanjay, et al. APPLIED PHYSICS LETTERS 171904 (2012)

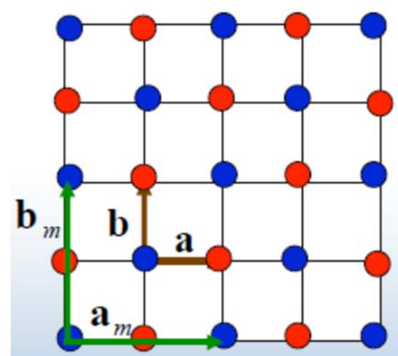
Diffraction from a simple cubic antiferromagnet I

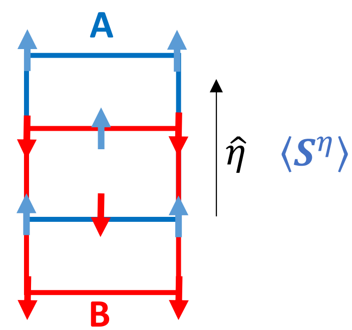


Reciprocal Space



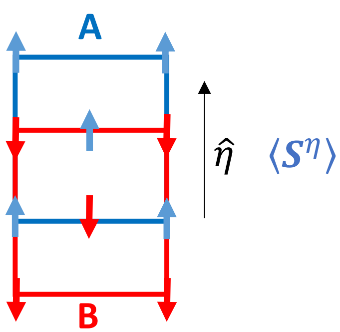
Real Space





$$\frac{d^2\sigma}{d\Omega dE_f} = \frac{k_f}{k_i} r_0^2 \left|\frac{g}{2}F(\vec{q})\right|^2 e^{-2W(k)} \sum_{\alpha\beta} (\delta_{\alpha\beta} - \hat{q}_\alpha \hat{q}_\beta) \frac{1}{2\pi\hbar}\int dt\, e^{-i\omega t} \sum_{ll'} e^{i\vec{q}.(\vec{r_{ld}} - \vec{r}_{ld'})} \left\langle S_l^\alpha(0) S_{l'}^\beta(t)\right\rangle$$

Diffraction from a simple cubic antiferromagnet II



$$\sum_{ll'} e^{i\vec{q}.(\overrightarrow{r_{ld}} - \vec{r}_{l'd'})} \langle S_l^\eta \rangle \langle S_{l'}^\eta \rangle = \langle S^\eta \rangle^2 N_m \sum_A e^{-i\vec{q}.l} \sum_d \sigma_d e^{-i\vec{q}.\vec{d}}$$

Sum over the ions in the sublattice A

Sum over the ions in the magnetic unit cell

$$\sum_A e^{-i\vec{q}.l} = \frac{(2\pi)^3}{v_{0m}} \sum_{\tau_m} \delta(\vec{q}.\overrightarrow{\tau_m})$$

$N_m = \frac{1}{2} N,$

$v_{0m} = 2v_0$

$\sigma_d = 1$, A

$\sigma_d = -1$, B

$$\frac{d^2\sigma}{d\Omega dE_f} = r_0^2 N_m \frac{(2\pi)^3}{v_{0m}} \sum_{\tau_m} |F_M(\overrightarrow{\tau_m})|^2 e^{-2W(k)} \{1 - (\widehat{\tau_m}.\hat{\eta})_{av}^2\} \delta(\vec{q}.\overrightarrow{\tau_m})$$

Magnetic structure factor:

$$F_M(\overrightarrow{\tau_m}) = \frac{1}{2} g \langle S^\eta \rangle F(\overrightarrow{\tau_m}) \sum_d \sigma_d e^{-i\overrightarrow{\tau_m}.\vec{d}}$$

Diffraction from a simple cubic antiferromagnet III

$$\sum_A e^{-i\vec{q}.\vec{r_l}} = \frac{(2\pi)^3}{v_{0m}} \sum_{\tau_m} \delta(\vec{q}.\overrightarrow{\tau_m})$$

$$\vec{q} = \overrightarrow{\tau_m} = t_1\tau_1 + t_2\tau_2 + t_3\tau_3$$

For a magnetic lattice: face centered cubic

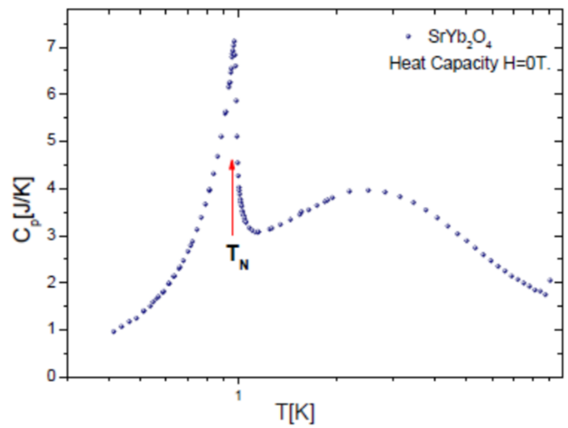
$$\sum_d \sigma_d e^{-i\vec{q}.\vec{d}} = \sum_d \sigma_d e^{-i\overrightarrow{\tau_m}.\vec{d}}$$

