Advanced Topics in Condensed Matter (ATCOMA): Lecture 14

for physics students for VF (Vertiefungsfächer)

- “Bio/Medical Physics“
- “Nanostructures“
- “Condensed Matter”

for NanoScience students

Today:

- Spin-resolved scattering of neutrons (i.e. polarization analysis)

… … first recap on scattering *without* polarization analysis

… … then what can be learned *with* polarization analysis

… … … for magnetic samples

… … … for *non*-magnetic samples

Main message:

Polarization analysis can add information even for non-magnetic samples !

Note KFN Webinar on Neutron Scattering with Polarization Analysis

Neutron polarization analysis:

An Introduction

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Rutherford Lab

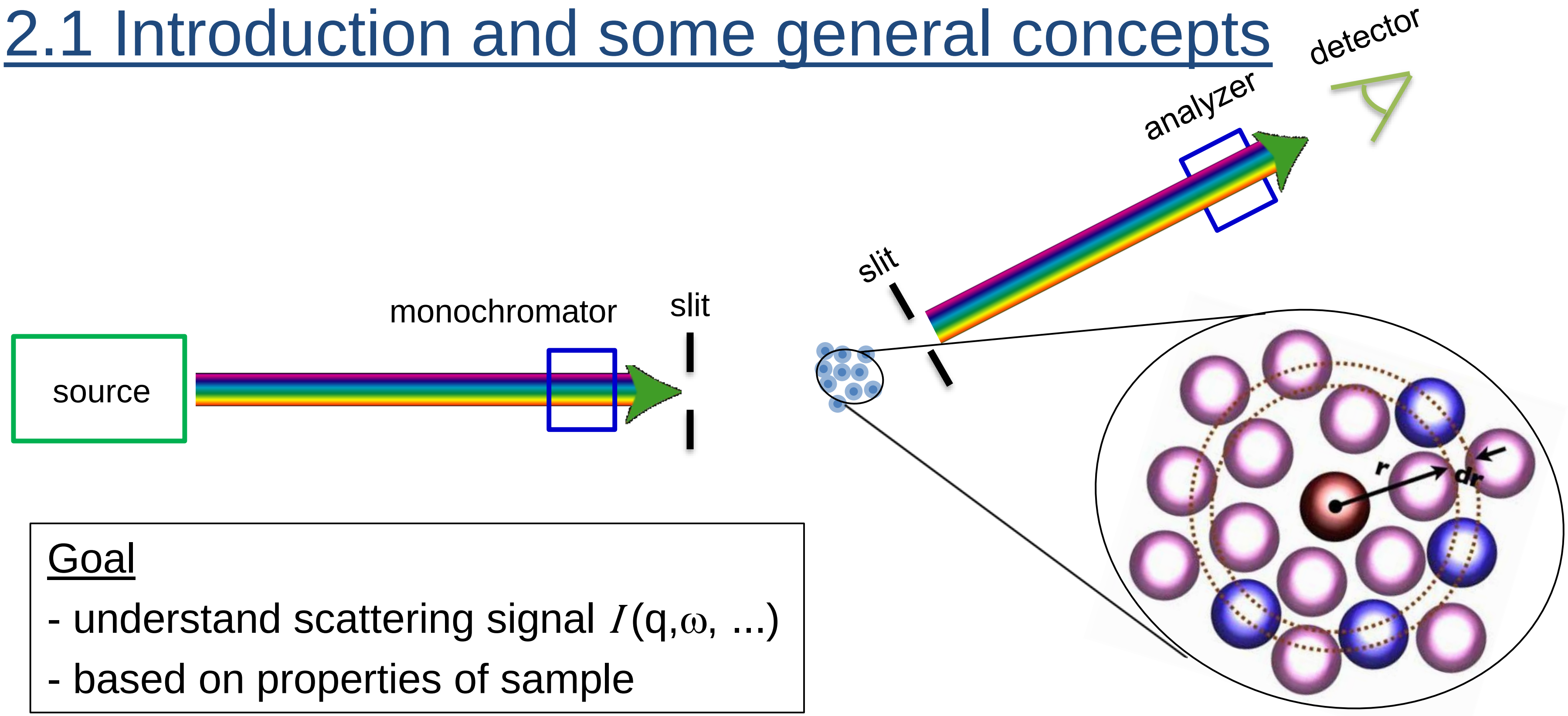
Friday, 30 January 2026, 11:00 - 12:00

https://www.sni-portal.de/en/user-committees/committee-research-with-neutrons/neutron-webinar

Generally, the KFN webinar takes place every last Friday of a month

Recap …

2.1 Introduction and some general concepts



<u>Goal</u>

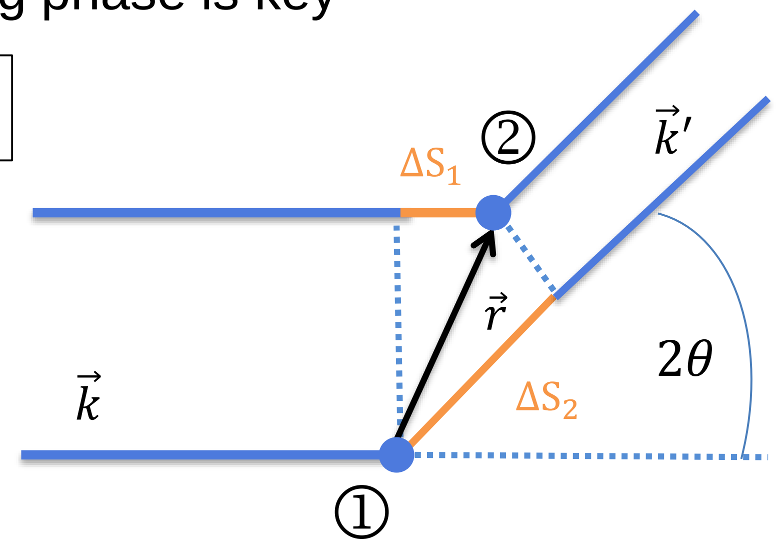
- understand scattering signal I(q,ω, ...)
- based on properties of sample

incident beam		sample	scattered beam
energy	$E = \hbar\omega_i$	N particles at positions $\overrightarrow{r_n}(t)$ with cross section σ_n	$E_f = \hbar\omega_f$
wavelength	λ_i		λ_f
wave vector	$\overrightarrow{k_i}$ (direction!)		$\overrightarrow{k_f}$
flux	$I_0 \quad \left[\frac{\text{quanta}}{\text{cm}^2\text{s}}\right]$		I

