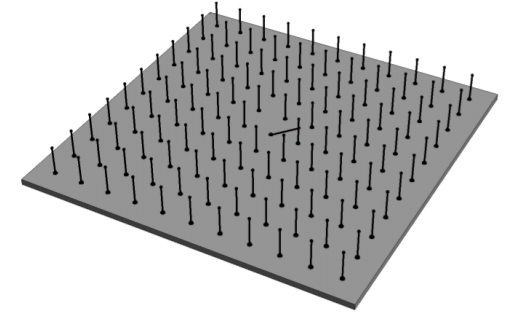
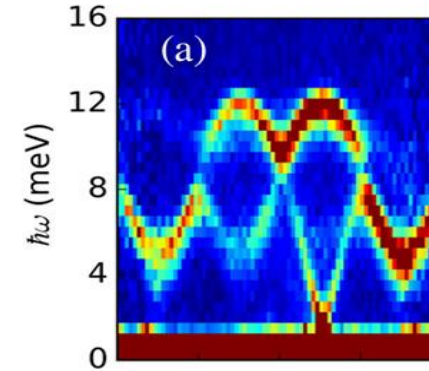
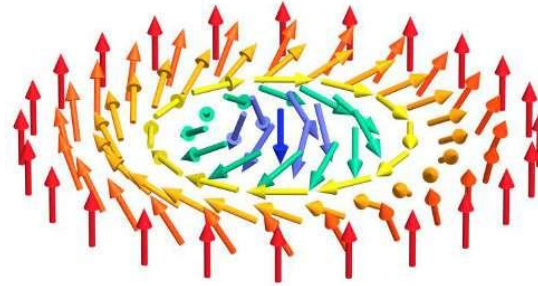
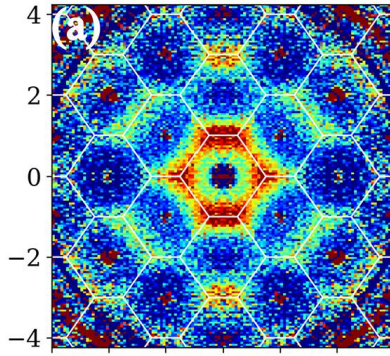
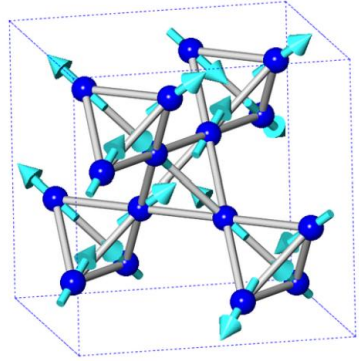




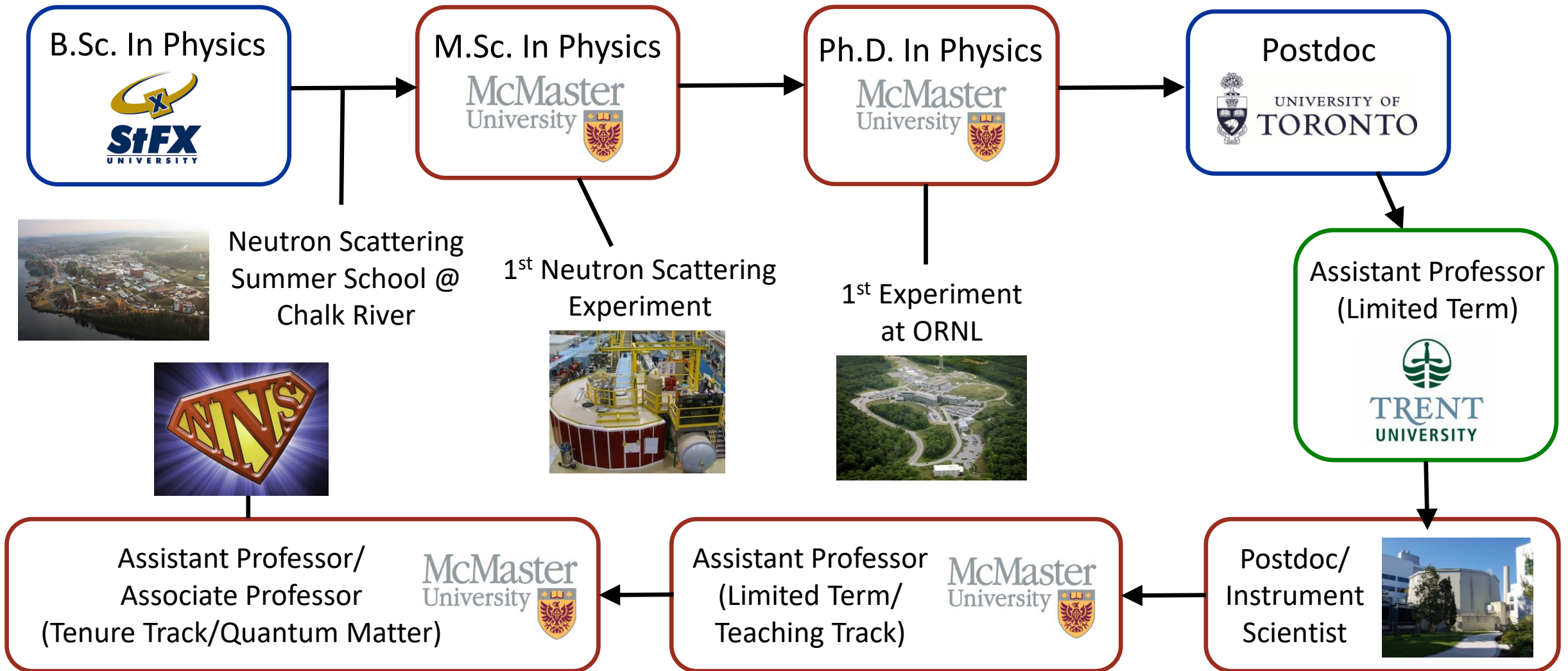
Introduction to Magnetic Scattering



Pat Clancy
Dept. of Physics & Astronomy
McMaster University

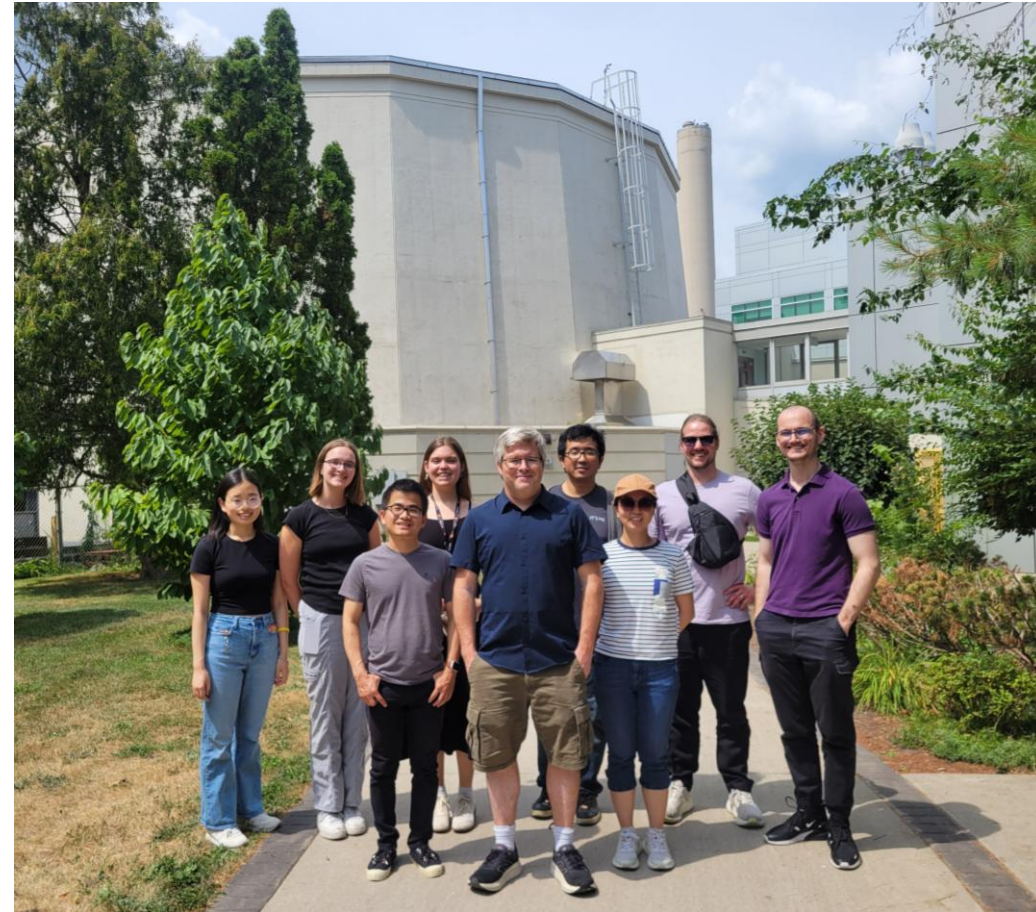
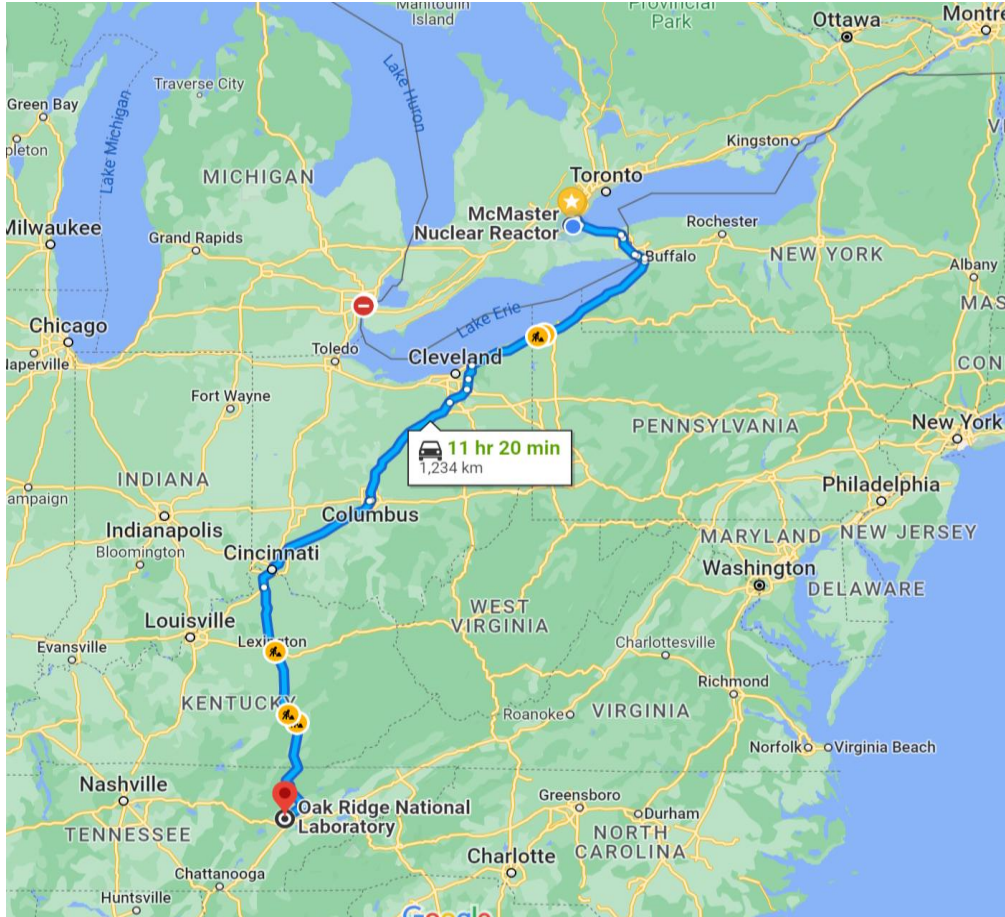


How did I get here?



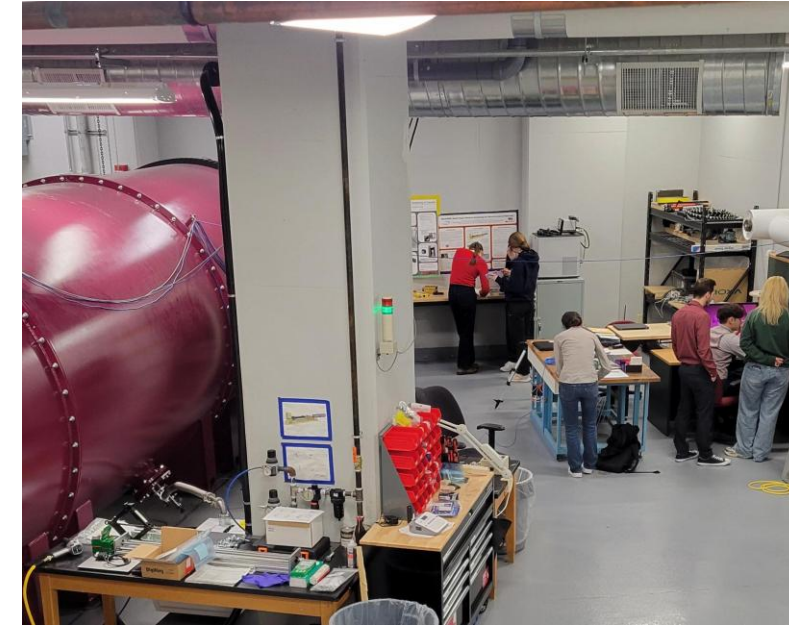
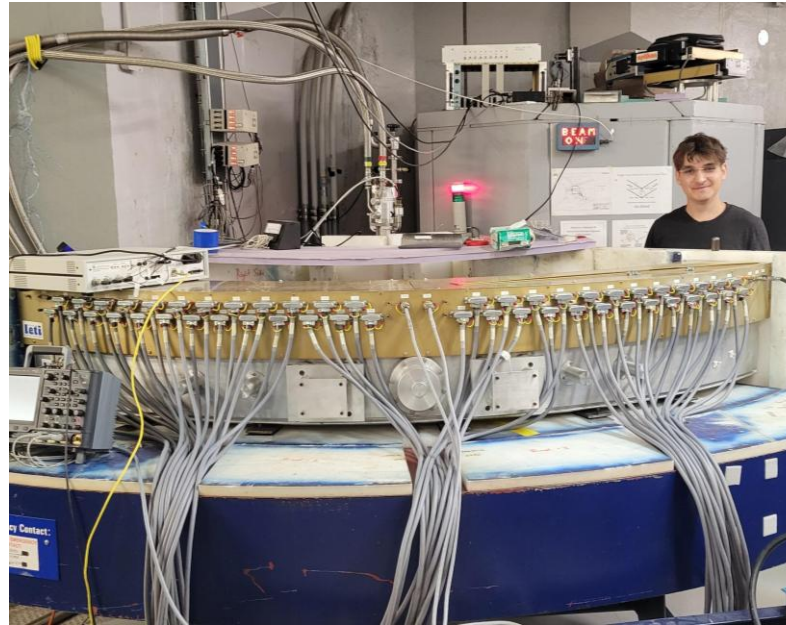
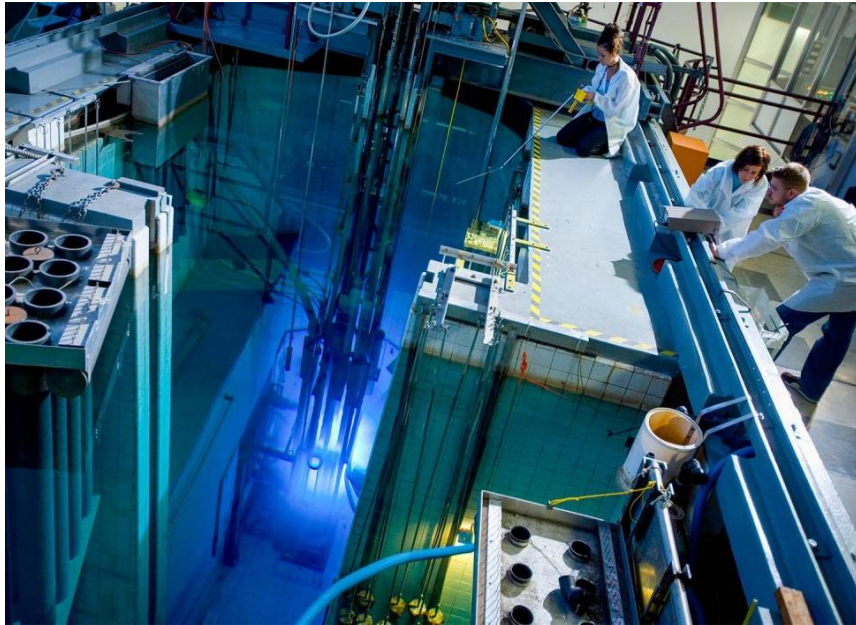
Neutron Scattering at McMaster