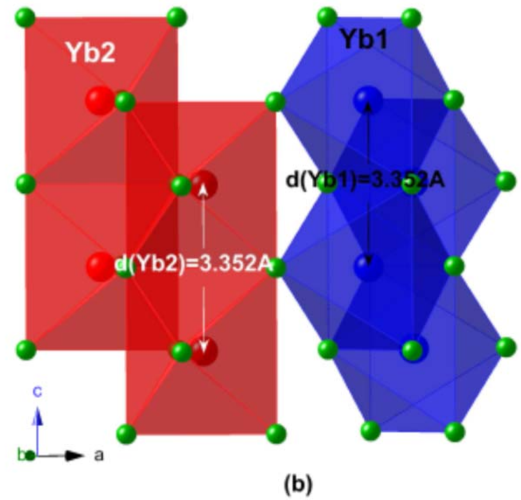
$$= 0, \tau_m = t_1, t_2, t_3$$

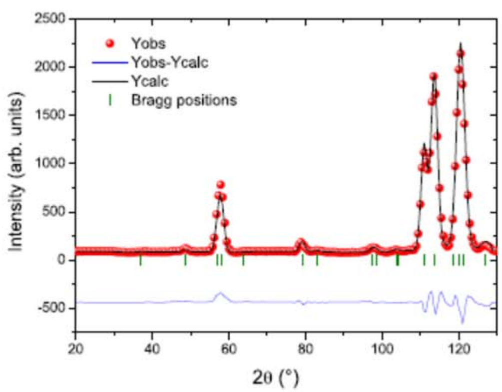
$$= 2, \tau_m = t_1 + \frac{1}{2}, t_2 + \frac{1}{2}, t_3 + \frac{1}{2}$$

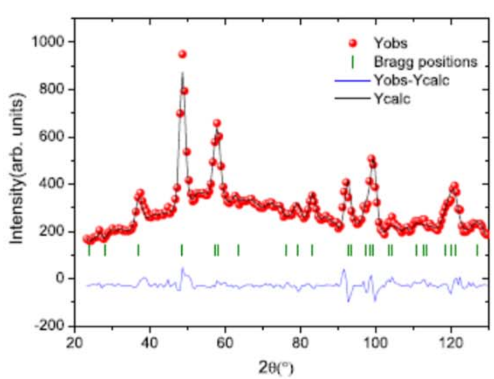
Nuclear and magnetic Bragg scatter ocurr at different points in the reciprocal lattice space