2.1 Introduction and some general concepts

Scattering phase is key

$$e^{i\vec{q}\cdot\vec{r}}$$



$$\vec{q} = \vec{k}' - \vec{k}$$

$$|\vec{q}| = \frac{4\pi}{\lambda}\sin\left(\frac{2\theta}{2}\right)$$

Roadmap

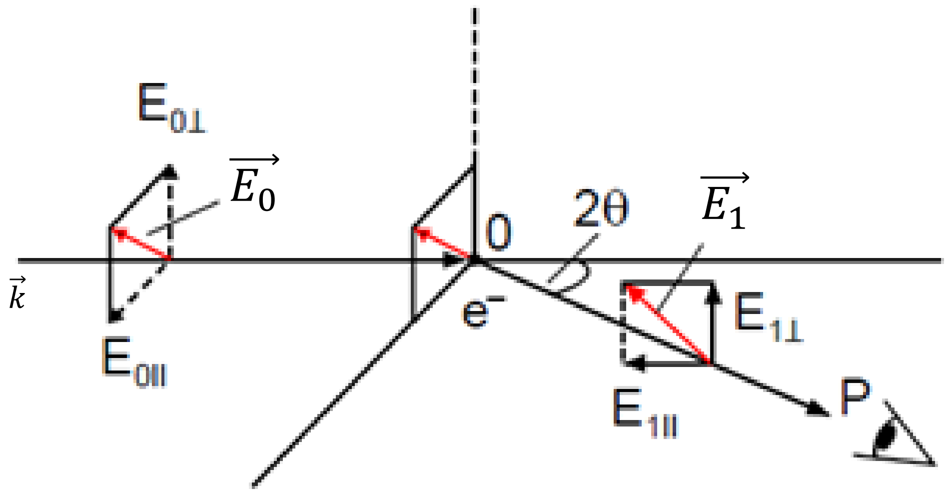
- understand elementary scattering process (individual atom)
- then “assemble“ atoms to a complete sample
- then resulting signal from scattering from all atoms with $e^{i\vec{q}\cdot\vec{r}}$

2.2 The elementary scattering process

2.2.1 X-rays

2.2 The elementary scattering process

2.2.1 X-rays



an electromagnetic wave stimulates an electron to forced oscillations

force on charge $\vec{F} = e\overrightarrow{E_0}$

acceleration $\vec{a} = \frac{\vec{F}}{m} = \frac{e\overrightarrow{E_0}}{m}$

accelerated charge radiates $E_1 \sim a\frac{e}{r}$

more precisely

$$E_1 = \frac{eE_0}{m}\left(\frac{\mu_0}{4\pi}\right)\frac{e}{r}\, sin(\overrightarrow{OP}, \vec{a})$$

$$E_{1\perp} = \frac{\mu_0}{4\pi}\frac{e^2}{m}\frac{E_{0\perp}}{r}$$

$$E_{1\parallel} = \frac{\mu_0}{4\pi}\frac{e^2}{m}\frac{E_{0\parallel}}{r}\, cos(2\theta)$$

$(= 0$ for $2\theta = 90°)$

2.2 The elementary scattering process

2.2.1 X-rays

... with the classical electron radius

$$r_e = \frac{\mu_0}{4\pi}\frac{e^2}{m} = \frac{e^2}{mc^2}\frac{1}{4\pi\epsilon_0} = 2.814 \cdot 10^{-5}\ \text{Å}$$

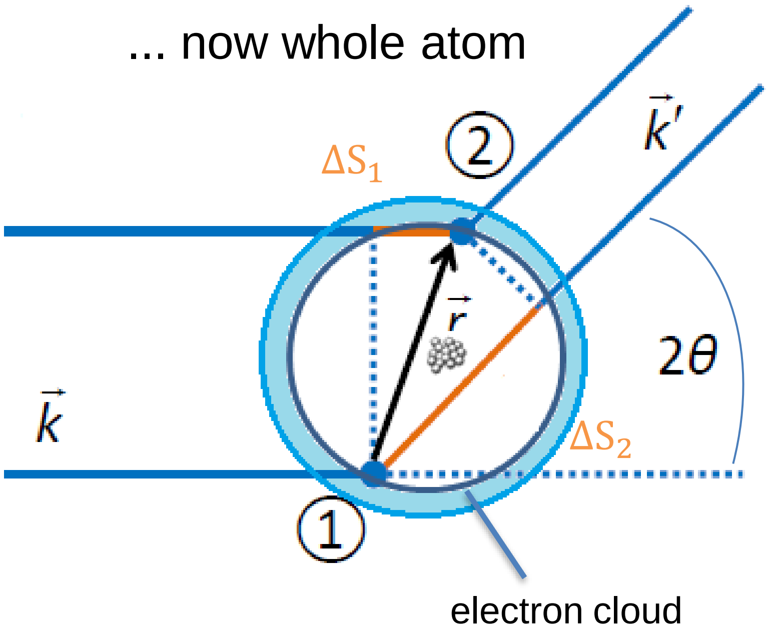
... and, after angular integration, the total scattering cross section

$$\sigma_{total} = \frac{8\pi}{3} r_e^2 \approx 6 \cdot 10^{-9}\ \text{Å}^2$$

2.2 The elementary scattering process

2.2.1 X-rays

... now whole atom



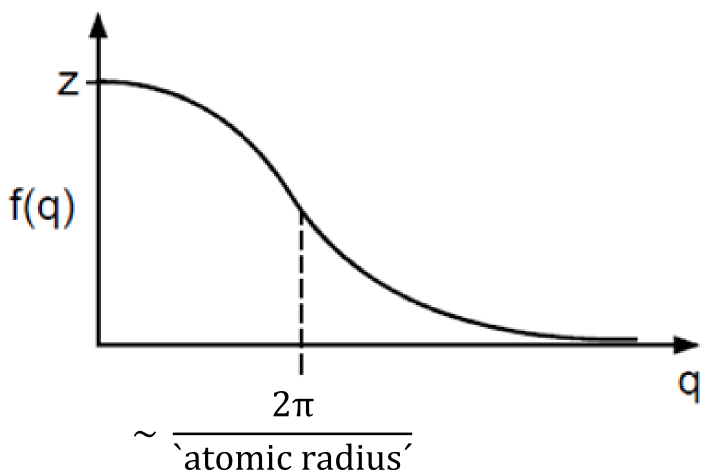
… sum of the scattering contributions from all volume elements of the electron cloud with their respective phase

Total scattered wave

$$A = r_e \int \rho(\vec{r})\, e^{i\vec{q}\vec{r}}\, d\vec{r}$$

'atomic form factor'
(Fourier transform of the electron cloud)

$$f(\vec{q}) = \int \rho(\vec{r})\, e^{i\vec{q}\vec{r}}\, d\vec{r}$$



$$f(q=0) = \sum_{n=1}^{Z} f_e^{(n)}(q=0) = \sum_{n=1}^{Z} 1 = Z$$

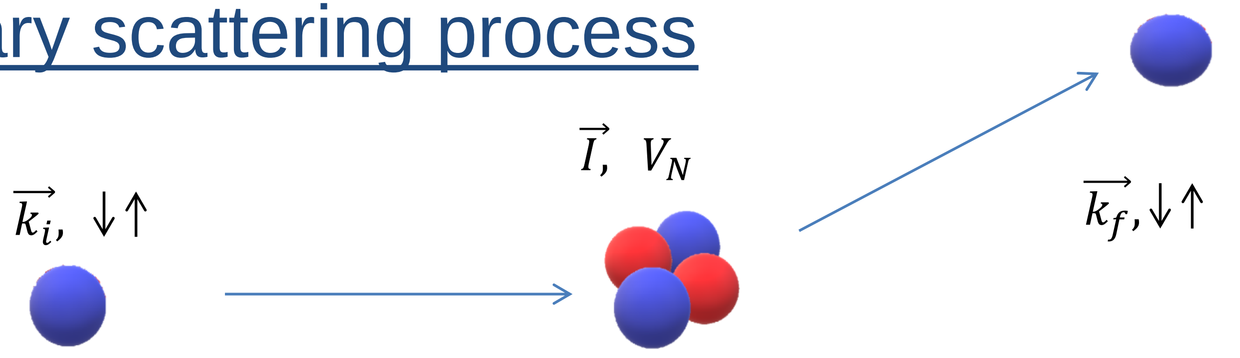
valency

2.2 The elementary scattering process

2.2.2 Neutrons

2.2 The elementary scattering process

2.2.2 Neutrons



Scattering due to nuclear interaction using Fermi's Golden Rule:

$$a = -\frac{m}{2\pi\hbar^2}\langle\Psi_f|V_N(\vec{r})|\Psi_i\rangle = -\frac{m}{2\pi\hbar^2}\int V_N(\vec{r})\, e^{i\vec{q}\cdot\vec{r}}\, d\vec{r}$$