Home to **McMaster Nuclear Reactor** – Canada's most powerful neutron source



Neutron Scattering at McMaster

Home to **McMaster Nuclear Reactor** – Canada's most powerful neutron source

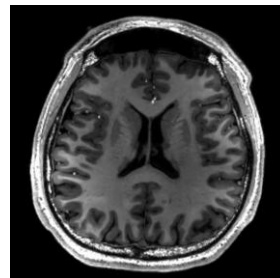
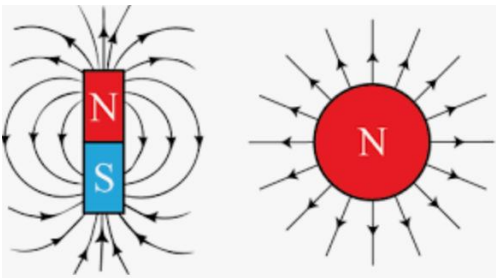
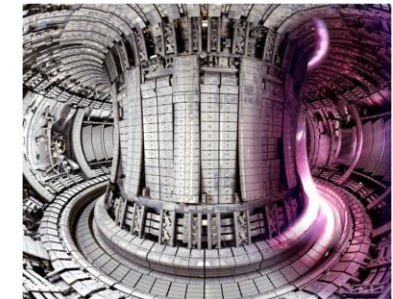
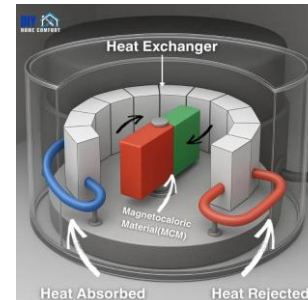
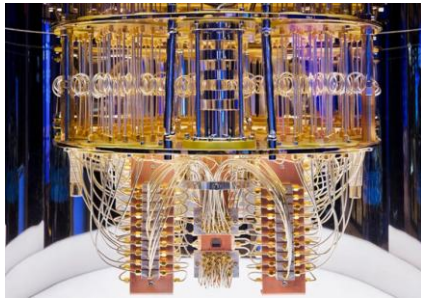
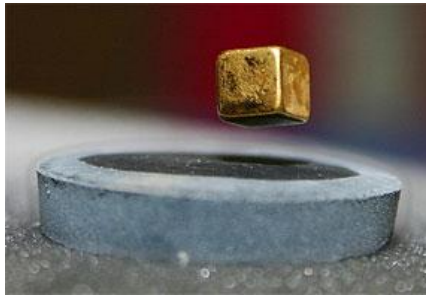


- 5 MW open-pool reactor used for **neutron scattering**, medical isotopes, neutron radiography, neutron activation/ irradiation studies, positron beams...
- Currently 2 neutron scattering beamlines: **MAD** and **MacSANS** (more coming soon)

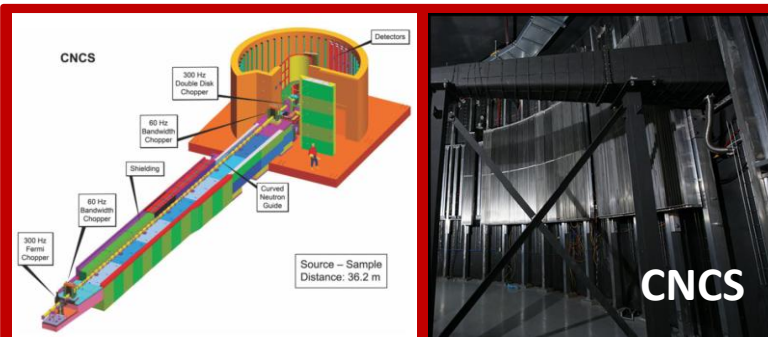
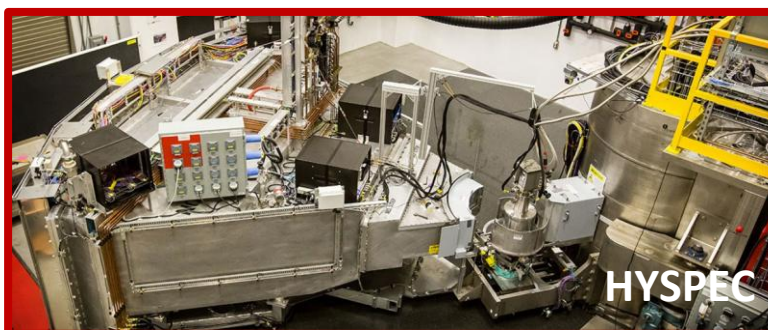
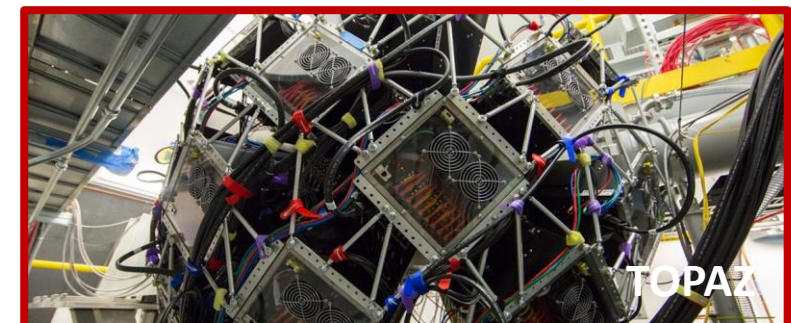
Introduction to Magnetic Scattering



- One of the “killer applications” of neutron scattering
- Neutron scattering is an essential tool for the study of magnetic materials
- **Elastic Scattering (diffraction)** – magnetic structure, phase transitions
- **Inelastic Scattering (spectroscopy)** – magnetic dynamics, excitations, interactions



What does magnetic scattering with neutrons look like?



Magnetic Scattering with Neutrons

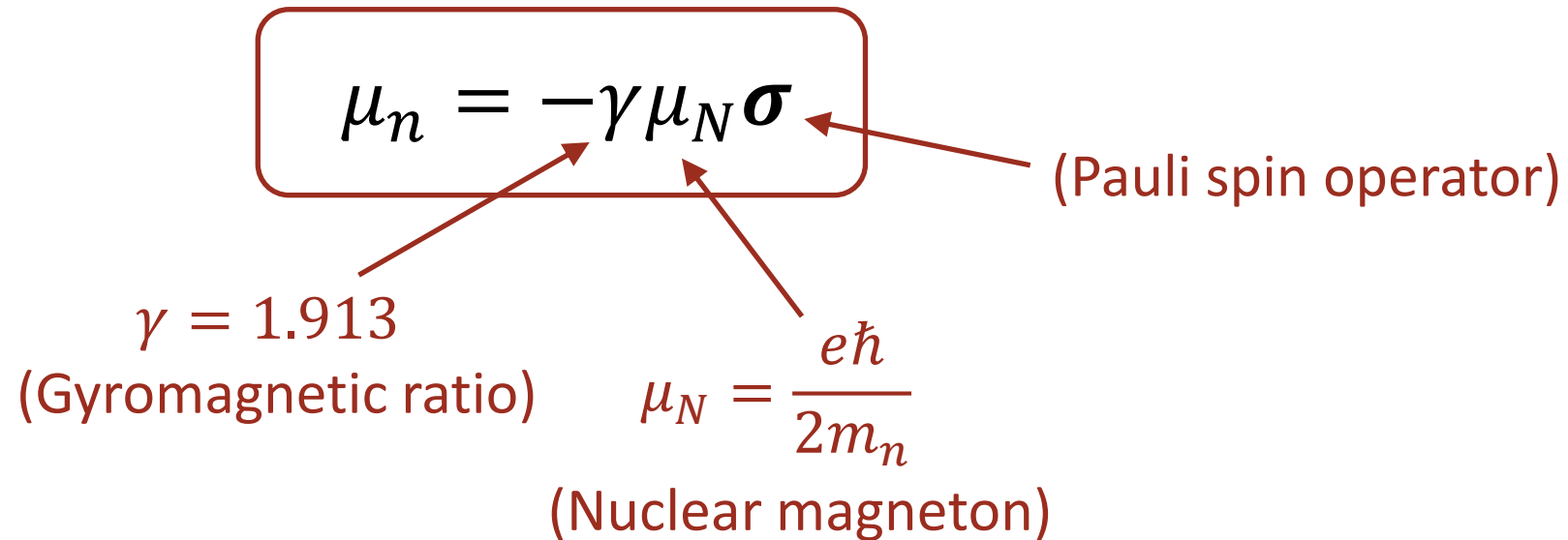
- Neutrons are spin $\frac{1}{2}$ particles
- They carry no charge, but do carry a **magnetic dipole moment**:

$$\mu_n = -\gamma \mu_N \boldsymbol{\sigma}$$

$\gamma = 1.913$
(Gyromagnetic ratio)

$\mu_N = \frac{e\hbar}{2m_n}$
(Nuclear magneton)

(Pauli spin operator)

A diagram illustrating the equation for the neutron magnetic dipole moment, $\mu_n = -\gamma \mu_N \boldsymbol{\sigma}$. The equation is enclosed in a rounded rectangle. Three arrows point from the components of the equation to their definitions: one from γ to $\gamma = 1.913$ (Gyromagnetic ratio), one from μ_N to $\mu_N = \frac{e\hbar}{2m_n}$ (Nuclear magneton), and one from $\boldsymbol{\sigma}$ to (Pauli spin operator).

- μ_n can interact with the electrons in a material via magnetic potentials
- **Scattering from these potentials can be comparable in strength to nuclear scattering**

Magnetic Materials

Transition Metals:
Up to 10 d-levels to fill

1 H Hydrogen	2 He Helium																
3 Li Lithium	4 Be Beryllium	5 B Boron	6 C Carbon	7 N Nitrogen	8 O Oxygen	9 F Fluorine	10 Ne Neon										
11 Na Sodium	12 Mg Magnesium	13 Al Aluminium	14 Si Silicon	15 P Phosphorus	16 S Sulfur	17 Cl Chlorine	18 Ar Argon										
19 K Potassium	20 Ca Calcium	21 Sc Scandium	22 Ti Titanium	23 V Vanadium	24 Cr Chromium	25 Mn Manganese	26 Fe Iron	27 Co Cobalt	28 Ni Nickel	29 Cu Copper	30 Zn Zinc	31 Ga Gallium	32 Ge Germanium	33 As Arsenic	34 Se Selenium	35 Br Bromine	36 Kr Krypton
37 Rb Rubidium	38 Sr Strontium	39 Y Yttrium	40 Zr Zirconium	41 Nb Niobium	42 Mo Molybdenum	43 Tc Technetium	44 Ru Ruthenium	45 Rh Rhodium	46 Pd Palladium	47 Ag Silver	48 Cd Cadmium	49 In Indium	50 Sn Tin	51 Sb Antimony	52 Te Tellurium	53 I Iodine	54 Xe Xenon
55 Cs Caesium	56 Ba Barium	57 La Lanthanum	72 Hf Hafnium	73 Ta Tantalum	74 W Tungsten	75 Re Rhenium	76 Os Osmium	77 Ir Iridium	78 Pt Platinum	79 Au Gold	80 Hg Mercury	81 Tl Thallium	82 Pb Lead	83 Bi Bismuth	84 Po Polonium	85 At Astatine	86 Rn Radon
87 Fr Francium	88 Ra Radium	89 Ac Actinium	104 Rf Rutherfordium	105 Db Dubnium	106 Sg Seaborgium	107 Bh Bohrium	108 Hs Hassium	109 Mt Meitnerium	110 Ds Darmstadtium	111 Rg Roentgenium	112 Cn Copernicium	113 Nh Nihonium	114 Fl Flerovium	115 Mc Moscovium	116 Lv Livermorium	117 Ts Tennessine	118 Og Oganesson

58 Ce Cerium	59 Pr Praseodymium	60 Nd Neodymium	61 Pm Promethium	62 Sm Samarium	63 Eu Europium	64 Gd Gadolinium	65 Tb Terbium	66 Dy Dysprosium	67 Ho Holmium	68 Er Erbium	69 Tm Thulium	70 Yb Ytterbium	71 Lu Lutetium
90 Th Thorium	91 Pa Protactinium	92 U Uranium	93 Np Neptunium	94 Pu Plutonium	95 Am Americium	96 Cm Curium	97 Bk Berkelium	98 Cf Californium	99 Es Einsteinium	100 Fm Fermium	101 Md Mendelevium	102 No Nobelium	103 Lr Lawrencium

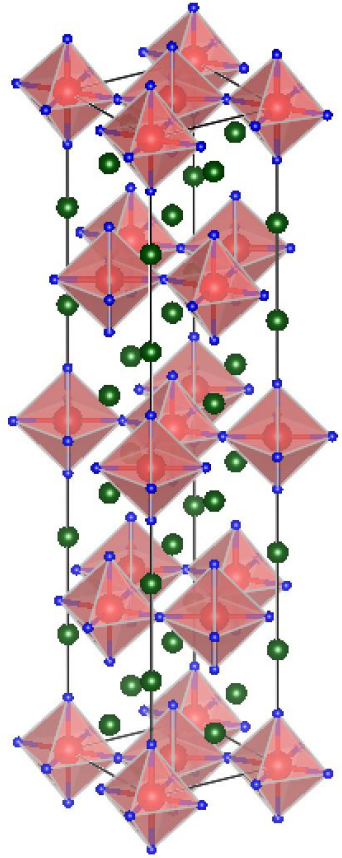
- **Magnetic moments** arise on atoms which have **unpaired electrons** in partially filled electronic orbitals

Lanthanides/Rare Earths and Actinides:
Up to 14 f-levels to fill

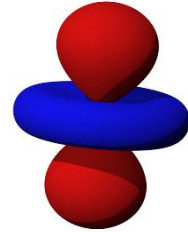
- Most common families of magnetic materials tend to be based on elements with partially filled d- or f-shells (e.g. **transition metals** or **rare earth/lanthanides**)