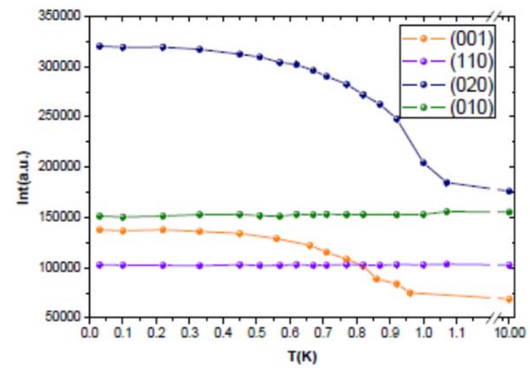
Example: $SrYb_2O_4$











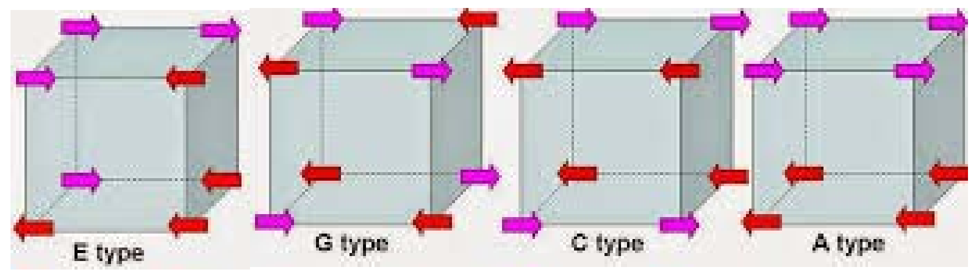
Example 2: $SrYb_2O_4$ II

$\mu(Yb1)$	$= \mu(Yb2)$										
(h,k,l)	$E4nucl$	$E4mag$	Gx	Gy	Gz	Ax	Ay	Az	Cx	Cy	Cz
(0, 1, 0)	55.6	3.4	0.2	0	2	0	0	0	471	0	0.1
(1, 0, 0)	100.9	1.1	0	0	0	0	481	481	0	1769	1770
(1, 1, 0)	158.53	74.5	0.1	0.2	0.3	0.1	0.1	0.3	1	0.1	0.1
(0, 2, 0)	635.19	615.4	0	0	0	690	0	696	0	0	0
(1, 2, 0)	2093.5	8.1	470	200	770	5	1.8	7	19	6	26
(2, 0, 0)	3467.5	82.8	0	330	330	0	0	0	0	0	0
(2, 1, 0)	85.87	24.3	0.1	0.2	0.2	0.1	0.1	0.2	0.1	0.1	0.1
(0, 3, 0)	60.18	5.36	0.1	0	0.1	0	0	0	0.2	0	0.2
(2, 2, 0)	1557.17	37.64	2.5	6	10	66	92	58	136	188	324
(1, 3, 0)	342.21	198.6	0.1	0.1	1	0.1	0.1	0.1	0.1	0.1	0.1
(0, 0, 1)	70.42	826.0	172	175	0	0	0	0	0.1	0	0
(3, 0, 0)	244.42	3.6	0	0	0	0	168	171	0	3	3
(0, 1, 1)	870.13	173.62	0	0	0	0.1	0.1	0	0	0	0
$\mu(Yb1)$	$\neq 0$	$\mu(Yb2)$	$= 0$								
(0, 1, 0)	55.6	3.4	314	0	314	0	0	0.2	0	0	471
(1, 0, 0)	100.9	1.1	0	0	0	0	126	126	0	437	437
(1, 1, 0)	158.53	74.5	35	50	85	43	115	198	24	32	56
(0, 2, 0)	635.19	615.4	0	0	0	173	0	73	0	0	0
(1, 2, 0)	2093.5	8.1	141	49	190	17	0.5	2.2	6	2	8
(2, 0, 0)	3467.5	82.8	0	85	85	0	0	0	0	0	0
(2, 1, 0)	85.87	24.3	4	21	24	12	71	84	6	31	37
(0, 3, 0)	60.18	5.36	53	0	53	0	0	0	15	0	15
(2, 2, 0)	1557.17	37.64	1.4	2	3.5	15	21	36	34	48	83
(1, 3, 0)	342.21	198.6	2.5	0.7	5	60	9	68	16	2.6	20
(0, 0, 1)	70.42	826.0	44	44	0	0	0	0	0	0	0
(3, 0, 0)	244.42	3.6	0	0	0	0	42	42	0	0.4	0.4
(0, 1, 1)	870.13	173.62	0	0	0	46	42	3.5	0	0	0

Representation Analysis

$$F(++++),\ C(++--),\ G(+--+)$$

$$A(+-+-)$$



$$\Gamma_1(C_xF_y),\ \Gamma_2(F_xC_y),\ \Gamma_3(G_xA_y),\ \text{and}\ \Gamma_4(A_xG_y),$$

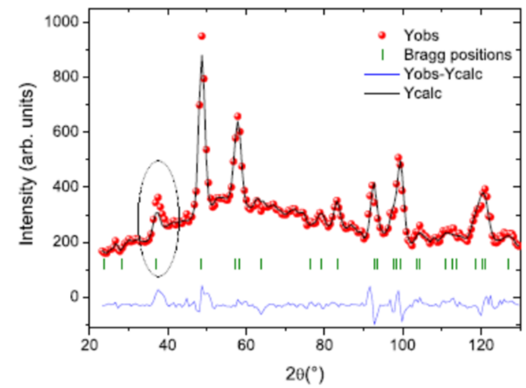
$$\Gamma_5(C_z),\ \Gamma_6(F_z),\ \Gamma_7(G_z), \Gamma_8(A_z)$$