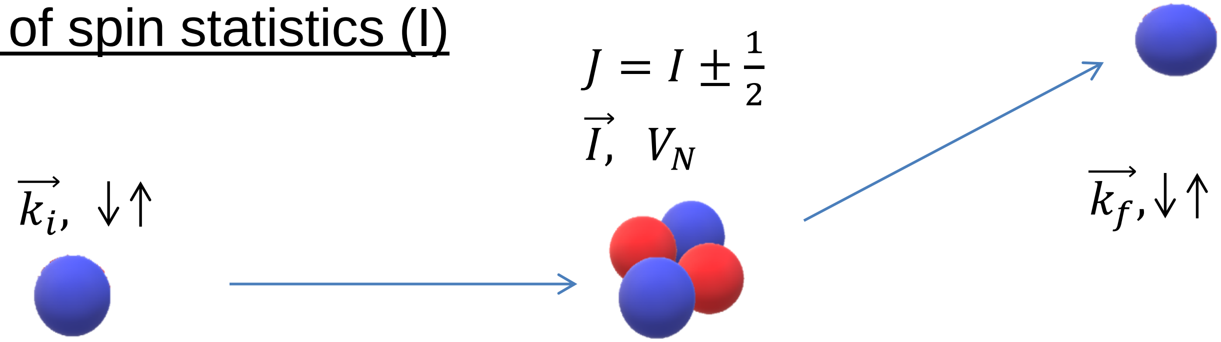
Potential V_N of nucleus is negligible for distance $r > 10^{-5}$Å;
with $q = 2\pi$Å^{-1} we have qr << 1 and thus

$$e^{i\vec{q}\cdot\vec{r}} \approx 1.$$

The scattering amplitude then becomes q independent, i.e. constant

$$b \equiv -a = \frac{m}{2\pi\hbar^2}\int V_N(\vec{r})\, d\vec{r}$$

Neutrons --- Influence of spin statistics (I)



spin of a neutron $s = \frac{1}{2}$

spin of nucleus I with ($2I$ +1) orientations

spin of total system (temporary compound = neutron + nucleus) $J = I \pm \frac{1}{2}$

Interaction V_N depends on relative spin orientation,
resulting in different scattering lengths with different probability

b_+	with probability	$w_+ = \frac{I+1}{2I+1}$
b_-		$w_- = \frac{I}{2I+1}$

Example: Scattering of a neutron on a proton (hydrogen nucleus)

$$b_+ = 10.4\ \mathrm{fm} \quad \mathrm{n}\uparrow\mathrm{p}\uparrow$$

$$b_- = -47.4\ \mathrm{fm} \quad \mathrm{n}\uparrow\mathrm{p}\downarrow$$

Neutrons --- Influence of spin statistics (II)

Considering a beam of unpolarized neutrons and nuclei

$$\mathrm{n}\ (\vec{k}_f)$$

$$\mathrm{n}\ (\vec{k}_i\ \uparrow\downarrow) \longrightarrow (\ldots, b_i, \ldots, b_j, \ldots) \nearrow$$

The intensity will be given by the weighted mean of every spin configuration

$$I = \langle AA^* \rangle = \sum_{i,j} \langle b_i b_j \rangle \, e^{i\vec{q}\cdot(\vec{r}_i - \vec{r}_j)}$$

With unpolarized nuclear spins we obtain:

$$i \neq j : \quad \langle b_i b_j \rangle = \langle b_i \rangle \langle b_j \rangle = \langle b \rangle^2$$

$$i = j : \quad \langle b_i b_i \rangle = \langle b^2 \rangle$$

Rewriting

$$\langle b_i b_j \rangle = \langle b \rangle^2 + \delta_{ij} \left(\langle b^2 \rangle - \langle b \rangle^2 \right)$$

gives

$$I = \langle b \rangle^2 \sum_{i,j} e^{i\vec{q}\cdot(\vec{r}_i - \vec{r}_j)} + \left(\langle b^2 \rangle - \langle b \rangle^2 \right) N$$

⇩ Coherent scattering

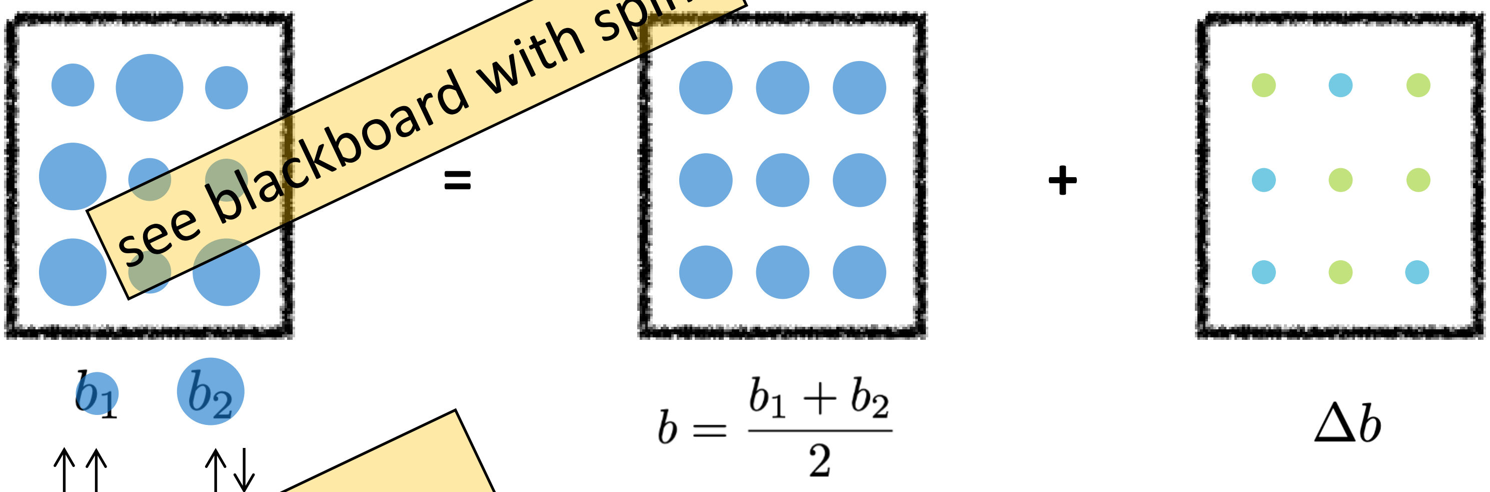
$$\sigma_{coh} = 4\pi \langle b \rangle^2$$