Magnetic Materials

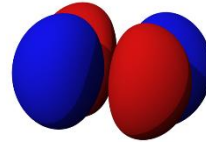
- Size of magnetic moments is determined by Hund's Rules:



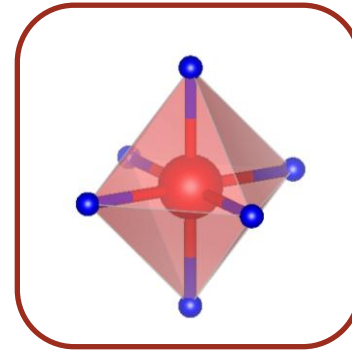
$$3z^2 - r^2$$



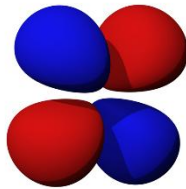
$$x^2 - y^2$$



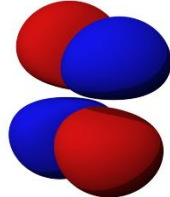
e_g orbitals



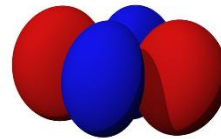
$$zx$$



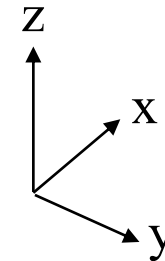
$$yz$$



$$xy$$

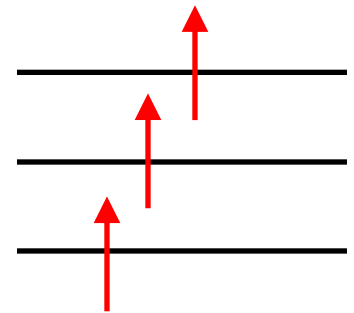
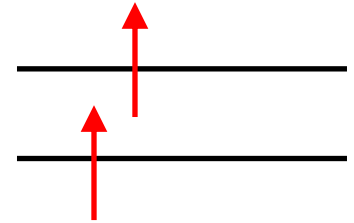


t_{2g} orbitals



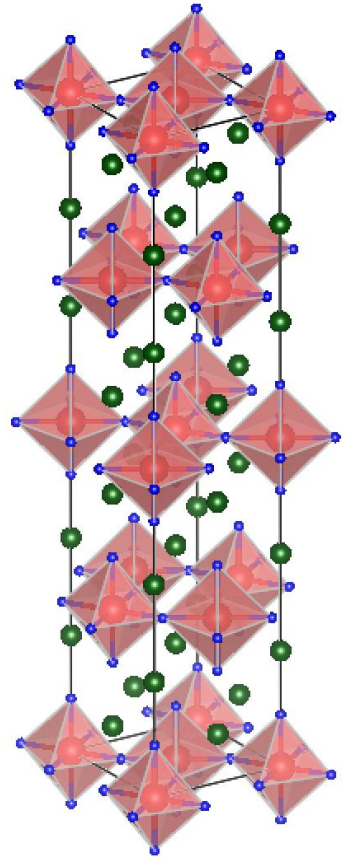
e.g. Mn^{2+} ($3d^5$)

$$S = 5/2$$

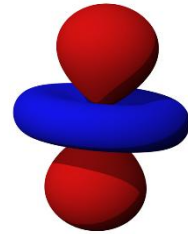


Magnetic Materials

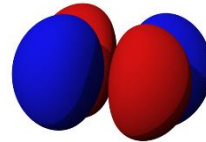
- Size of magnetic moments is determined by Hund's Rules:



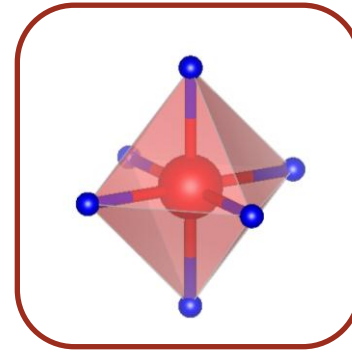
$$3z^2 - r^2$$



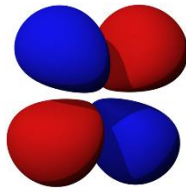
$$x^2 - y^2$$



e_g orbitals



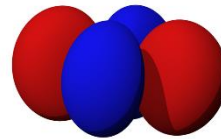
$$zx$$



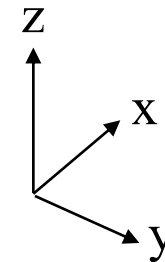
$$yz$$



$$xy$$

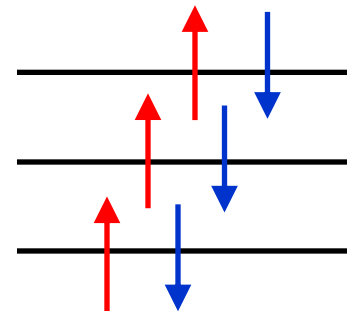
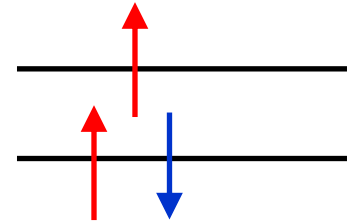


t_{2g} orbitals



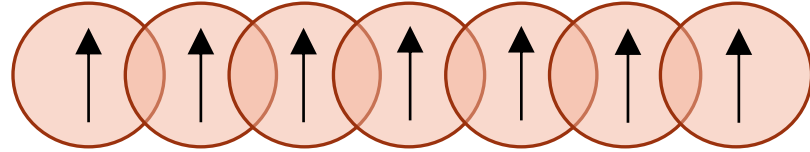
e.g. Cu^{2+} ($3d^9$)

$$S = 1/2$$

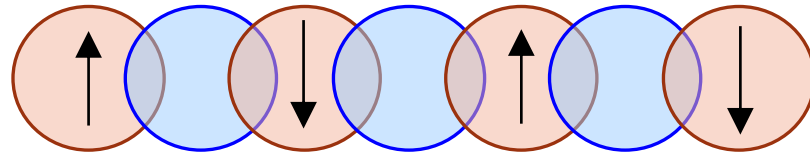


Magnetic Interactions

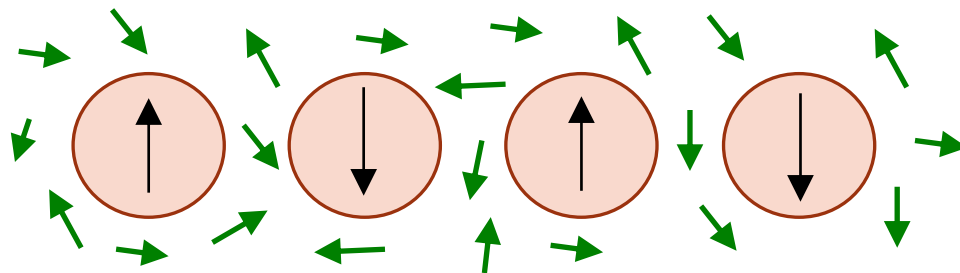
- Direct exchange:



- Superexchange:



- RKKY exchange:

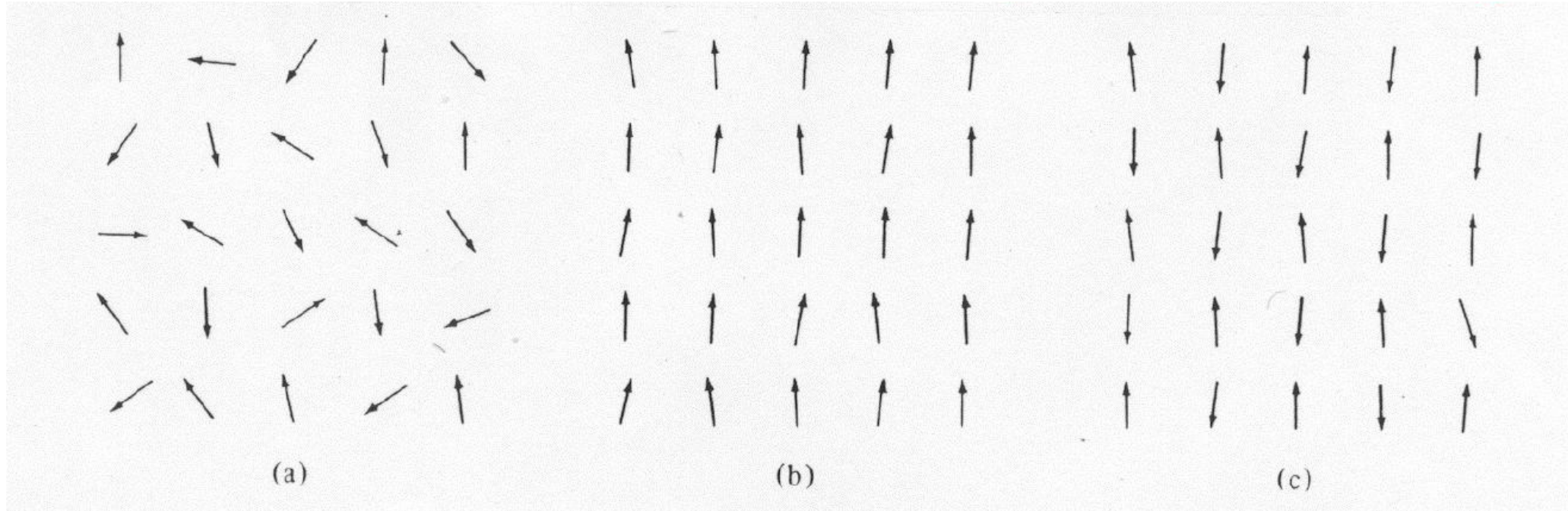


Describe interactions by
a magnetic Hamiltonian:

$$\text{e.g. } H = J \sum_{i,j} S_i \cdot S_j$$

(exchange parameter)

Magnetic Order



Paramagnet
 $(T > T_c)$

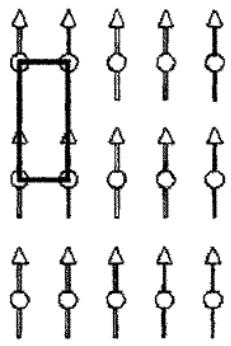
Ferromagnet
 $(T < T_c)$

Antiferromagnet
 $(T < T_N)$

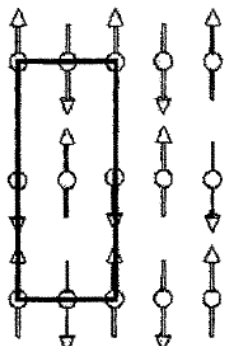
Magnetic Structures

- Magnetically ordered structure that develops in a material depends on nature of underlying magnetic interactions

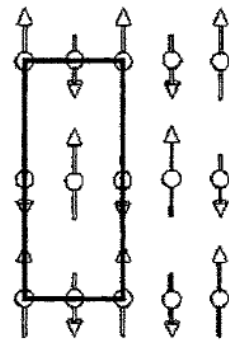
Structures can be relatively simple...



A) ferromagnetic

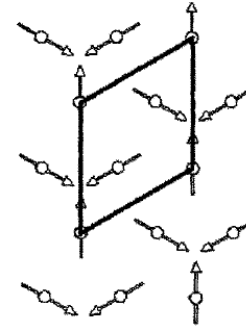


b) antiferromagnetic

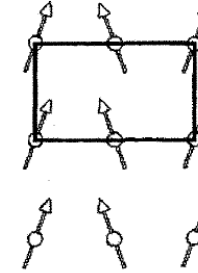


c) ferrimagnetic

... or more complex



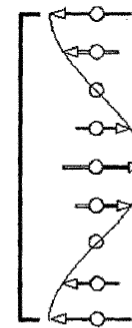
d) triangular



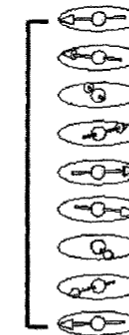
e) canted



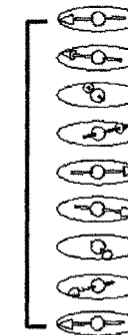
f) umbrella



h) sine or cosine



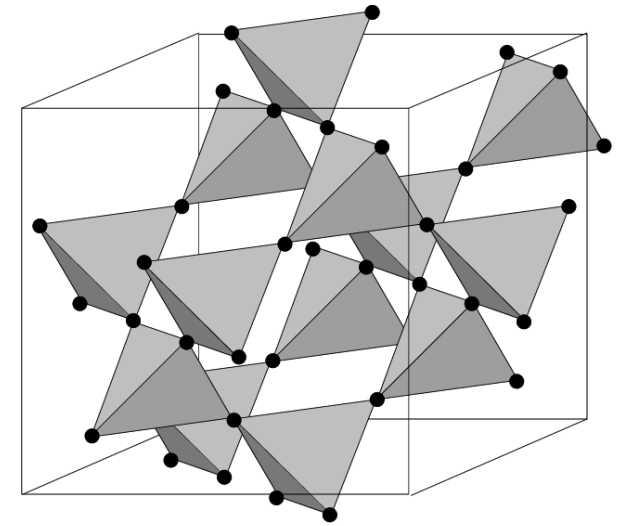
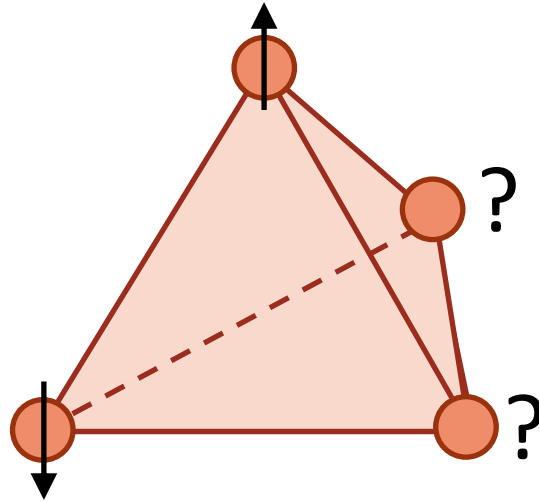
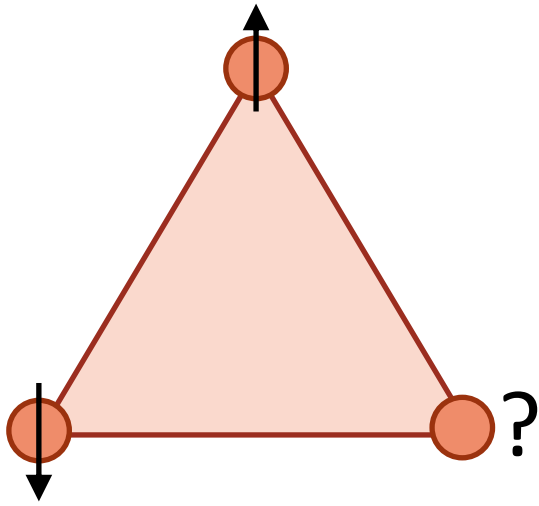
i) circular helix



j) elliptical helix

Geometric Frustration

- We can also try to design magnetic materials which don't order at all:

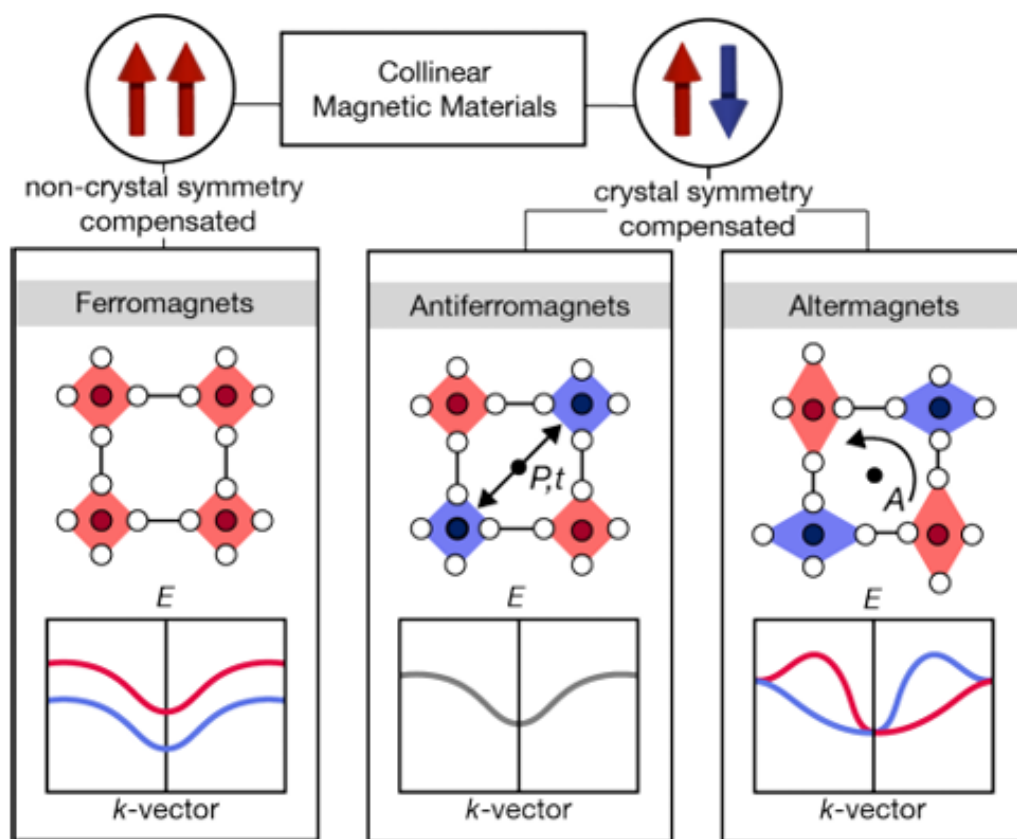


The Pyrochlore Lattice

- Geometrically frustrated magnets can display exotic quantum ground states at low temperatures, e.g. **quantum spin liquids**, **spin ices**, **spin glasses**...

New Forms of Magnetism?

Altermagnetism: Initially proposed in 2019-2021 (*Smejkal/Hayami/Yuan/Mazin et al*)

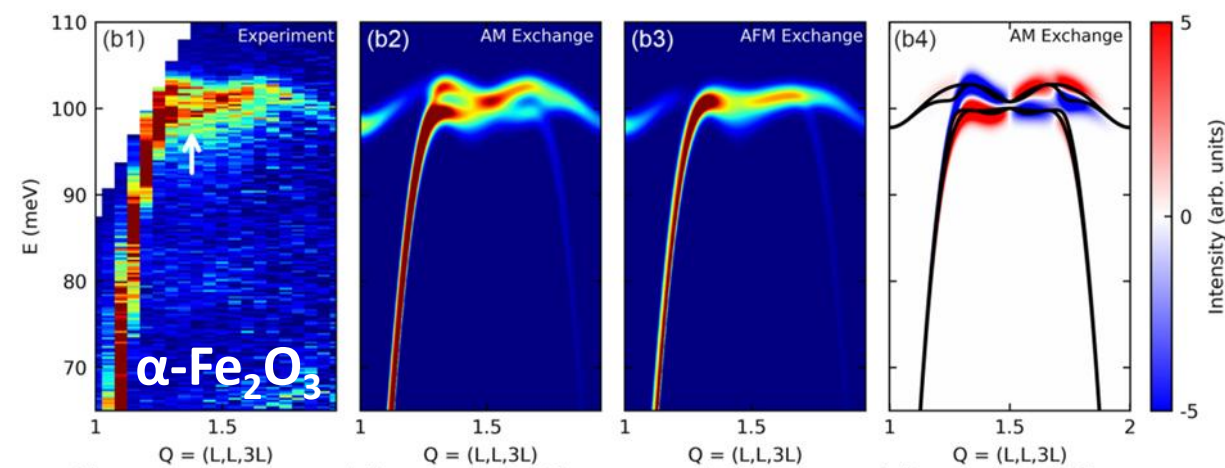


S. S. Fender et al, JACS (2025)

First experimental observations:

MnTe – *J. Krempasky et al, Nature (2024)*

RuO₂ – *O. Fedchenko et al, Sci. Adv. (2024)*

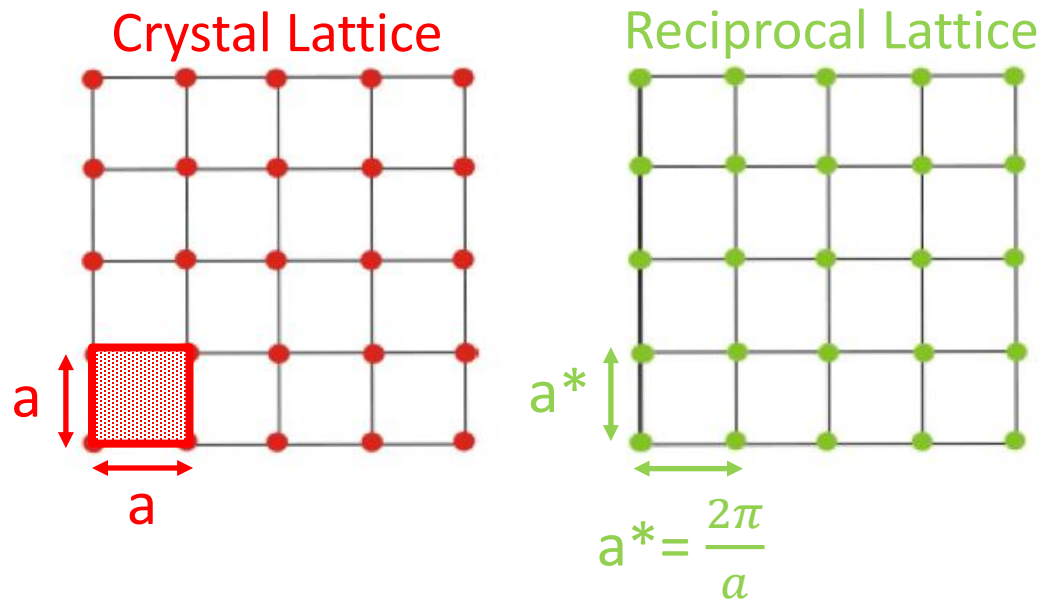


Q. Sun et al, PRL (2025) – ARCS @ ORNL

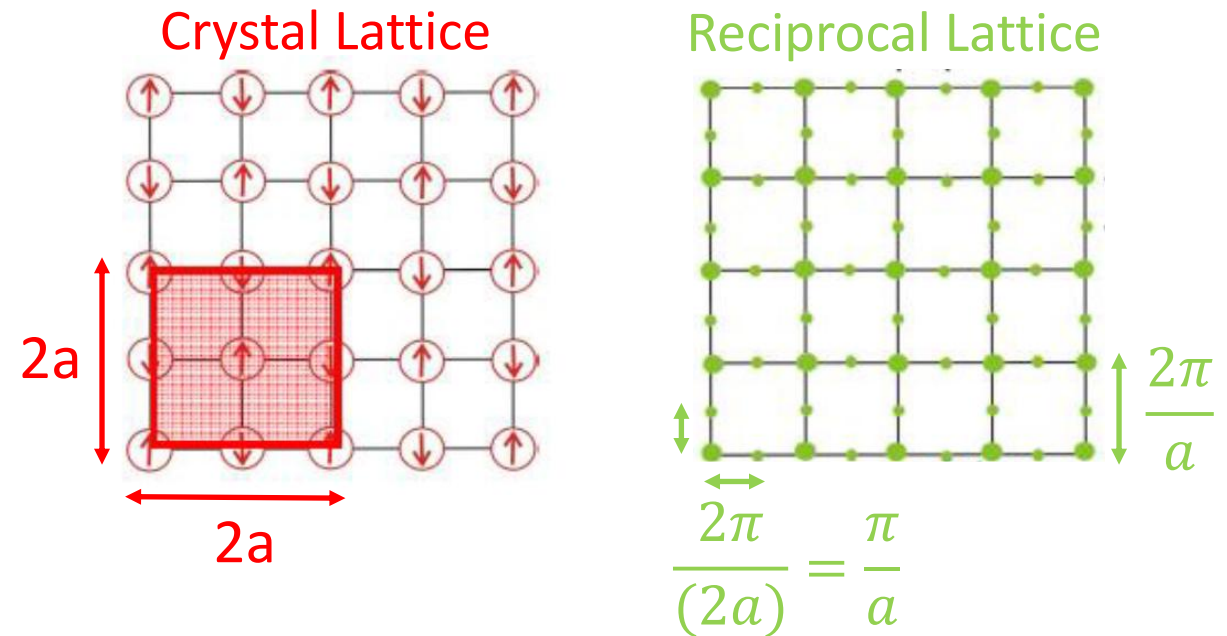
Scattering from a Magnetically Ordered Crystal

- How can we detect magnetic order in a neutron scattering experiment?

Paramagnetic State ($T > T_N$)



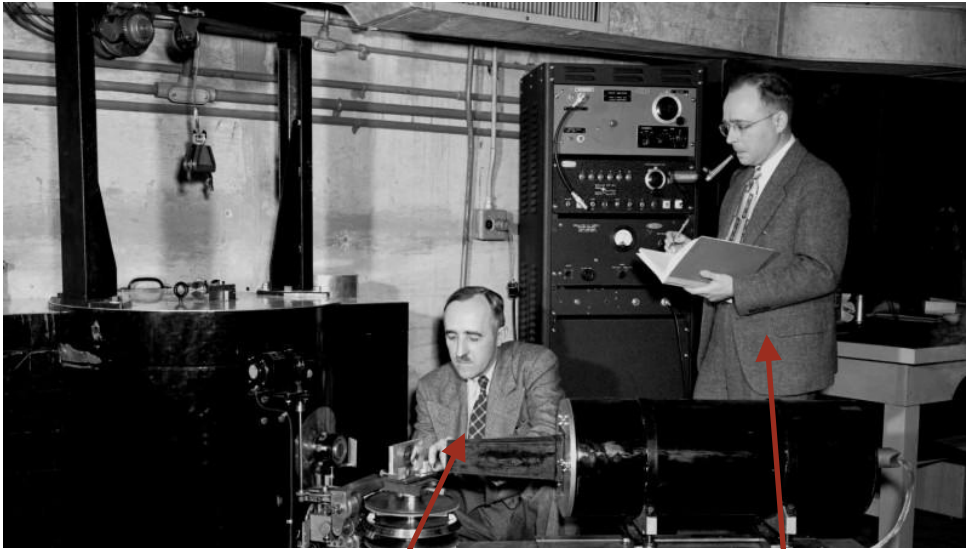
Antiferromagnetic State ($T < T_N$)



- Development of AF order increases size of unit cell → **new magnetic Bragg peaks appear**

First Observation: Magnetic Neutron Scattering from MnO

- Early neutron diffraction experiments at the ORNL X-10 Graphite Reactor:



Ernest Wollan

Clifford Shull

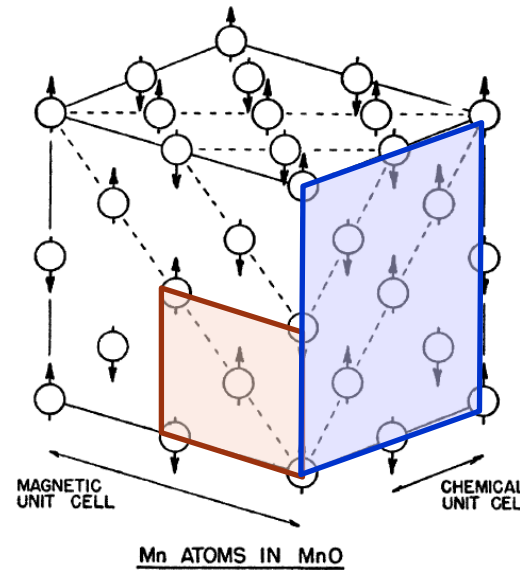


FIG. 5. Antiferromagnetic structure existing in MnO below its Curie temperature of 120°K. The magnetic unit cell has twice the linear dimensions of the chemical unit cell. Only Mn ions are shown in the diagram.

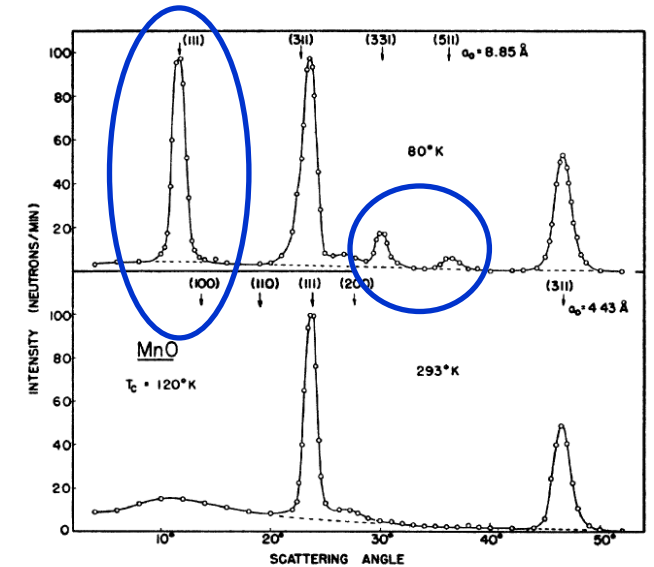


FIG. 4. Neutron diffraction patterns for MnO taken at liquid nitrogen and room temperatures. The patterns have been corrected for the various forms of extraneous, diffuse scattering mentioned in the text. Four extra antiferromagnetic reflections are to be noticed in the low temperature pattern.

First direct evidence of antiferromagnetism

*Shull, Strauser, and Wollan, Phys. Rev. **83**, 333 (1951)*

First Observation: Magnetic Neutron Scattering from MnO

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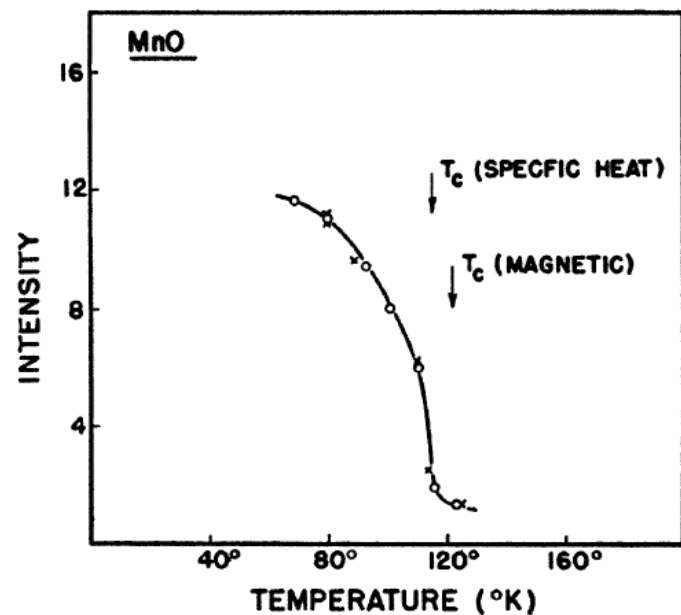


FIG. 7. Temperature dependence of magnetic intensity for MnO. The Curie temperatures suggested by specific heat and magnetic susceptibility data are shown.