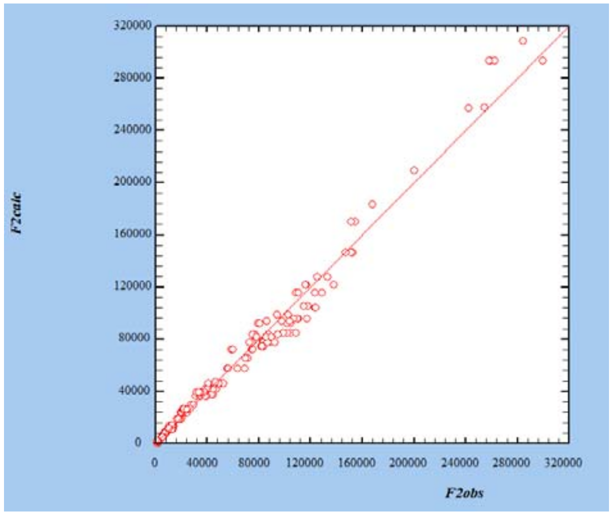
Basireps -Fullprof

Example 2: $SrYb_2O_4$ III

```
!-------------------------------------------------------------------------------
!  Data for PHASE number:   2  ==> Current R_Bragg for Pattern#  1:    62.93
!-------------------------------------------------------------------------------
SrYb2O4 magnetic
!
!Nat Dis Mom Pr1 Pr2 Pr3 Jbt Irf Isy Str Furth       ATZ    Nvk Npr More
   8   0   0 0.0 0.0 1.0   1   4  -1   0   0       823.842   0   0   1
!
!Jvi Jdi Hel Sol Mom Ter  Brind   RMua    RMub    RMuc   Jtyp  Nsp_Ref Ph_Shift N_Domains
   0   0   0   0   0   0  1.0000  1.0000  0.0000  0.0000    1      0       0       0
!
P -1                        <--Space group symbol for hkl generation
!Nsym Cen Laue MagMat
   1   1   1   1
!
SYMM x,y,z
MSYM u,v,w,0.0
!
!Atom   Typ  Mag Vek    X      Y      Z       Biso    Occ      Rx      Ry      Rz
!     Ix     Iy     Iz    beta11  beta22  beta33   MagPh
YB11   MMN2  1  0  0.42170 0.10900 0.25000 0.20000  1.00000   3.370   1.900   0.000  #color 1 0 0 1 scale 2.3
                    0.00    0.00    0.00    0.00     0.00    0.00    0.00    0.00
     0.000   0.000   0.000   0.000   0.000   0.000  0.00000
      0.00    0.00    0.00    0.00    0.00    0.00     0.00
YB12   MMN2  1  0  0.57830 0.89100 0.75000 0.20000  1.00000   3.370  -1.900   0.000  #color 1 0 0 1 scale 2.3
                    0.00    0.00    0.00    0.00     0.00    0.00    0.00    0.00
     0.000   0.000   0.000   0.000   0.000   0.000  0.00000
      0.00    0.00    0.00    0.00    0.00    0.00     0.00
YB13   MMN2  1  0  0.92170 0.39100 0.25000 0.20000  1.00000  -3.370   1.900   0.000  #color 1 0 0 1 scale 2.3
                    0.00    0.00    0.00    0.00     0.00    0.00    0.00    0.00
     0.000   0.000   0.000   0.000   0.000   0.000  0.00000
      0.00    0.00    0.00    0.00    0.00    0.00     0.00
YB14   MMN2  1  0  0.07830 0.60900 0.75000 0.20000  1.00000  -3.370  -1.900   0.000  #color 1 0 0 1 scale 2.3
                    0.00    0.00    0.00    0.00     0.00    0.00    0.00    0.00
     0.000   0.000   0.000   0.000   0.000   0.000  0.00000
      0.00    0.00    0.00    0.00    0.00    0.00     0.00
YB21   MMN2  1  0  0.42530 0.61230 0.25000 0.20000  1.00000   0.810   1.900   0.000  #color 1 0 0 1 scale 2.3
                    0.00    0.00    0.00    0.00     0.00    0.00    0.00    0.00
     0.000   0.000   0.000   0.000   0.000   0.000  0.00000
      0.00    0.00    0.00    0.00    0.00    0.00     0.00
YB22   MMN2  1  0  0.57470 0.38730 0.75000 0.20000  1.00000   0.810  -1.900   0.000  #color 1 0 0 1 scale 2.3
                    0.00    0.00    0.00    0.00     0.00    0.00    0.00    0.00
     0.000   0.000   0.000   0.000   0.000   0.000  0.00000
      0.00    0.00    0.00    0.00    0.00    0.00     0.00
YB23   MMN2  1  0  0.92530 0.88770 0.25000 0.20000  1.00000  -0.810   1.900   0.000  #color 1 0 0 1 scale 2.3
                    0.00    0.00    0.00    0.00     0.00    0.00    0.00    0.00
     0.000   0.000   0.000   0.000   0.000   0.000  0.00000
      0.00    0.00    0.00    0.00    0.00    0.00     0.00
YB24   MMN2  1  0  0.07470 0.11230 0.75000 0.20000  1.00000  -0.810  -1.900   0.000  #color 1 0 0 1 scale 2.3
                    0.00    0.00    0.00    0.00     0.00    0.00    0.00    0.00
     0.000   0.000   0.000   0.000   0.000   0.000  0.00000
      0.00    0.00    0.00    0.00    0.00    0.00     0.00
```

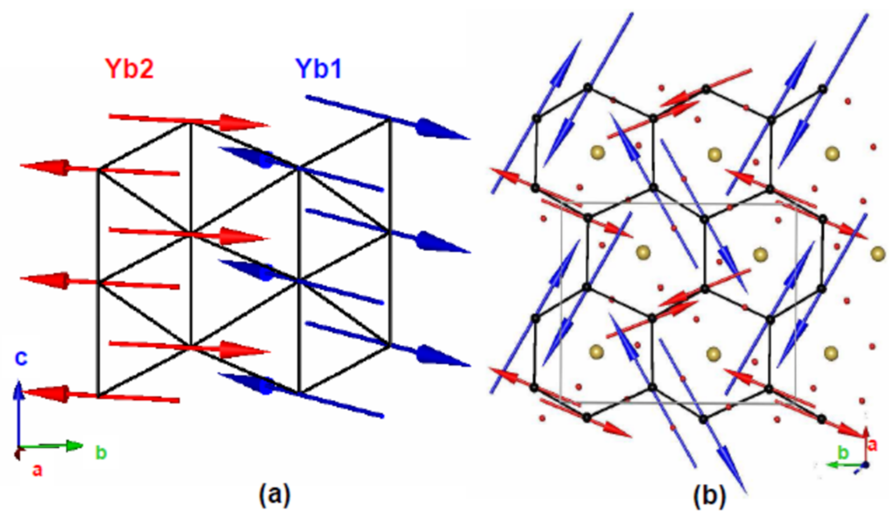
Rietvel Refinement





Example 2: $SrYb_2O_4$ IV

Name	$\mu_x(\mu_B)$	$\mu_y(\mu_B)$	$\mu(\mu_B)$
Yb11	3.37(5)	−1.9(1)	3.90(8)
Yb12	−3.37(5)	1.9(1)	3.90(8)
Yb13	−3.37(5)	−1.9(1)	3.90(8)
Yb14	3.37(5)	1.9(1)	3.90(8)
Yb21	0.81(5)	−2.0(1)	2.2(1)
Yb22	−0.81(5)	2.0(1)	2.2(1)
Yb23	−0.81(5)	−2.0(1)	2.2(1)
Yb24	0.81(5)	2.0(1)	2.2(1)
$R_p = 3.53$,	R_{exp}=5.18,	R_{exp}=5.76	