⇩ Incoherent scattering

$$\sigma_{inc} = 4\pi \left(\langle b^2 \rangle - \langle b \rangle^2 \right)$$

Neutrons --- Illustration of coherent and incoherent scattering

nuclear scattering ... decompose into two contributions:



$$b = \frac{b_1 + b_2}{2}$$

Δb

Coherent	Incoherent
→ Pair-correlation	→ Self-correlation

see blackboard with spins

Do not confuse this "coherent scattering" of neutrons by the sample with "coherence" of the X-ray beam

similarity to X-ray scattering from disordered alloy:

"Bragg" + "diffuse scattering"

("coherent") ("incoherent")

Figure courtesy of Michihiro Nagao

Neutrons --- Remarks on the scattering cross sections

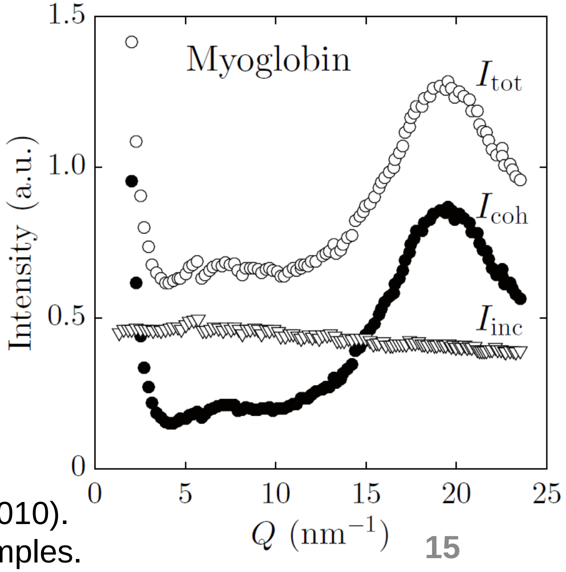
1. Every isotope has both coherent and incoherent scattering (σ_{coh} and σ_{inc}) except when $I = 0$ (e.g. ^{58}Ni)
2. The most famous example for the difference between two isotopes is hydrogen ($I = 1/2$) and deuterium ($I = 1$)

	σ_{coh} (barn)	σ_{inc} (barn)
H	2.0	80
D	5.6	2.0

1 barn = 10^{-28} m^2

The incoherent cross section of hydrogen is highest.

The big difference between H and D is used in organic matter for a high contrast (H/D substitution, deuteration of selected components)



Separation of coherent and incoherent nuclear scattering from a solution of myoglobin in D2O.

Gaspar, A. M., Busch, S., Appavou, M-S., Haeussler, W., Georgii, R., Su, Y., and Doster, W. (2010). Using polarization analysis to separate the coherent and incoherent scattering from protein samples. Biochim. Biophys. Acta 1804, 76–82; after Boothroyd, p.114

Neutrons --- Remarks on the scattering cross sections

Column	Symbol	Unit	Quantity
1			element
2	Z		atomic number
3	A		mass number
4	$I(p)$		spin (parity) of the nuclear ground state
5	c	%	natural abundance (For radioisotopes the half-life is given instead.)
6	b_c	fm	bound coherent scattering length
7	b_i	fm	bound incoherent scattering length
8	s_c	barn[1]	bound coherent scattering cross section
9	s_i	barn	bound incoherent scattering cross section
10	s_s	barn	total bound scattering cross section
11	s_a	barn	absorption cross section for 2200 m/s neutrons[2]