Peak intensity $\propto$ staggered magnetization

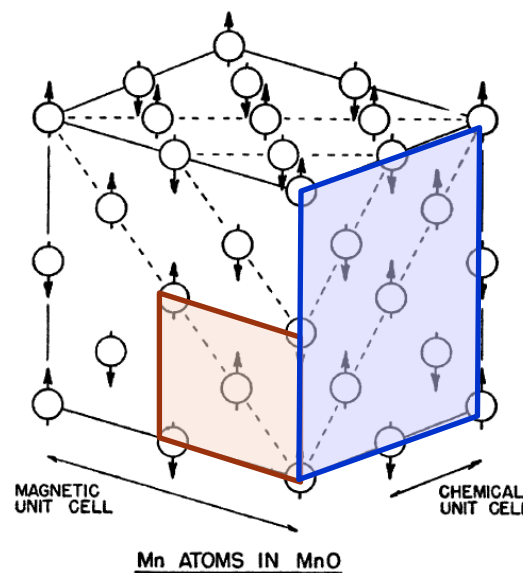


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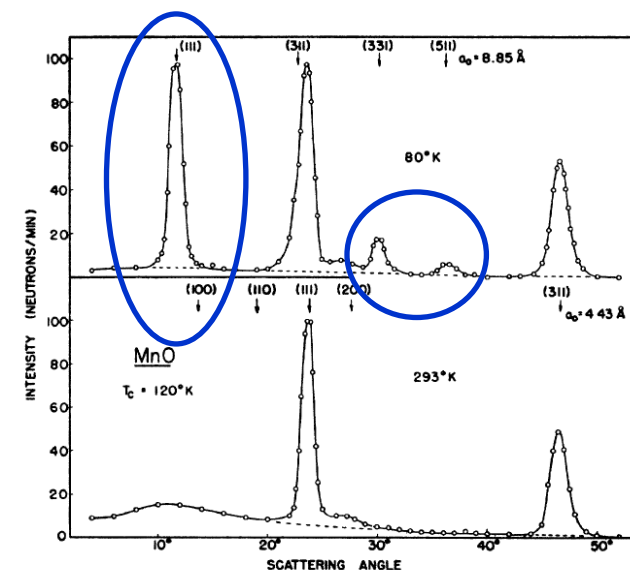


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First direct evidence of antiferromagnetism

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(More on magnetic order in MnO in Experiment N8 on HB-2A)

Magnetic Scattering Cross Section

- What fraction of neutrons will scatter off a sample with a particular change in energy and momentum?
- Change in momentum: $\vec{Q} = \vec{k} - \vec{k}'$
- Change in energy: $\Delta E = \hbar\omega = \frac{\hbar^2 k^2}{2m} - \frac{\hbar^2 k'^2}{2m}$
- Apply Fermi's Golden Rule (1st order perturbation theory):

$$\frac{d^2\sigma}{d\Omega dE'}_{k,\sigma,\lambda \rightarrow k',\sigma',\lambda'} = \underbrace{\left(\frac{m}{2\pi\hbar^2}\right)^2 \frac{k'}{k}}_{\text{(Kinematics)}} \underbrace{|\langle k' \sigma' \lambda' | V_m | k \sigma \lambda \rangle|^2}_{\text{(Interaction Term)}} \underbrace{\delta(E_\lambda - E_{\lambda'} + \hbar\omega)}_{\text{(Energy Conservation)}}$$

The Magnetic Potential

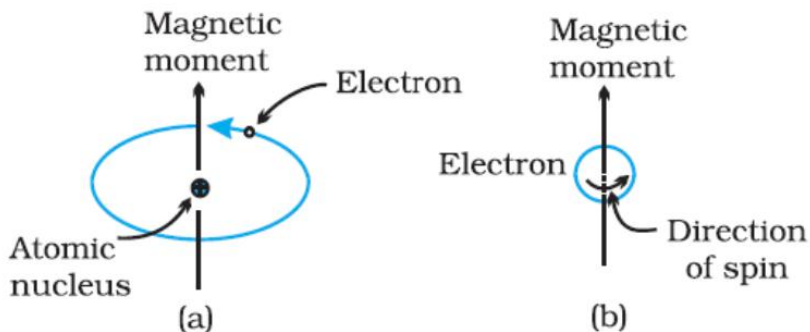
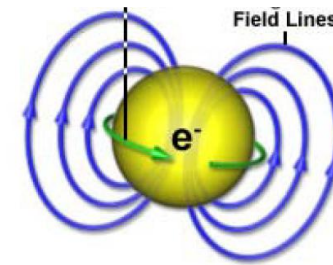
- In order to evaluate the matrix element in the interaction term, we need to determine the magnetic potential produced by all of the unpaired electrons in the material:

$$V_m = \vec{\mu}_n \cdot \vec{B}$$

(Magnetic Potential)

(Magnetic Dipole Moment of Neutron)

(Magnetic Field Produced by Unpaired Electrons)



Must consider:

B_l = Magnetic field from **orbital motion** of an electron

B_s = Magnetic field from **spin** of an electron

Magnetic Scattering Cross Section

- Evaluating the interaction term $|\langle k' \sigma' \lambda' | V_m | k \sigma \lambda \rangle|^2$ can be quite complicated.
- Jumping to the final result:

$$\frac{d^2\sigma}{d\Omega dE'} = \frac{(\gamma r_0)^2}{2\pi\hbar} \frac{k'}{k} N \left[\frac{1}{2} g F(\vec{Q}) \right]^2 \sum_{\alpha\beta} (\delta_{\alpha\beta} - \hat{Q}_\alpha \hat{Q}_\beta) \\ \times \sum_l e^{i\vec{Q}\cdot\vec{l}} \int \left\langle e^{-i\vec{Q}\cdot\vec{u}_0(0)} e^{i\vec{Q}\cdot\vec{u}_l(t)} \right\rangle \left\langle S_0^\alpha(0) S_l^\beta(t) \right\rangle e^{-i\omega t} dt$$

Key features:

1. From constants – magnetic scattering comparable in strength to nuclear scattering ($\sim r_0^2$)
2. Proportional to square of **magnetic form factor**, $F(\vec{Q})^2$

Magnetic Scattering Cross Section

- Evaluating the interaction term $|\langle k' \sigma' \lambda' | V_m | k \sigma \lambda \rangle|^2$ can be quite complicated.
- Jumping to the final result:

$$\frac{d^2\sigma}{d\Omega dE'} = \frac{(\gamma r_0)^2}{2\pi\hbar} \frac{k'}{k} N \left[\frac{1}{2} gF(\vec{Q}) \right]^2 \sum_{\alpha\beta} (\delta_{\alpha\beta} - \hat{Q}_\alpha \hat{Q}_\beta) \\ \times \sum_l e^{i\vec{Q}\cdot\vec{l}} \int \left\langle e^{-i\vec{Q}\cdot\vec{u}_0(0)} e^{i\vec{Q}\cdot\vec{u}_l(t)} \right\rangle \left\langle S_0^\alpha(0) S_l^\beta(t) \right\rangle e^{-i\omega t} dt$$

Key features:

3. **Polarization factor** – describes dependence on spin direction. Term vanishes if components of spin are parallel to scattering vector $\vec{Q} \rightarrow$ only sensitive to $S \perp \vec{Q}$

Magnetic Scattering Cross Section

- Evaluating the interaction term $|\langle k' \sigma' \lambda' | V_m | k \sigma \lambda \rangle|^2$ can be quite complicated.
- Jumping to the final result:

$$\frac{d^2\sigma}{d\Omega dE'} = \frac{(\gamma r_0)^2}{2\pi\hbar} \frac{k'}{k} N \left[\frac{1}{2} g F(\vec{Q}) \right]^2 \sum_{\alpha\beta} (\delta_{\alpha\beta} - \hat{Q}_\alpha \hat{Q}_\beta) \times \sum_l e^{i\vec{Q}\cdot\vec{l}} \int \left\langle e^{-i\vec{Q}\cdot\vec{u}_0(0)} e^{i\vec{Q}\cdot\vec{u}_l(t)} \right\rangle \left\langle S_0^\alpha(0) S_l^\beta(t) \right\rangle e^{-i\omega t} dt$$

Key features:

4. **Dynamic spin pair correlation function** – measures correlation between spin α at origin and $t = 0$ and spin β at position l and time t . The Fourier transform of this term is the **dynamic structure factor**, $S(\vec{Q}, \omega)$

Magnetic Form Factor

- $F(\vec{Q})$ = Fourier transform of the spin distribution in real space

$$F(\vec{Q}) = \int S(\vec{r}) e^{i\vec{Q} \cdot \vec{r}} d^3r$$

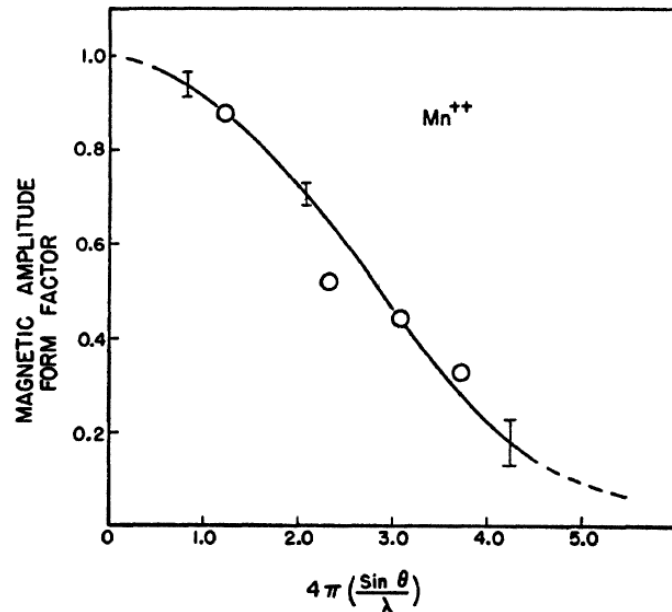
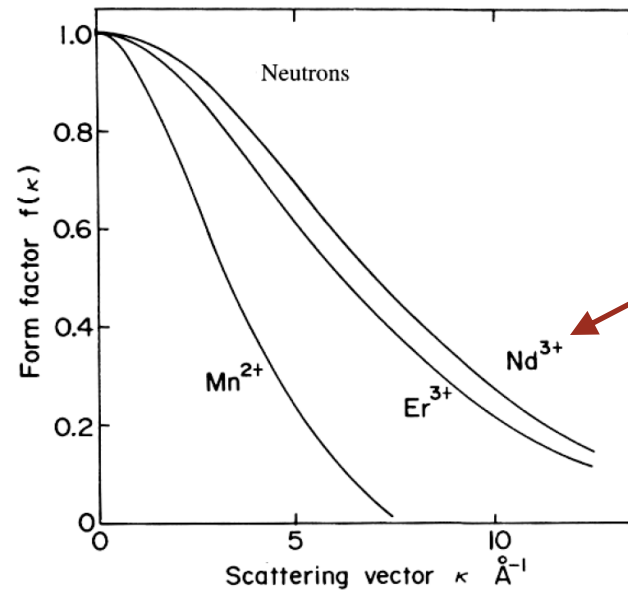


FIG. 2. Magnetic amplitude form factor for Mn²⁺ ions. The curve is that obtained from paramagnetic diffuse scattering with estimated error as shown. The points represent values of the form factor obtained from the low temperature antiferromagnetic reflections of MnO.



$F(\vec{Q})$ decreases faster as wavefunctions become more spatially extended

- Analogous to chemical form factor for x-ray scattering
- Typically drops off monotonically as $\vec{Q}$ increases

Shull, Strauser, and Wollan, *Phys. Rev.* **83**, 333 (1951)

Elastic Magnetic Scattering

- For elastic scattering (i.e. diffraction), we have: $\Delta E = \hbar\omega = \frac{\hbar^2 k^2}{2m} - \frac{\hbar^2 k'^2}{2m} = 0$
- What we measure is the **time-independent** structure factor, $S(\vec{Q})$

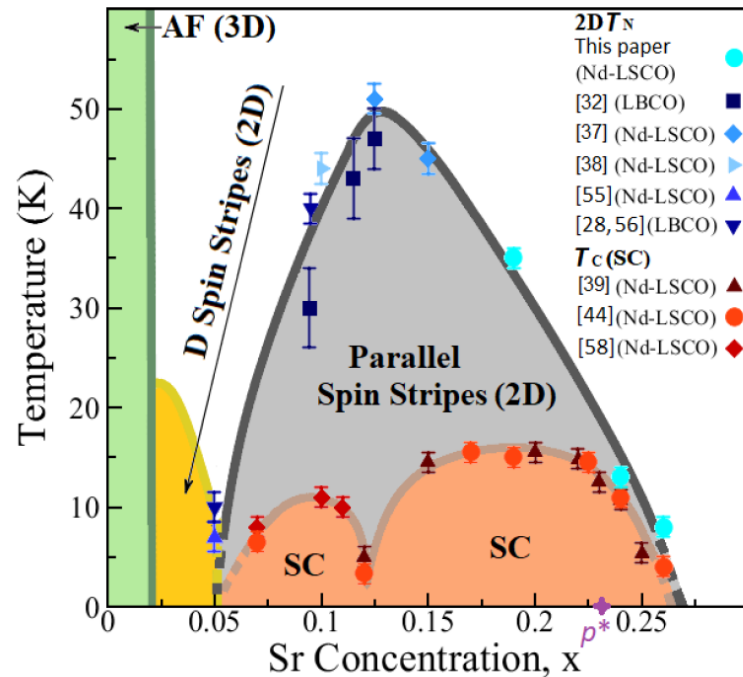
$$\frac{d\sigma}{d\Omega} = (\gamma r_0)^2 \frac{k'}{k} N \left[\frac{1}{2} g^F(\vec{Q}) \right]^2 e^{-2W} \sum_{\alpha\beta} (\delta_{\alpha\beta} - \hat{Q}_\alpha \hat{Q}_\beta) \times \sum_l e^{i\vec{Q} \cdot \vec{l}} \int \langle S_0^\alpha \rangle \langle S_l^\beta \rangle$$