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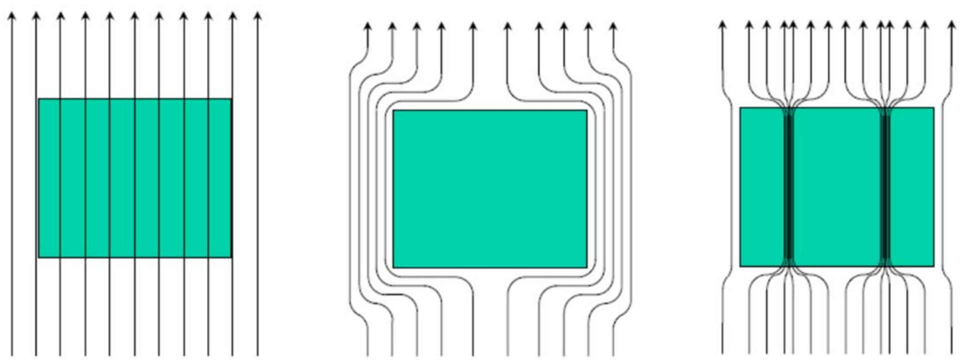
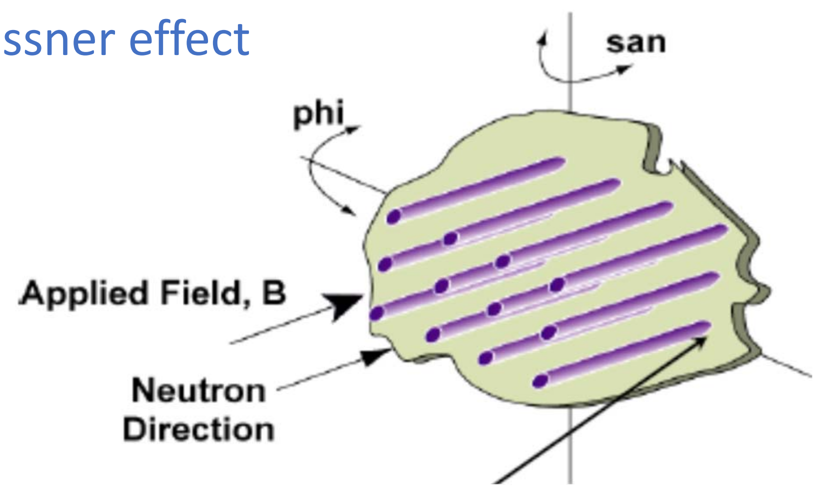
Flux line lattices in Superconductors