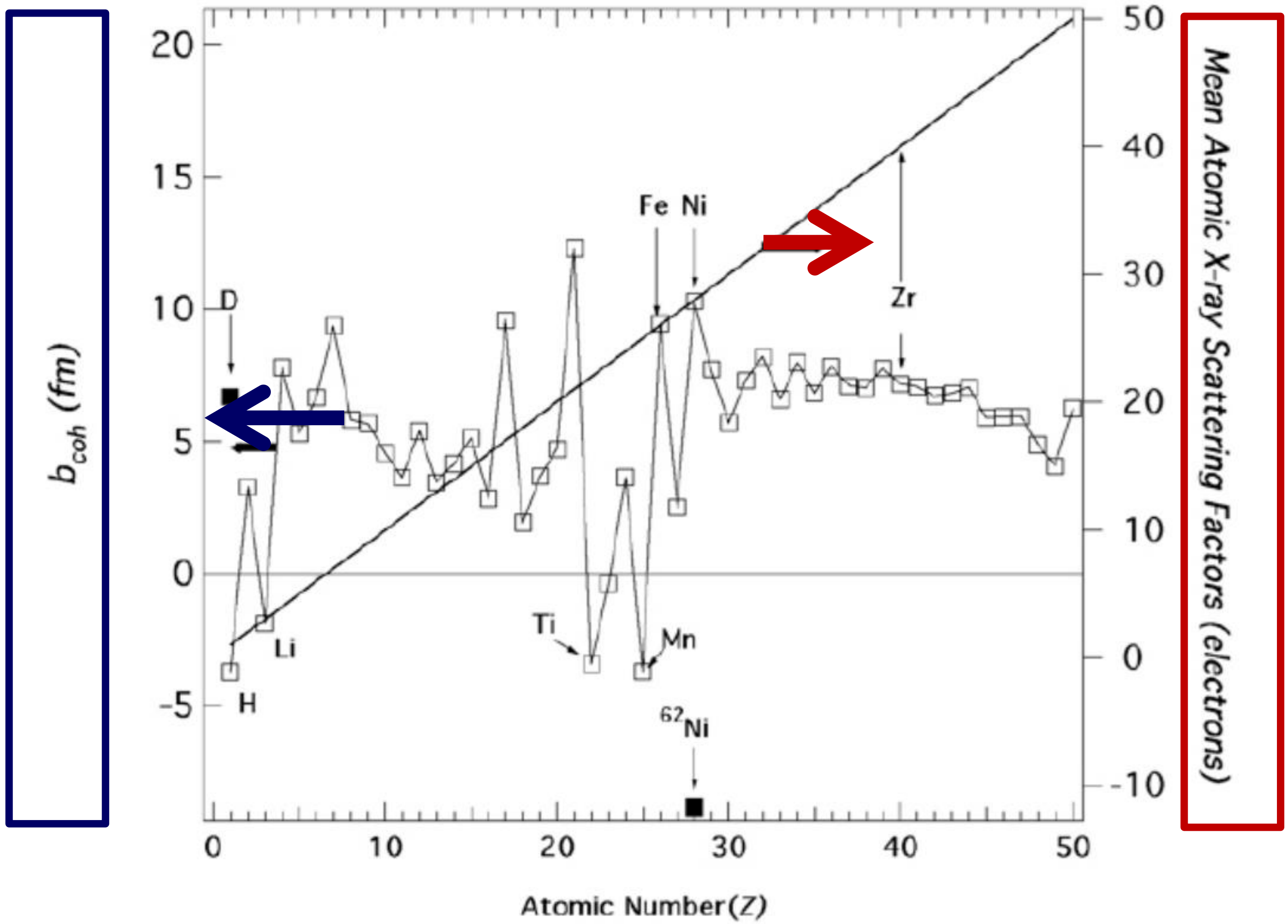
(1) 1 barn = 100 fm^2

(2) E = 25.30 meV, k = 3.494 $Å^{-1}$, l = 1.798 Å

	Z	A	$I(\pi)$	c	b_c	b_i	σ_c	σ_i	σ_s	σ_a
H	1				−3.7390(11)		1.7568(10)	80.26(6)	82.02(6)	0.3326(7)
		1	1/2(+)	99.985	−3.7406(11)	25.274(9)	1.7583(10)	80.27(6)	82.03(6)	0.3326(7)
		2	1(+)	0.015	6.671(4)	4.04(3)	5.592(7)	2.05(3)	7.64(3)	0.000519(7)
		3	1/2(+)	(12.32 a)	4.792(27)	−1.04(17)	2.89(3)	0.14(4)	3.03(5)	0
He	2				3.26(3)		1.34(2)	0	1.34(2)	0.00747(1)
		3	1/2(+)	0.00014	5.74(7) −1.483(2)i	−2.5(6) +2.568(3)i	4.42(10)	1.6(4)	6.0(4)	5333.(7.)
		4	0(+)	99.99986	3.26(3)	0	1.34(2)	0	1.34(2)	0
Li	3				−1.90(2)		0.454(10)	0.92(3)	1.37(3)	70.5(3)
		6	1(+)	7.5	2.00(11) −0.261(1)i	−1.89(10) +0.26(1)i	0.51(5)	0.46(5)	0.97(7)	940.(4.)
		7	3/2(−)	92.5	−2.22(2)	−2.49(5)	0.619(11)	0.78(3)	1.40(3)	0.0454(3)
Be	4	9	3/2(−)	100	7.79(1)	0.12(3)	7.63(2)	0.0018(9)	7.63(2)	0.0076(8)

Comparison of neutrons and X-rays

For neutrons no monotonic dependence on *Z* as for X-rays



John B. Parise "Introduction to neutron science"

Comparison of neutrons and X-rays

Interactions different on the fundamental level, cross sections similarly weak.

Thus, many aspects of the scattering theory are similar for X-rays and neutrons, including kinematic theory, i.e. no multiple scattering, which is good.

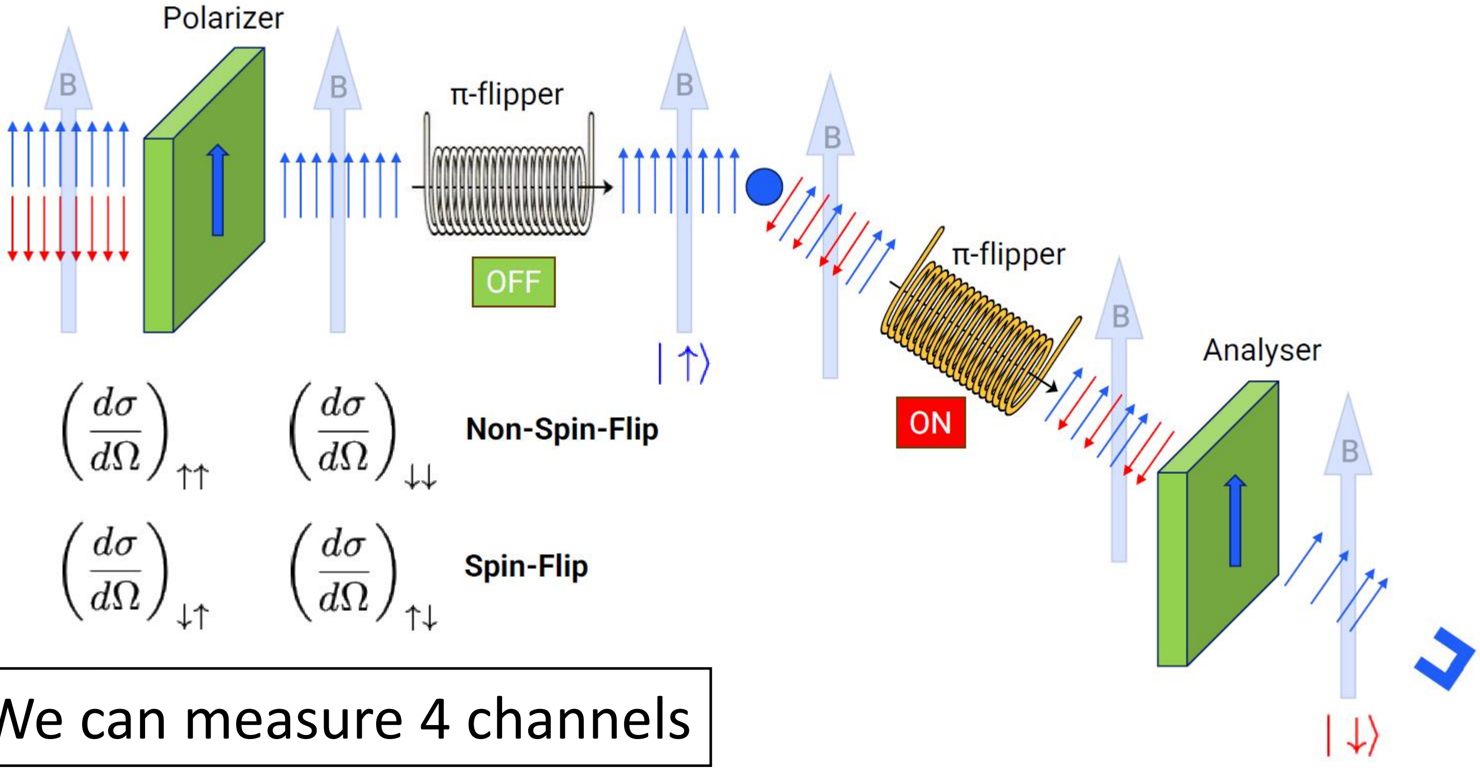
This makes a common summer school particularly suitable!

It also makes it easier to cover both in this lecture and to use both in one's research.