↑
↑
↑

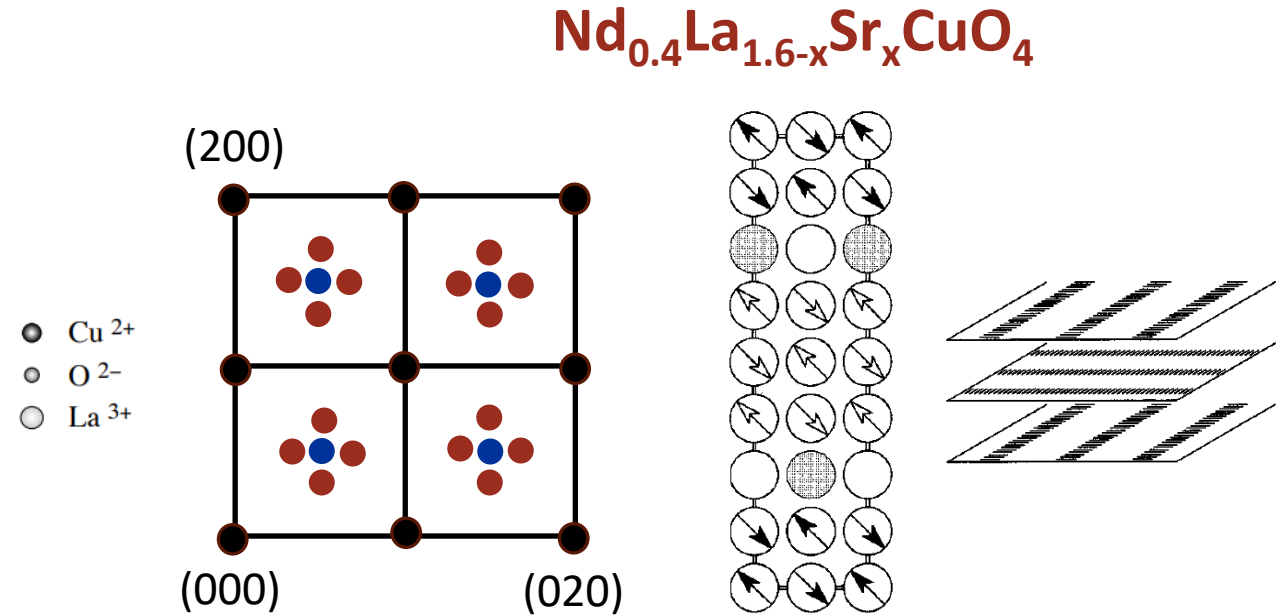
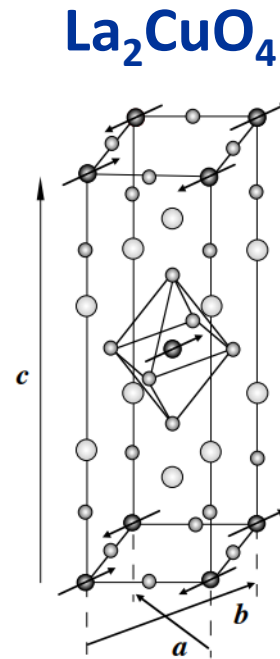
Debye-Waller Effect
Polarization Factor:
Only sensitive to $S \perp \vec{Q}$
Add up spins with a
phase factor of $e^{i\vec{Q} \cdot \vec{l}}$

Elastic Magnetic Scattering: Examples

- Magnetic order in High T_c cuprate superconductors (e.g. $\text{Nd}_{0.4}\text{La}_{1.6-x}\text{Sr}_x\text{CuO}_4$)



Q. Ma et al, Phys. Rev. Res. (2021)

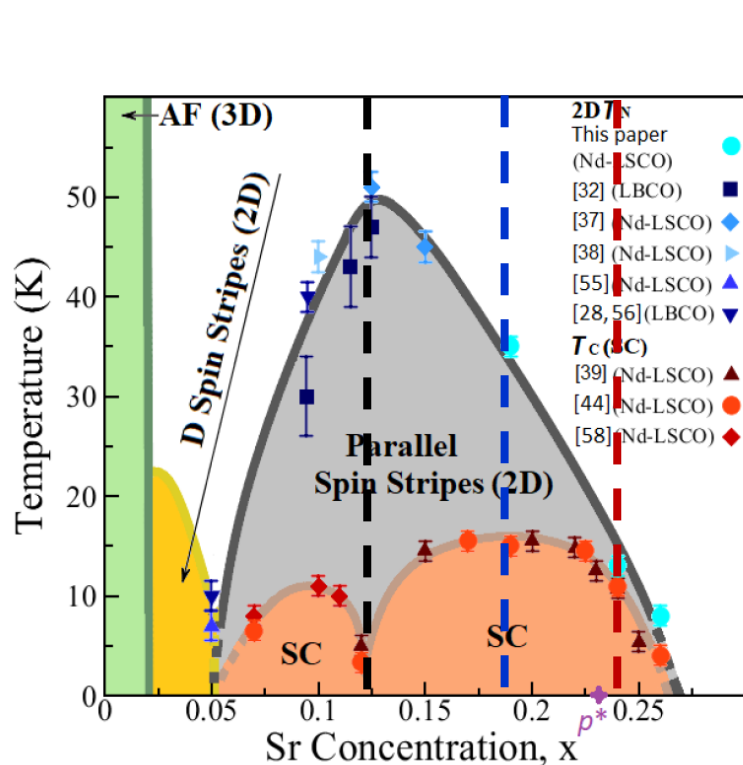


J. Tranquada et al, Phys. Rev. B (1996)

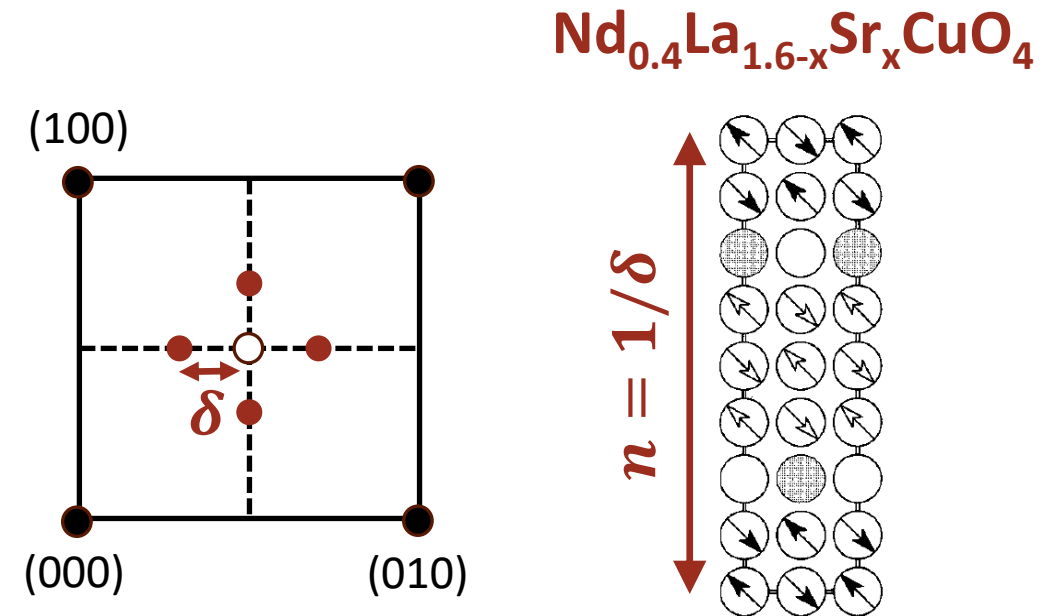
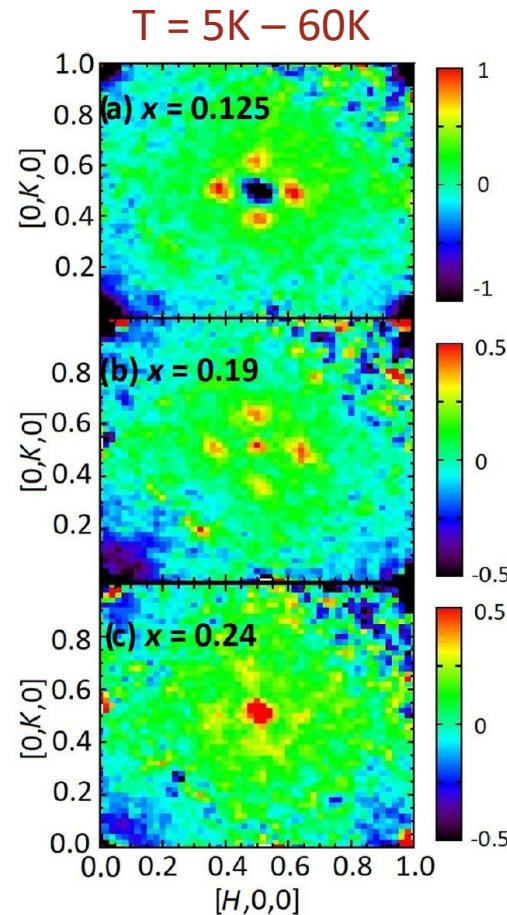
- Undoped parent compound: **commensurate** antiferromagnetic order, $\mathbf{Q}_{\text{AF}} = (0.5, 0.5, L)$
- For $x > 0.02$: **incommensurate "stripe"** order, $\mathbf{Q}_{\text{AF}} = (0.5 \pm \delta, 0.5, L)$ and $(0.5, 0.5 \pm \delta, L)$

Elastic Magnetic Scattering: Examples

- Magnetic order in High T_c cuprate superconductors (e.g. $\text{Nd}_{0.4}\text{La}_{1.6-x}\text{Sr}_x\text{CuO}_4$)



Q. Ma et al, Phys. Rev. Res. (2021)
 SEQUOIA @ ORNL

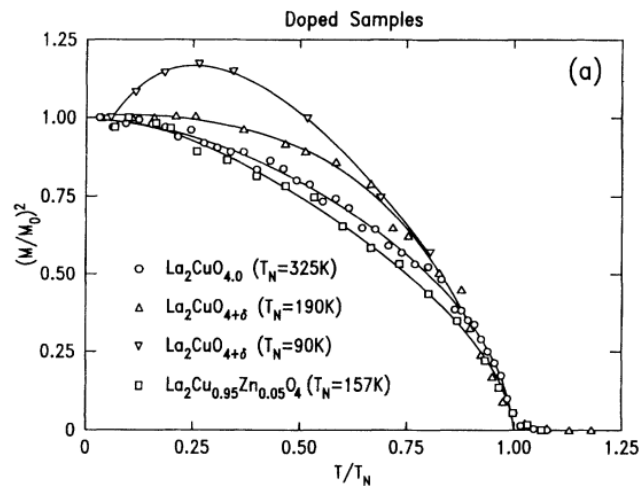


Peaks at $\mathbf{Q}_{\text{AF}} = (0.5 \pm \delta, 0.5, L)$ imply modulation of magnetic structure along [100] with period of $n = 1/\delta$ unit cells

Elastic Magnetic Scattering: Examples



Well-defined Bragg peaks:
Long-range 3D magnetic order



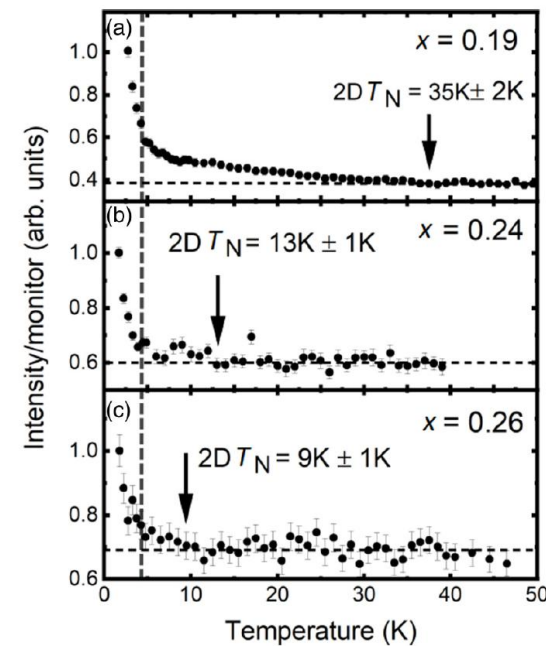
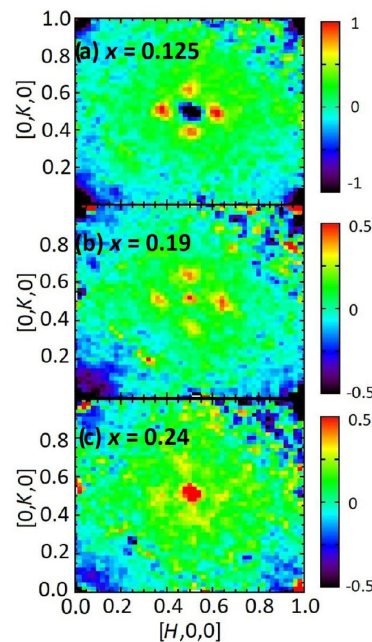
Keimer et al, PRB (1992)

$$I \propto M^2 = M_0^2 \left(1 - \frac{T}{T_C}\right)^{2\beta}$$

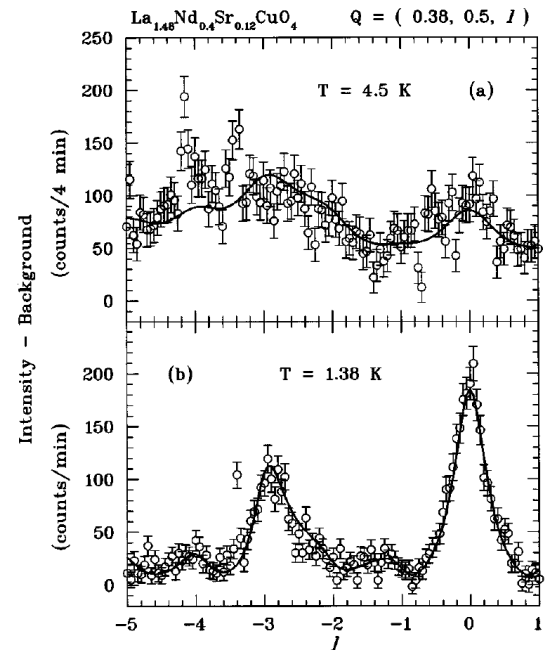
$$\xi \propto \frac{1}{Q} = \text{correlation length}$$



Diffuse “rods” of magnetic scattering:
Quasi-2D magnetic order



Ma et al, PRR (2021)
HB-3 @ ORNL



Tranquada et al, PRB (1996)

Inelastic Magnetic Scattering

- For inelastic scattering (i.e. spectroscopy), we have: $\Delta E = \hbar\omega = \frac{\hbar^2 k^2}{2m} - \frac{\hbar^2 k'^2}{2m} \neq 0$
- This implies that $|\vec{k}| \neq |\vec{k}'| \rightarrow$ change in both $\vec{Q}$ and ω
- What we measure is the **dynamical structure factor** $S(\vec{Q}, \omega)$

• Key points:

- Study **dynamic** magnetic moments (on time scales of 10^{-9} to 10^{-12} sec)

Bose (Temperature) Factor

Imaginary part of dynamic susceptibility

$$S(\vec{Q}, \omega) = \frac{1}{1 - e^{-\beta\hbar\omega}} \frac{\chi''(\vec{Q}, \omega)}{\pi(g\mu_B)^2} = \boxed{n(\omega)} \boxed{\chi''(\vec{Q}, \omega)} \quad (\text{Fluctuation-Dissipation Theorem})$$

- Intensity integrated over all $\vec{Q}, \omega$ is constant: $\int d\omega \int_{BZ} d\vec{Q} S(\vec{Q}, \omega) \sim S(S + 1)$
(Total Moment Sum Rule)

(More on inelastic scattering in Martin Mourigal's lectures on Wednesday)