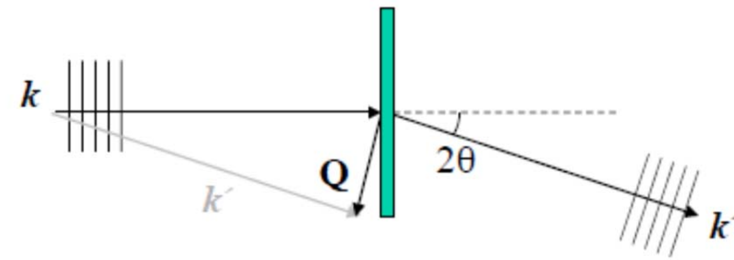


Normal state | Superconducting state | Flux line lattice

Meissner effect

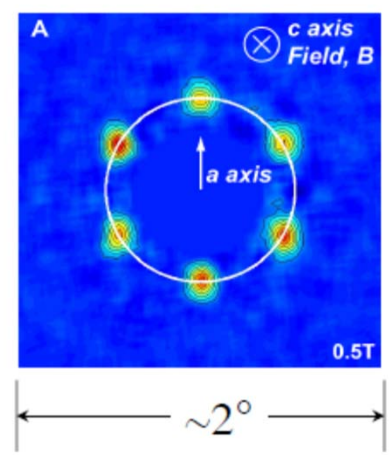


Scattering geometry

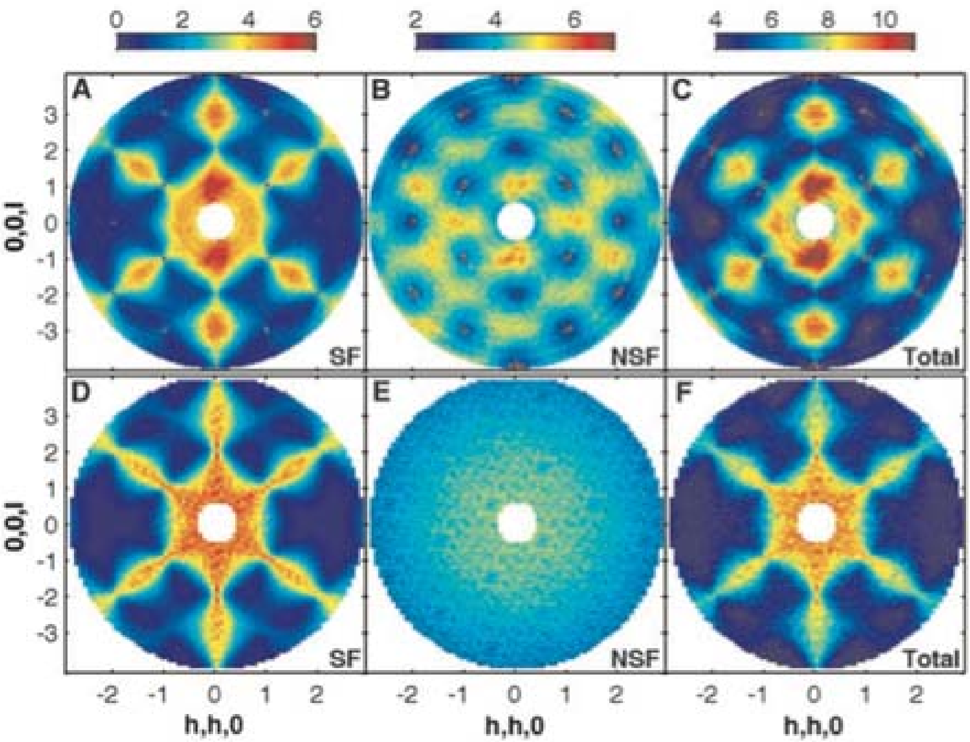


The momentum transfer, **Q**, is roughly perpendicular to the flux lines, therefore all the magnetization is seen.

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

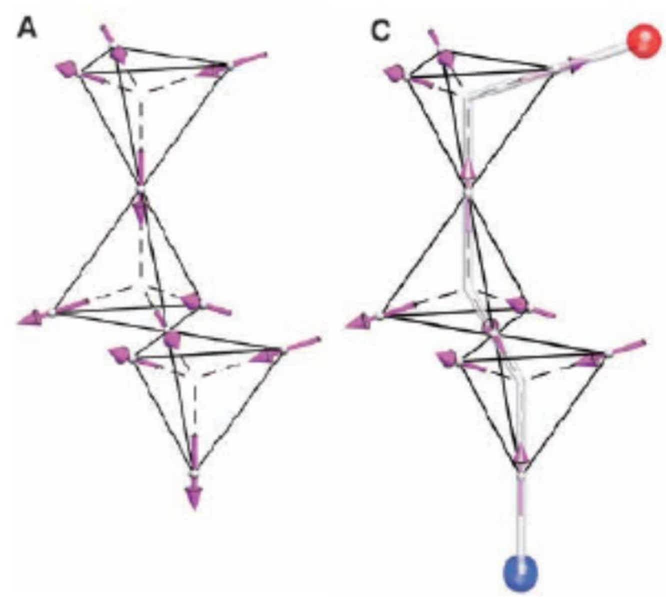


Diffuse elastic magnetic scattering



Magnetic Coulomb Phase in the Spin Ice $Ho_2Ti_2O_7$

T. Fennell,[1*] P. P. Deen,[1] A. R. Wildes,[1] K. Schmalzl,[2] D. Prabhakaran,[3] A. T. Boothroyd
R. J. Aldus,[4] D. F. McMorrow,[4] S. T. Bramwell[4]