Nevertheless, some differences neutrons vs.	X-rays
e.g.	
- penetration depth typically still higher	slightly less for X-rays
- stronger interaction with light elements	---------------
- contrast variation by isotopic substitution	absorption edges
- incoherent cross section (used for QENS)	---------------
- high energy resolution	possible, but less common
- magnetic scattering	different mechanism for X-rays
- flux lower for neutrons	higher for synchrotrons

Now something new …

14 Spin-resolved scattering of neutrons



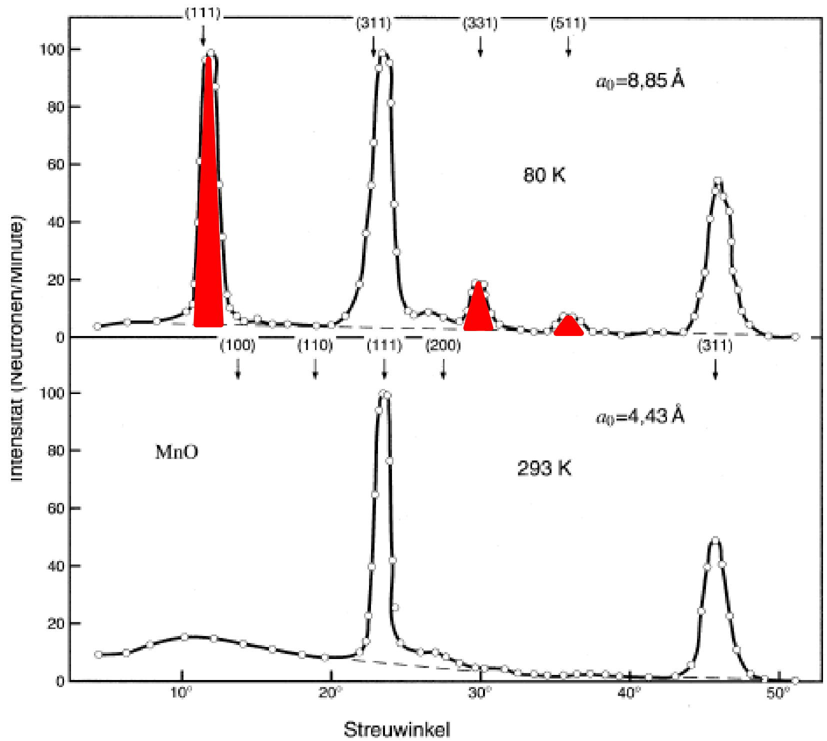
$$\left(\frac{d\sigma}{d\Omega}\right)_{\uparrow\uparrow} \quad \left(\frac{d\sigma}{d\Omega}\right)_{\downarrow\downarrow}$$ **Non-Spin-Flip**

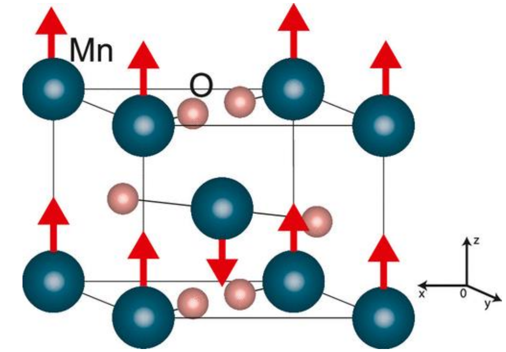
$$\left(\frac{d\sigma}{d\Omega}\right)_{\downarrow\uparrow} \quad \left(\frac{d\sigma}{d\Omega}\right)_{\uparrow\downarrow}$$ **Spin-Flip**

We can measure 4 channels

14.1 Magnetic structures

Antiferromagnet MnO

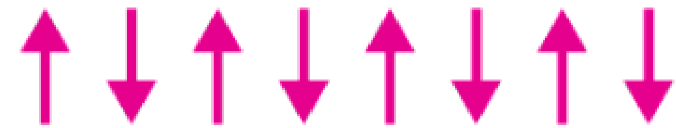




neutrons:

magnetic structure

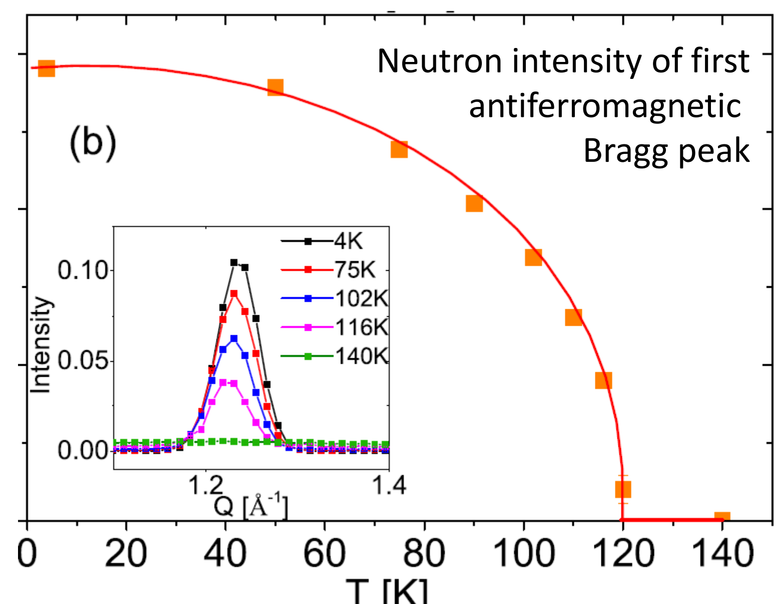
$T_N \approx 120$ K



X-rays & neutrons:

chemical structure

$T_{melt} \approx 2000$ K

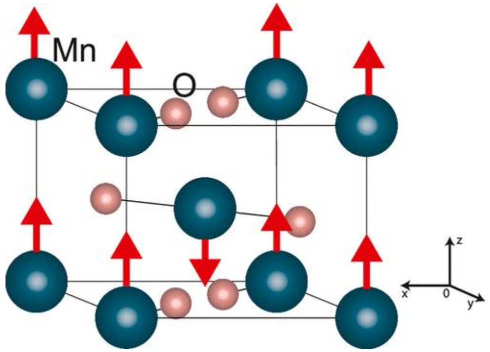


See also C. G. Shull et al. (Nobel prize 1994)

X. Sun et al. J. Phys.: Conf. Ser. 862 (2017) 012027

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

14.1 Magnetic structures



Resolving magnetic structures

(ferromagnets, antiferromagnets, ferrimagnets, etc.)

… is what one typically has in mind for spin-resolved neutron scattering

… is indeed the direct way of demonstrating, e.g.

the antiferromagnetic order by an additional Bragg peak (superstructure)

(remember that the net macroscopic magnetization of the antiferromagnet is zero,

so macroscopic measurements are not enough)

Note that there are many more features and subleties associated with neutron scattering from magnetic samples, both re magnetic structures as well as excitations.