Inelastic Magnetic Scattering: Spin Waves

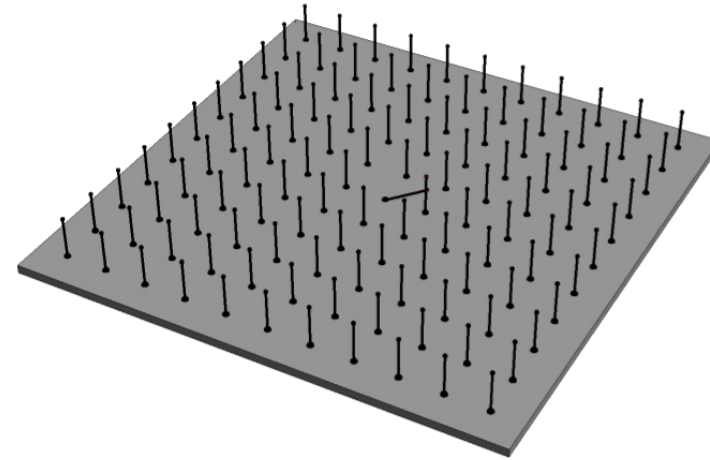
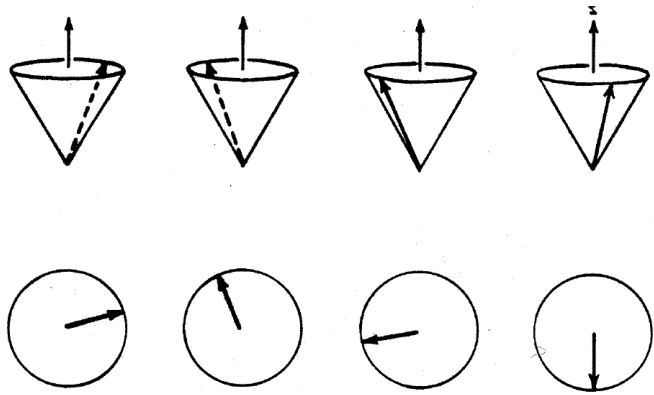
- When a neutron scatters off a sample it can create or destroy an excitation
- If sample is magnetically ordered (e.g. a FM spin chain), the incident neutron can create a spin “defect” which is distributed over all possible sites
- We call this collective excitation a **spin wave** or **magnon**



Spins are coupled through magnetic Hamiltonian:
$$H = J \sum_{i,j} S_i \cdot S_j$$

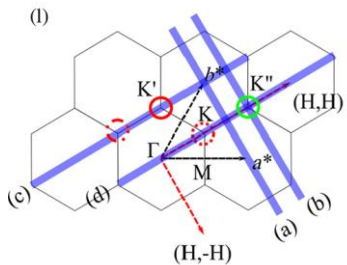
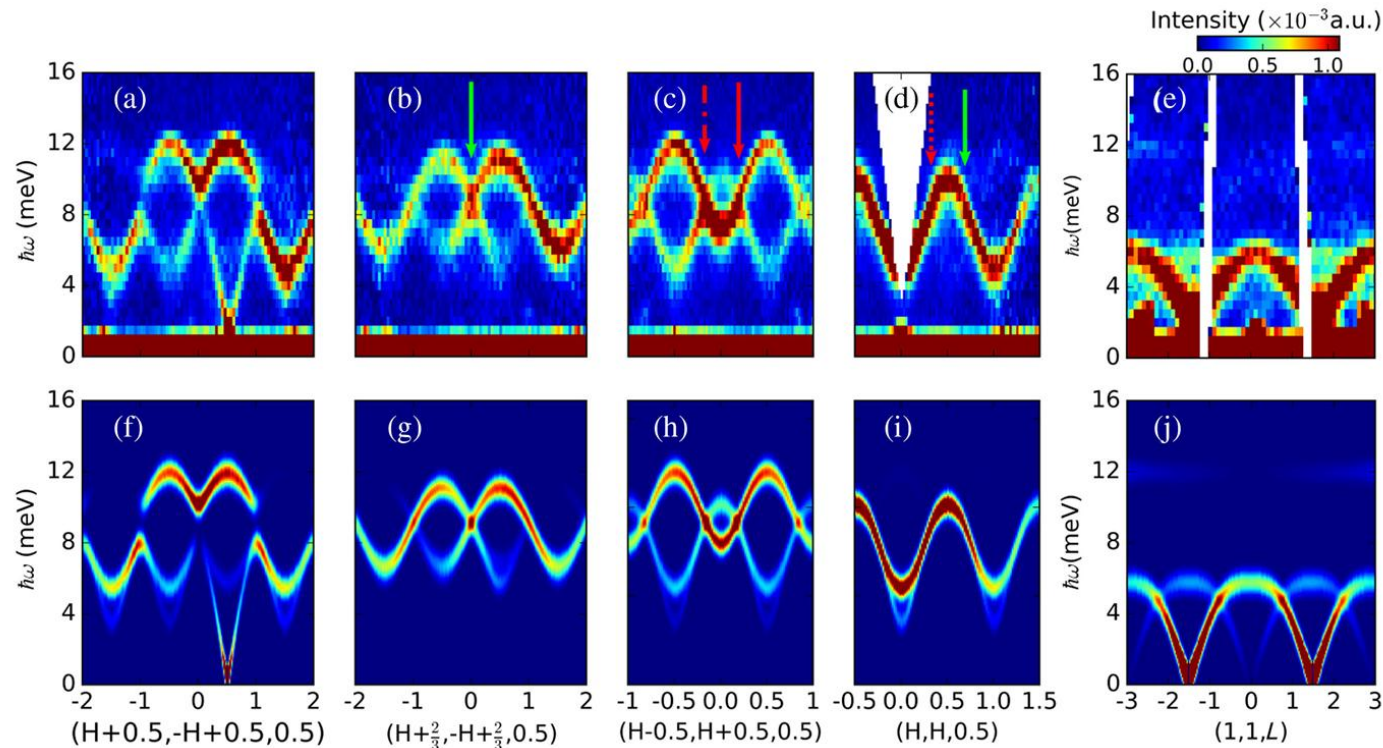
Inelastic Magnetic Scattering: Spin Waves

- When a neutron scatters off a sample it can create or destroy an excitation
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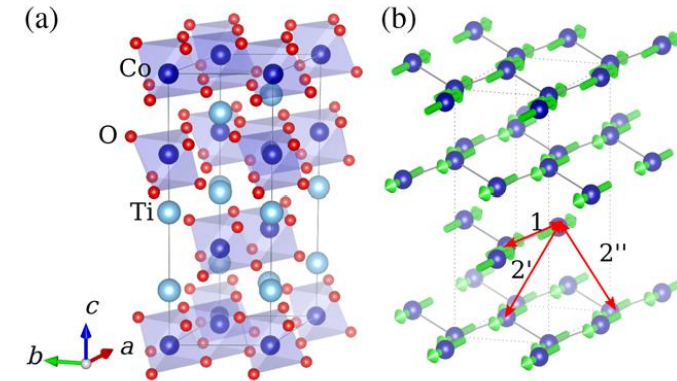
Inelastic Magnetic Scattering: Examples



B. Yuan et al, PRX (2020) – SEQUOIA @ ORNL

$$H = J_{\parallel}(\tilde{S}_{x,i}\tilde{S}_{x,j} + \tilde{S}_{y,i}\tilde{S}_{y,j}) + J_{\perp}\tilde{S}_{z,i}\tilde{S}_{z,j}$$

• Spin waves in a honeycomb magnet



• **CoTiO₃** Single Crystal

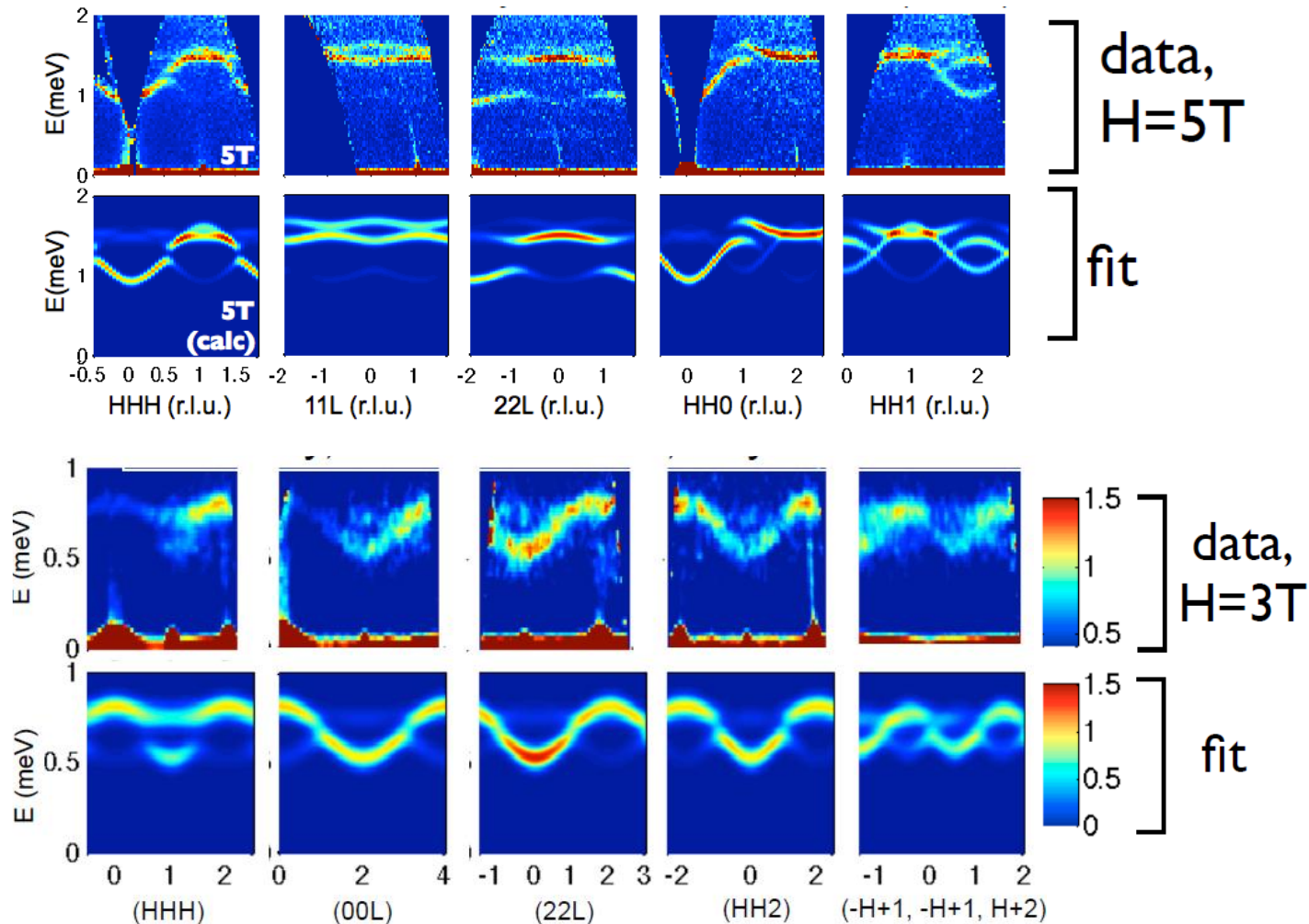
• Measured on SEQUOIA at ORNL

• Fit spin wave dispersion to theoretical model and extract detailed exchange parameters:

$$J_{\parallel,1} = 4.41 \text{ meV}, J_{\perp,1} = 0,$$

$$J_{\parallel,2'=2''} = J_{\perp,2'=2''} = 0.57 \text{ meV}$$

Inelastic Magnetic Scattering: Examples

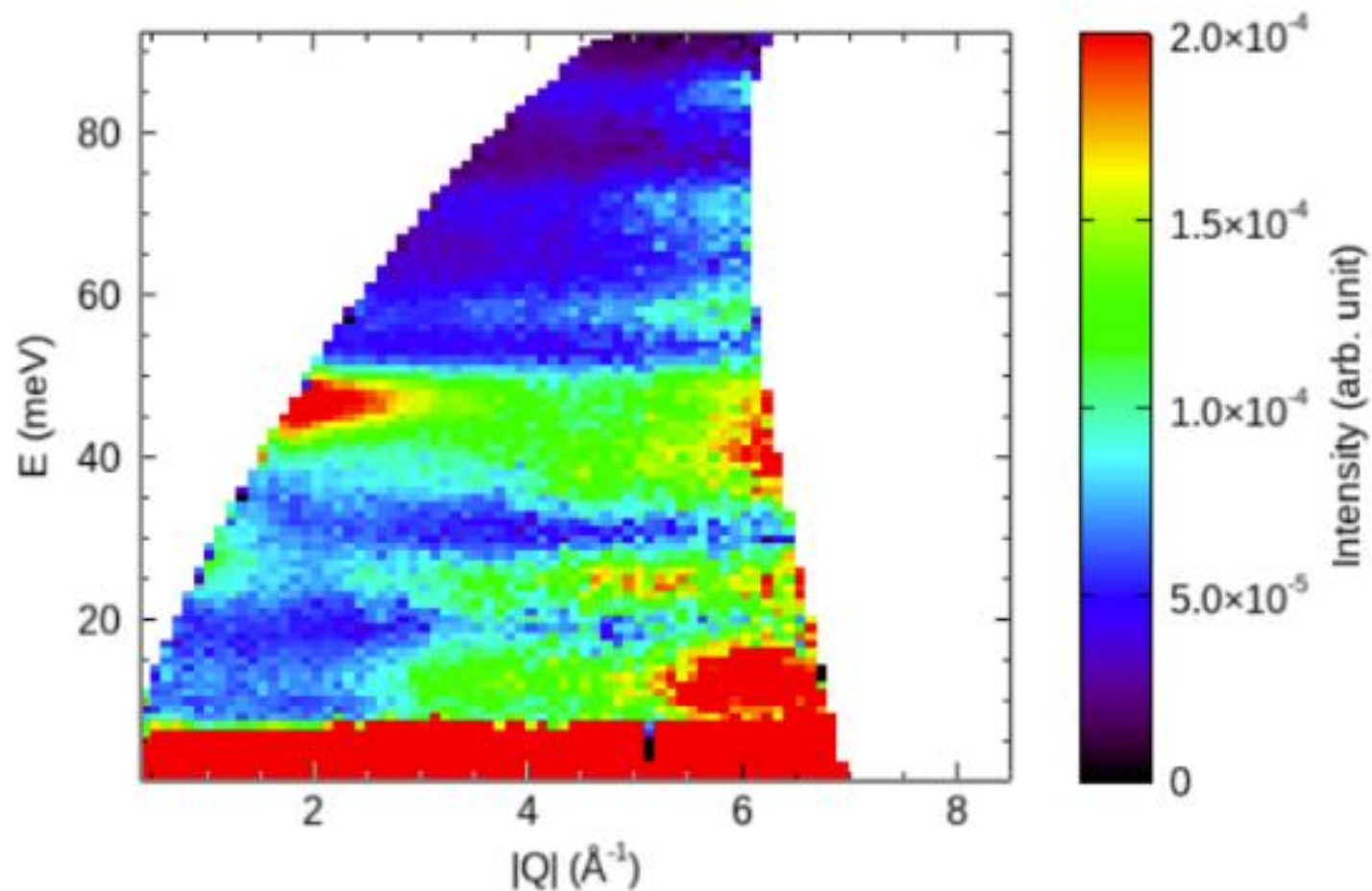


- **Frustrated magnetism in pyrochlores**
- $\text{Yb}_2\text{Ti}_2\text{O}_7$ (top) and $\text{Er}_2\text{Ti}_2\text{O}_7$ (bottom) Single Crystals
- Measured on DCS at NIST
- Fit spin wave dispersion to theoretical model and extract detailed exchange parameters (J_1, J_2, J_3, J_4)
- Magnetic interactions explain low temperature magnetic ground states

K. Ross et al, Phys. Rev. X **1**, 021002 (2011)

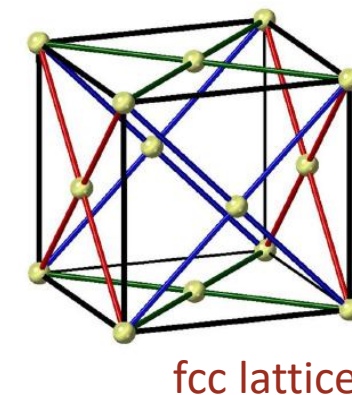
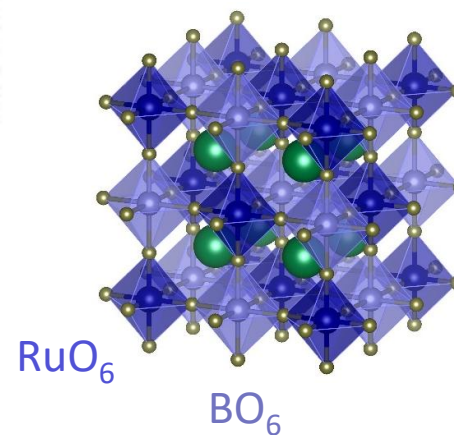
L. Savary et al, Phys. Rev. Lett. **109**, 167201 (2012)

How can we distinguish magnetic scattering?