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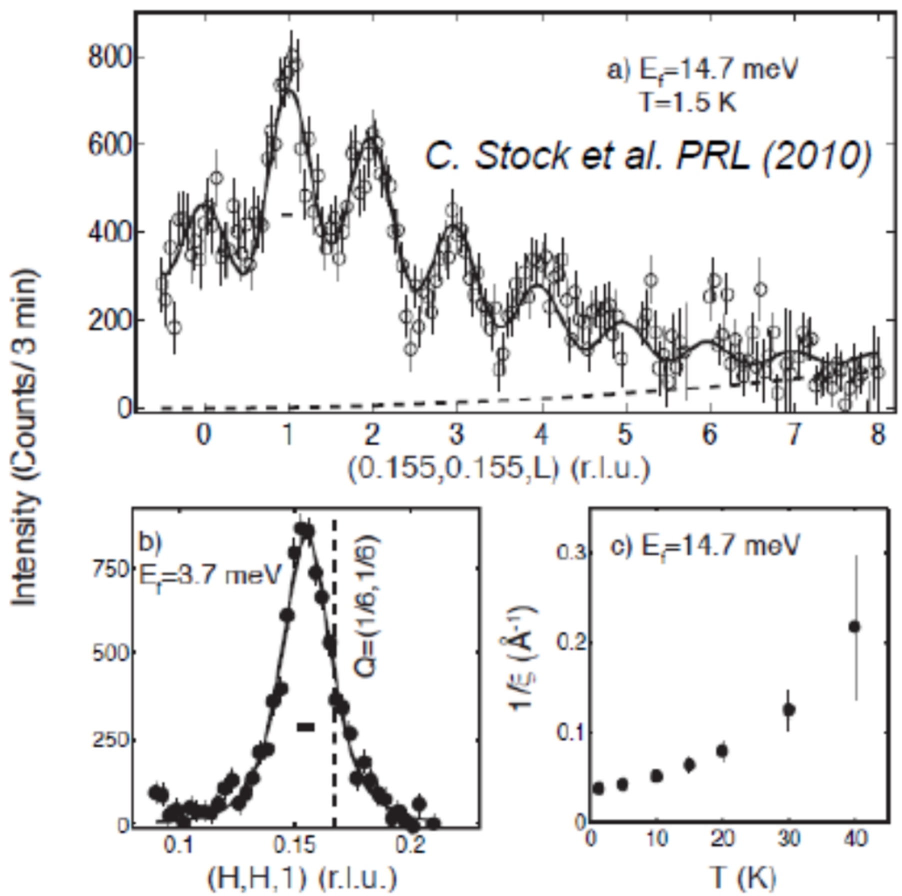
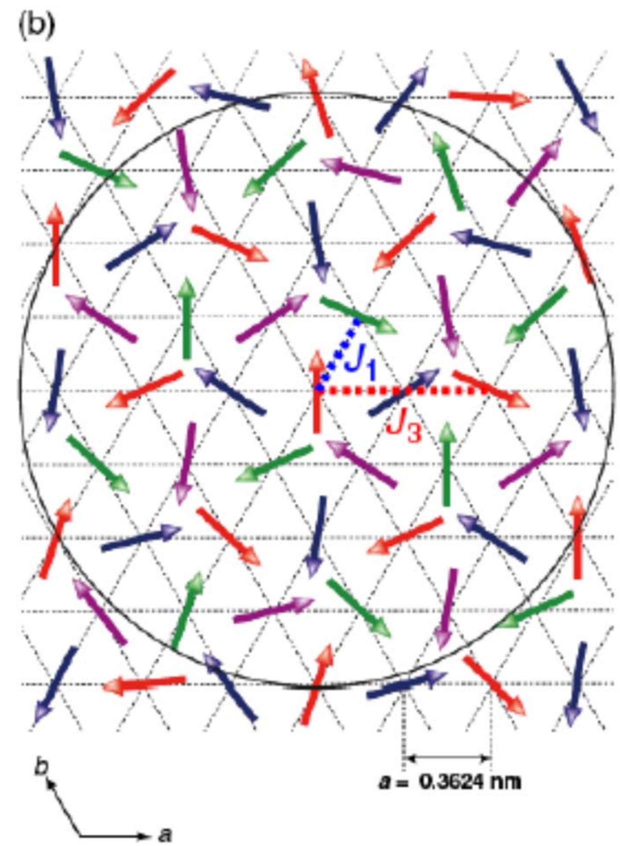
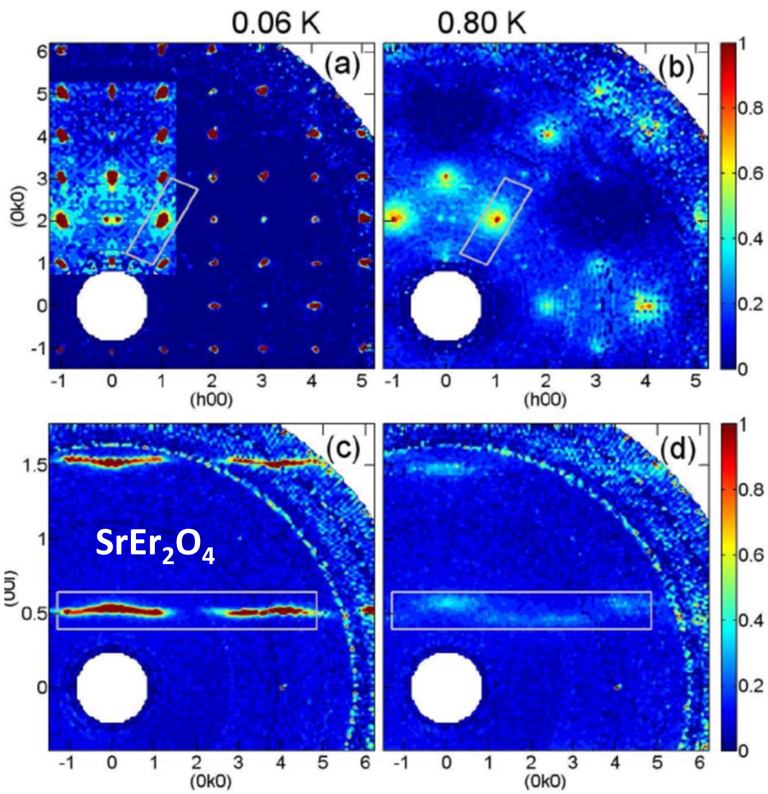
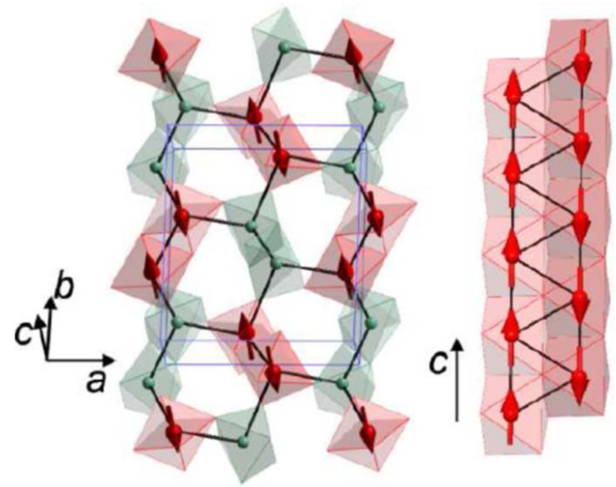
Short range magnetic order





Short range magnetic order II





Petrenko, et al., Phys. Rev. B **78**, 184410 (2008)
Hayes, et al., Phys. Rev. B **84**, 174435 (2011).