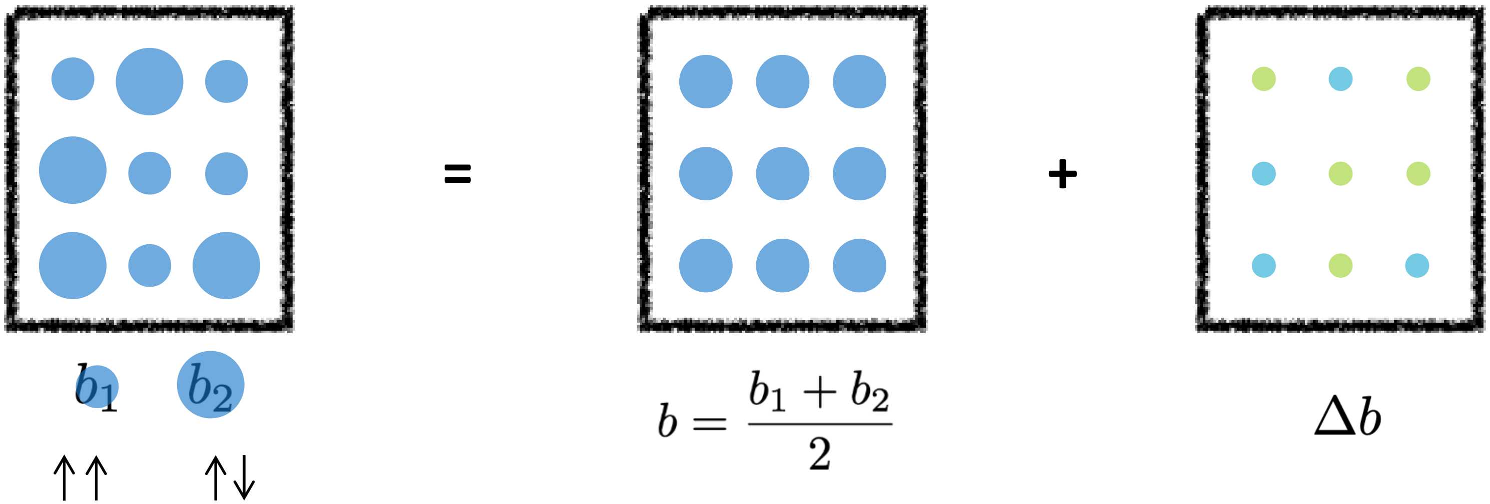
We will postpone the discussion of these for the time being.

Now

We show that spin-resolved neutron scattering also contains

additional information for non-magnetic samples !

14.2 Spin-resolved scattering of neutrons / Theory



Coherent → Pair-correlation	Incoherent → Self-correlation

In conventional (non-polarized) neutron scattering the common wisdom is that there is a coherent and an incoherent scattering cross section, as derived in ATCOMA at the start of term (I recommend you look this up to refresh your memory).

The most famous example is neutron scattering from hydrogen (1H) atoms, for which the scattering length differs depending on relative spin state of the proton and the neutron.

This gives rise to an inhomogeneous sample of hydrogens as seen by the neutron,

and thus an _average_ scattering (--> "coherent" scattering")

and a deviation from the average (--> "incoherent" scattering).

(Note: Remember that the incoherent scattering is not necessarily bad; it gives access famously to the self-diffusion in energy-resolved experiments).

If you imagine you are using polarized neutrons, then this will be extra experimental effort (plus more beamtime required etc etc),

but you can be rewarded by removing this "inhomogeneity", or, more precisely, you can hope to separate coherent and incoherent scattering.

It is also relevant in some reflectometry experiments, and, importantly, not only those which study magnetism.

Furthermore, again in particular in the context of reflectometry, the polarization analysis can give additional information,

in particular with a magnetic reference layer, even if the layered structure of interest is non-magnetic.

14.2 Spin-resolved scattering of neutrons / Theory

Can we gain information by considering spin-resolved scattering of neutrons ?

Importantly, this is relevant not only for magnetic samples !

First, we remember that the reason for the incoherent cross section in particular for 1H (hydrogen) is difference of the scattering length between ↑↑ and ↑↓ for the relative spin orientation of neutron and nucleus.

If, hypothetically, we could eliminate this "inhomogeneity“ (i.e. different spin orientations in the sample), we could measure the purely coherent scattering.
However, the polarizing of the nuclei in the sample by an external field B is far too weak

$$\mu B / k_B T \text{ is only} \sim 10^{-5}$$

for T = 300 K and B =1 T for ^{1}H and less for most other nuclei.

Alternatively, we could polarize the neutrons and analyze different scattering channels (which will be extra experimental effort, but possible).
Let us now see how we benefit from this.

14.2 Spin-resolved scattering of neutrons / Theory

The polarization-dependent scattering cross-sections can be calculated from the following **Moon-Riste-Koehler** equations

$$\left(\frac{d\sigma}{d\Omega}\right)_{ss'} = |\sum_n U_n^{ss'} \exp\left(i\vec{Q}.\vec{r}_n\right)|^2$$

where,

$$\left.\begin{aligned} U^{\uparrow\uparrow} &= \bar{b} - pM_{\perp z} + BI_z \\ U^{\downarrow\downarrow} &= \bar{b} + pM_{\perp z} - BI_z \end{aligned}\right\} U^{\mathrm{NSF}}$$

$$\left.\begin{aligned} U^{\uparrow\downarrow} &= -p\left(M_{\perp x} + iM_{\perp y}\right) + B\left(I_x + iI_y\right) \\ U^{\downarrow\uparrow} &= -p\left(M_{\perp x} - iM_{\perp y}\right) + B\left(I_x - iI_y\right) \end{aligned}\right\} U^{\mathrm{SF}}$$

$$\bar{b} = \frac{(I+1)b_+ + Ib_-}{2I+1}$$

$$B = \frac{b_+ - b_-}{2I+1}$$

$$p = 1.913\frac{\mu_0}{4\pi}\frac{e^2}{m_e}$$

- The *z*-direction is along the direction of the neutron polarization
- I is the nuclear spin quantum number and I_x, I_y and I_z are the components of the nuclear spin angular momentum
- $M_{\perp x}$, $M_{\perp y}$, and $M_{\perp z}$ are the components of the magnetic field perpendicular to the scattering vector
- b_+ and b_- are the spin-dependent scattering lengths - tabulated in https://www.tuwien.at/en/phy/ati/neutron-and-quantum-physics/research/techniques-of-neutron-physics/table-of-neutron-scattering-lengths

*Moon, Riste and Koehler, Physical Review **181**, 920 (1969) // courtesy Ross Stewart*

Coherent (nuclear) Scattering

Assuming no magnetism in the sample – we can work out the **coherent** nuclear scattering, just by taking the average of the amplitudes

$$\overline{U^{\mathrm{NSF}}} = \bar{\bar{b}} \pm \overline{BI_z}$$

$$\overline{U^{\mathrm{SF}}} = \overline{BI_x \pm BiI_y}$$

Now, if the nuclear spins are randomly oriented, then the average over any one component of ***I*** is zero. Therefore

$$\overline{U^{\mathrm{NSF}}} = \bar{b}$$

$$\overline{U^{\mathrm{SF}}} = 0$$

All the nuclear coherent scattering appears in the Non-Spin-Flip measurements.

courtesy Ross Stewart

Incoherent (nuclear) Scattering

Again, assuming no magnetism we can work out the **incoherent** scattering, which is given by the variance in the scattering amplitudes

$$\overline{U^2} - \overline{U}^2$$

Applying this to the NSF amplitudes, we get

$$\overline{(\bar{b} + BI_z)^2} - \overline{(\bar{b} + BI_z)}^2$$

$$= \overline{b^2} + \overline{B^2 I_z^2} + 2\overline{bBI_z} - \overline{(b + BI_z)}^2$$

Again, we assume that the nuclei are randomly oriented

Nuclear isotope incoherent $\overline{b^2} - \overline{b}^2 + \overline{B^2 I_z^2}$ **Nuclear spin incoherent**

Note that $\mathbf{I}^2 = I(I+1) = I_x^2 + I_y^2 + I_z^2$, so for isotropic nuclear spins

$$I_x^2 = I_y^2 = I_z^2 = 1/3\ I(I+1)$$

and thus

$$\left(\overline{U^2} - \overline{U}^2\right)^{\mathrm{NSF}} = \overline{b^2} - \overline{b}^2 + {}^1\!/\!{}_3 B^2 I(I+1)$$

Incoherent (nuclear) Scattering

Again, assuming no magnetism we can work out the **incoherent** scattering, which is given by the variance in the scattering amplitudes

$$\overline{U^2} - \overline{U}^2$$

Applying this to the SF amplitudes, we get

$$\overline{B^2(I_x + iI_y)^2} - \left(\overline{B(I_x + iI_y)}\right)^2$$

$$= \overline{B^2(I_x^2 + I_y^2)}$$

So assuming randomly oriented nuclear spins again, we get

$$\left(\overline{U^2} - \overline{U}^2\right)^{\mathrm{SF}} = {}^2\!/_3 B^2 I(I+1)$$

which is exactly twice the non-spin-flip spin-incoherent scattering !