(B. Yuan et al, SEQUOIA @ ORNL)

- **Spin and Orbital Excitations in Ru Double Perovskites**
- Powder samples of A_2BRuO_6
- Measured on SEQUOIA at SNS



How can we distinguish magnetic scattering?

(1) Momentum dependence:

- Magnetic scattering **decreases** with increasing $|Q|$ ($\propto |F(Q)|^2$)
- Phonon scattering **increases** with increasing $|Q|$ ($\propto |e \cdot Q|^2$)

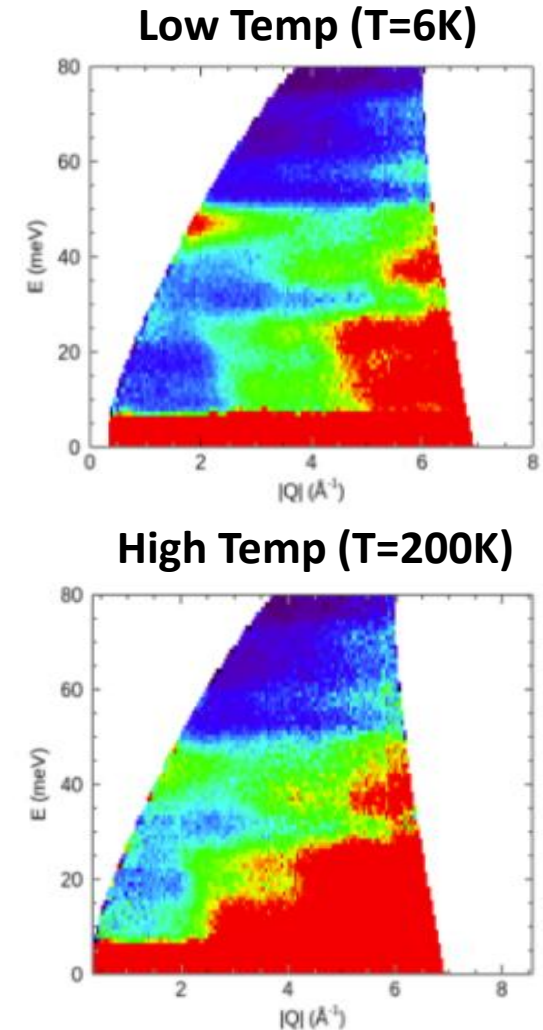
(2) Temperature dependence:

- Magnetic scattering **decreases** with increasing T (disappears at $T > T_C$)
- Phonon scattering **increases** with increasing T ($\propto$ thermal population)

(3) Polarization dependence (with polarized beam):

- Magnetic scattering **mostly spin flip**
- Nuclear scattering **mostly non-spin flip**

More on polarized neutrons in experiments N2 (HYSPEC) and N23 (MAGREF), and Barry Winn's lecture on Wednesday



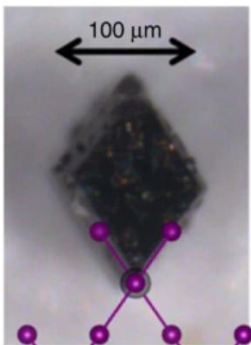
What if neutrons aren't an (easy) option?

- Magnetic neutron scattering can be challenging for:
- Very small samples (e.g. sub-mm sized crystals, thin films, heterostructures, diamond anvil or strain cells)
- Highly absorbing elements (e.g. Gd, Sm, Eu, B, Ir)
- Very expensive elements (e.g. >\$1000/g)



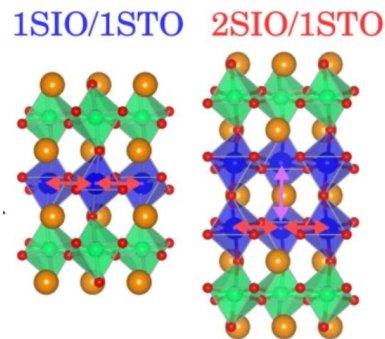
Magnetic scattering is also possible with **x-rays**...

*Harmonic
honeycomb
 β -Li₂IrO₃*

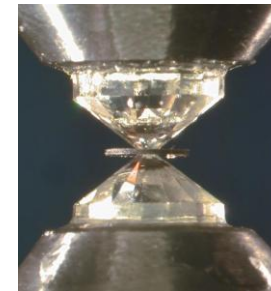


*K.A. Modic et al,
Nat. Comm. (2014)*

*(nSrIrO₃/SrTiO₃)
heterostructures*



*D. Meyers et al,
Sci. Rep. (2019)*



*α -Li₂IrO₃ in
diamond anvil cell*

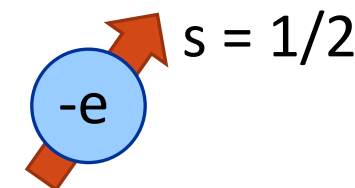
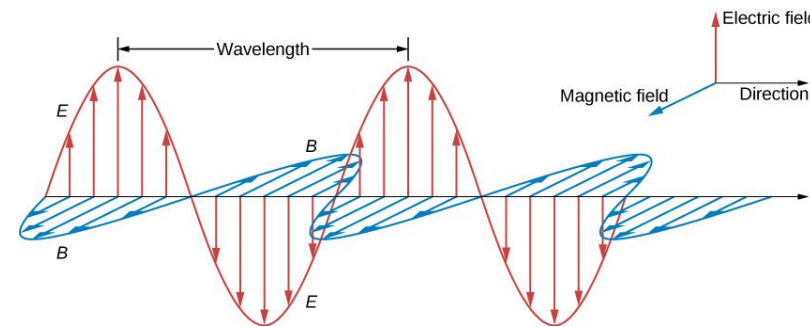
Magnetic Scattering with X-rays

- X-rays carry no magnetic moment
- Primary interaction with matter: **E-field** of x-ray + **charge** of electrons
- Also interacts through: **B-field** of x-ray + **spin** of electrons
- Unlike neutrons:

1. Magnetic scattering is MUCH weaker than charge scattering

$$\text{Amplitude ratio: } \frac{A(\text{magnetic})}{A(\text{charge})} = \frac{\hbar\omega}{mc^2} \quad (\text{for } \textit{single electron})$$

2. X-ray photon energies (**~0.5 to 50 keV**) are orders of magnitude larger than typical energy scales for magnetic excitations (**~0.5 to 500 meV**)



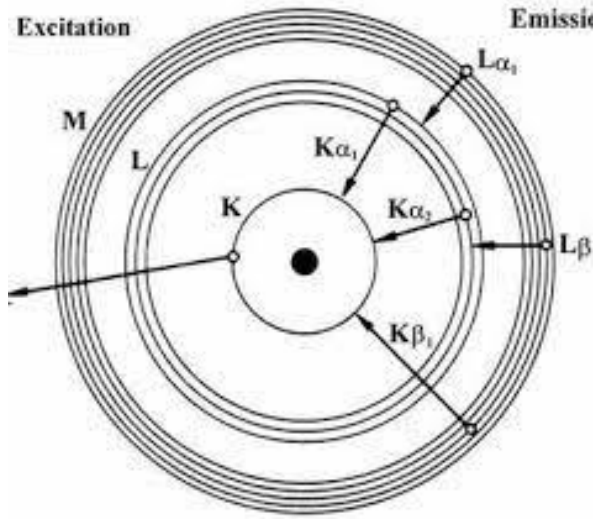
At $E_i \sim 5$ keV:
Amplitude ratio $\sim 10^{-2}$
Intensity ratio $\sim 10^{-4}$

Resonant Magnetic X-ray Scattering

Hard x-rays (> 5 keV)

Tender x-rays (1-5 keV)

Soft x-rays (< 1 keV)



1 H Hydrogen	2 He Helium																
3 Li Lithium	4 Be Beryllium	5 B Boron	6 C Carbon	7 N Nitrogen	8 O Oxygen	9 F Fluorine	10 Ne Neon									11 Na Sodium	12 Mg Magnesium
13 Al Aluminium	14 Si Silicon	15 P Phosphorus	16 S Sulfur	17 Cl Chlorine	18 Ar Argon									19 K Potassium	20 Ca Calcium	21 Sc Scandium	22 Ti Titanium
23 V Vanadium	24 Cr Chromium	25 Mn Manganese	26 Fe Iron	27 Co Cobalt	28 Ni Nickel	29 Cu Copper	30 Zn Zinc	31 Ga Gallium	32 Ge Germanium	33 As Arsenic	34 Se Selenium	35 Br Bromine	36 Kr Krypton	37 Rb Rubidium	38 Sr Strontium	39 Y Yttrium	40 Zr Zirconium
41 Nb Niobium	42 Mo Molybdenum	43 Tc Technetium	44 Ru Ruthenium	45 Rh Rhodium	46 Pd Palladium	47 Ag Silver	48 Cd Cadmium	49 In Indium	50 Sn Tin	51 Sb Antimony	52 Te Tellurium	53 I Iodine	54 Xe Xenon	55 Cs Caesium	56 Ba Barium	57 La Lanthanum	58 Ce Cerium
59 Pr Praseodymium	60 Nd Neodymium	61 Pm Promethium	62 Sm Samarium	63 Eu Europium	64 Gd Gadolinium	65 Tb Terbium	66 Dy Dysprosium	67 Ho Holmium	68 Er Erbium	69 Tm Thulium	70 Yb Ytterbium	71 Lu Lutetium	72 Hf Hafnium	73 Ta Tantalum	74 W Tungsten	75 Re Rhenium	76 Os Osmium
77 Ir Iridium	78 Pt Platinum	79 Au Gold	80 Hg Mercury	81 Tl Thallium	82 Pb Lead	83 Bi Bismuth	84 Po Polonium	85 At Astatine	86 Rn Radon	87 Fr Francium	88 Ra Radium	89 Ac Actinium	90 Th Thorium	91 Pa Protactinium	92 U Uranium	93 Np Neptunium	94 Pu Plutonium
95 Am Americium	96 Cm Curium	97 Bk Berkelium	98 Cf Californium	99 Es Einsteinium	100 Fm Fermium	101 Md Mendelevium	102 No Nobelium	103 Lr Lawrencium					104 Rf Rutherfordium	105 Db Dubnium	106 Sg Seaborgium	107 Bh Bohrium	108 Hs Hassium
109 Mt Meitnerium	110 Ds Darmstadtium	111 Rg Roentgenium	112 Cn Copernicium	113 Nh Nihonium	114 Fl Flerovium	115 Mc Moscovium	116 Lv Livermorium	117 Ts Tennessine	118 Og Oganesson								

- Scattering tensor for magnetic x-ray scattering:

$$F_j(E) = \sigma^{(0)}(E) \varepsilon_i \cdot \varepsilon_0^* + \sigma^{(1)}(E) \varepsilon_i \times \varepsilon_0^* \cdot M_j + \sigma^{(2)}(E) \left[(\varepsilon_i \cdot M_j)(\varepsilon_0^* \cdot M_j) - \frac{1}{3} \varepsilon_i \cdot \varepsilon_0^* \right]$$

- Intensity of magnetic Bragg peaks:
$$I = \left| \sum_j e^{ig \cdot r_j} \sigma_j^{(1)}(E) \varepsilon_i \times \varepsilon_0^* \cdot M_j \right|^2$$

Magnetic X-ray Scattering

Advantages:

- Element (and even orbital) specificity
- Smaller samples (ideal for thin films, high pressure diamond anvil cell experiments)
- Better resolution in momentum

Disadvantages:

- More complicated theory/modeling
- Magnetic scattering much weaker than charge scattering
- Worse resolution in energy
- Restricted momentum transfer (soft x-ray)

X-ray and neutron scattering are highly complementary techniques for the study of magnetic materials
(But **neutrons** should almost always be your 1st choice)

Suggestions for Further Reading...

Textbooks:

G.L. Squires – *Introduction to the Theory of Thermal Neutron Scattering* (2012)

S.W. Lovesey – *Theory of Neutron Scattering from Condensed Matter, Vol. 2* (1984)

T. Chatterji – *Neutron Scattering from Magnetic Materials* (2006)

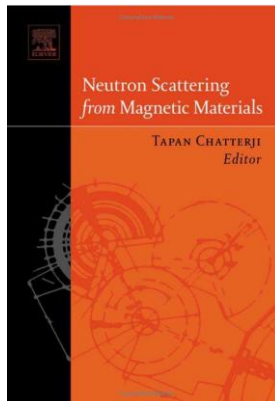
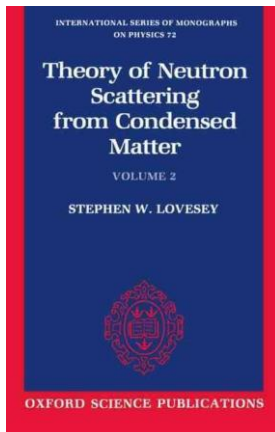
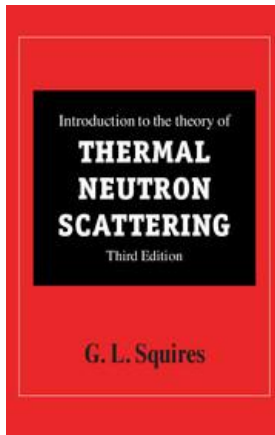
Reviews:

J.W. Lynn – [Magnetic Neutron Scattering](#) from *Characterization of Materials, Vol. 2* (2012)

I.A. Zaliznyak and S.-H. Lee – [Magnetic Neutron Scattering](#) from *Modern Techniques for Characterizing Magnetic Materials* (2005)

S.M. Yusuf and A. Kumar – [Neutron Scattering of Advanced Magnetic Materials](#), Appl. Phys. Rev. (2017)

S. Mühlbauer et al – [Magnetic Small-Angle Neutron Scattering](#), Rev. Mod. Phys. (2019)



Any Questions?



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