Parametric studies

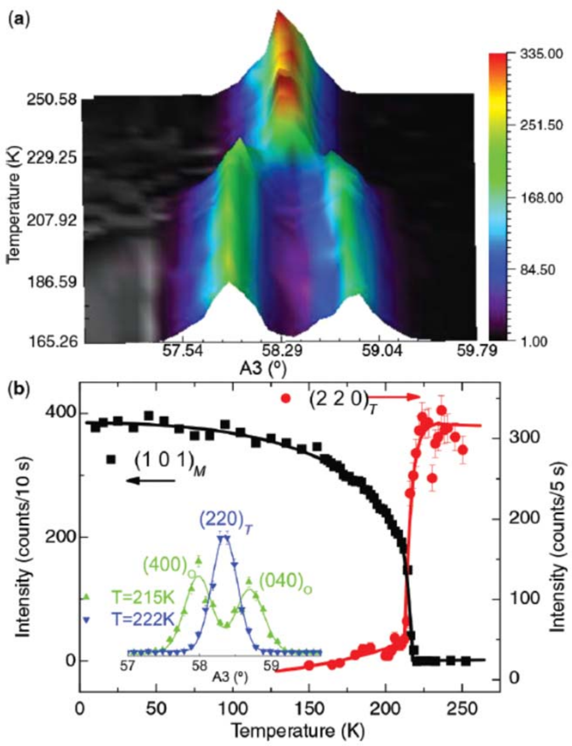


Figure 8. Structural and magnetic phase transition as a function of temperature in a single crystal of $SrFe_2As_2$.

Zhao 2008 *Phys. Rev. B* 78: 140504(R), 1–4..

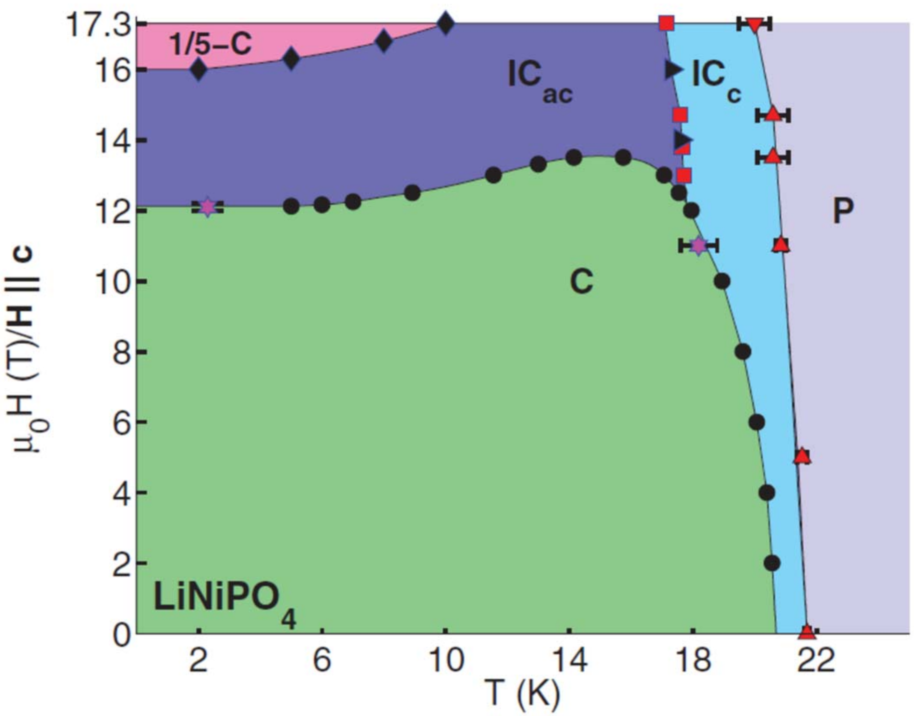


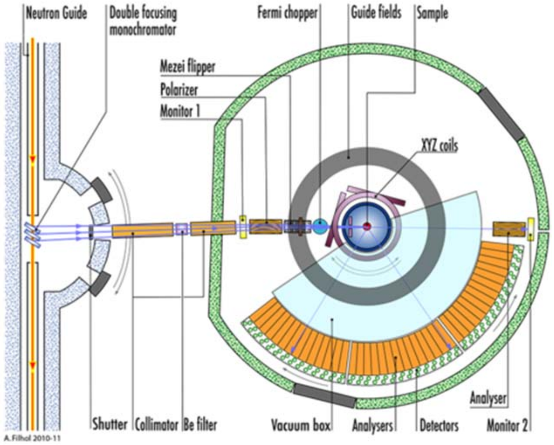
FIG. 4. (Color online) $(\mu_0 H, T)$-phase diagram of $LiNiPO_4$ for

Toft-Petersen PHYSICAL REVIEW B **84**, 054408 (2011)

Experimental methods

Diffractometers

Polarized diffractometers



Triple axis spectrometers

SANS