(Non-magnetic) polarization analysis

$$\left(\frac{d\sigma}{d\Omega}\right)^{\mathrm{NSF}} = \left(\frac{d\sigma}{d\Omega}\right)_{\mathrm{coh}} + \left(\frac{d\sigma}{d\Omega}\right)_{\mathrm{II}} + \frac{1}{3}\left(\frac{d\sigma}{d\Omega}\right)_{\mathrm{SI}}$$

$$\left(\frac{d\sigma}{d\Omega}\right)^{\mathrm{SF}} = \frac{2}{3}\left(\frac{d\sigma}{d\Omega}\right)_{\mathrm{SI}}$$

- if the scattering is fully coherent/isotope incoherent – then scattered polarization is preserved
- if the scattering is fully spin-incoherent then, the polarization of the scattered beam is 1/3 of the incoming beam

$$\vec{P}' = -{}^{1}\!/_{3}\vec{P}$$

(Non-magnetic) polarization analysis

$$\left(\frac{d\sigma}{d\Omega}\right)_{\mathrm{coh}} + \left(\frac{d\sigma}{d\Omega}\right)_{\mathrm{II}} = \left(\frac{d\sigma}{d\Omega}\right)^{\mathrm{NSF}} - \frac{1}{2}\left(\frac{d\sigma}{d\Omega}\right)^{\mathrm{SF}}$$

$$\left(\frac{d\sigma}{d\Omega}\right)_{\mathrm{SI}} = \frac{3}{2}\left(\frac{d\sigma}{d\Omega}\right)^{\mathrm{SF}}$$

- Polarization analysis can never fully isolate the purely coherent scattering
- Even if it could – the coherent scattering still contains the self-correlation terms
- However – the incoherent scattering can be fully separated from coherent contributions !

14.2 Spin-resolved scattering of neutrons / Theory

See Boothroyd, p.125 / summary / Ross Stewart

Remember that "normally" (i.e. without polarization analysis)
the inc and coh scattering is "always on top of each other" and cannot be separated
(even if 1H is employed and sigma_inc dominates, we do not have sigma_coh = 0 !)

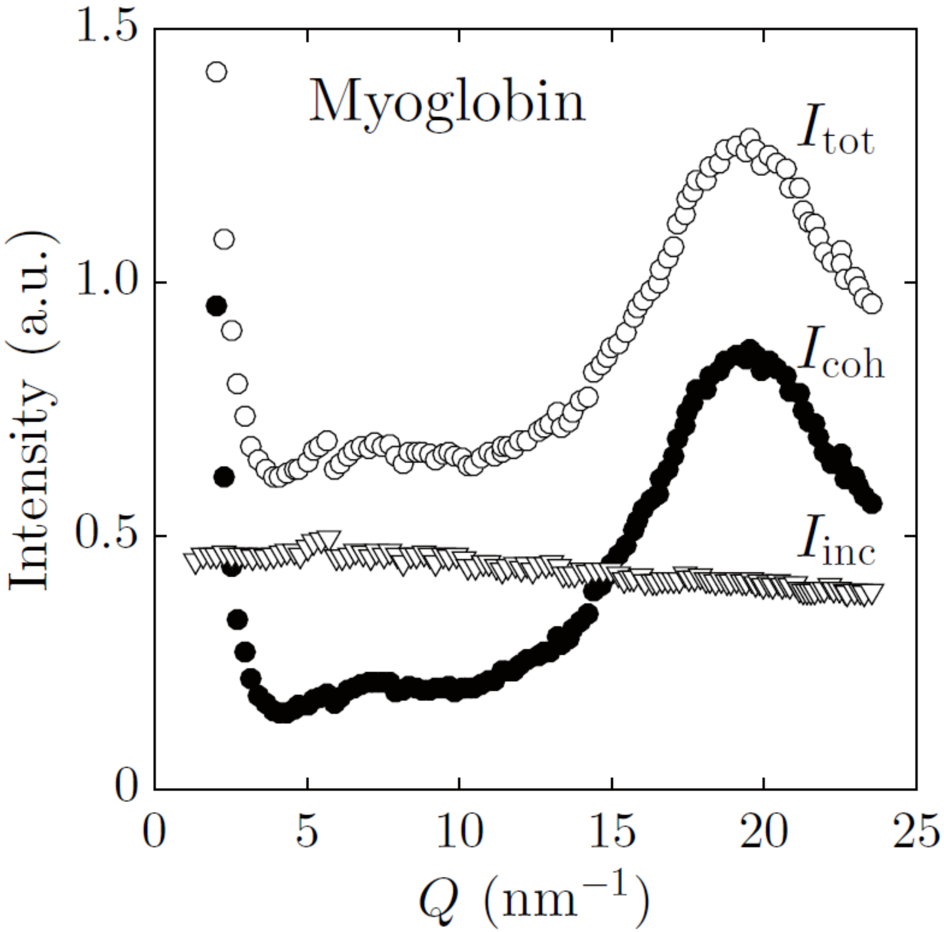
Spin-resolved scattering can help to separate the contributions.

1) Nuclear coherent and isotopic incoherent scattering are both NSF
2) nuclear spin incoherent scattering is 1/3 NSF and 2/3 SF

14.3 Spin-resolved scattering of neutrons / Examples

Partly based on Ross Stewart lecture on Oxford school 2024

14.3 Spin-resolved scattering of neutrons / Examples



Separation of coherent and incoherent nuclear scattering from a solution of myoglobin in D2O.

Since nuclear coherent scattering does not change the polarization of the neutron no new information on structural correlations can be obtained by performing polarization analysis. However, one potentially useful application of polarization analysis is to separate nuclear coherent from nuclear incoherent scattering in systems where the spin incoherence dominates the isotopic incoherence. Then the coherent scattering is

$$I_{NSF} - ½\, I_{SF}.$$

An obvious case is hydrogen-containing systems, since the proton has a spin incoherent cross-section an order of magnitude larger than for any other nucleus. This method has been applied to myoglobin, for which the coherent scattering tends to be diffusive and difficult to separate from the incoherent scattering by other methods.

Gaspar, A. M., Busch, S., Appavou, M-S., Haeussler, W., Georgii, R., Su, Y., and Doster, W. (2010). Using polarization analysis to separate the coherent and incoherent scattering from protein samples. Biochim. Biophys. Acta 1804, 76–82; after Boothroyd, p.114

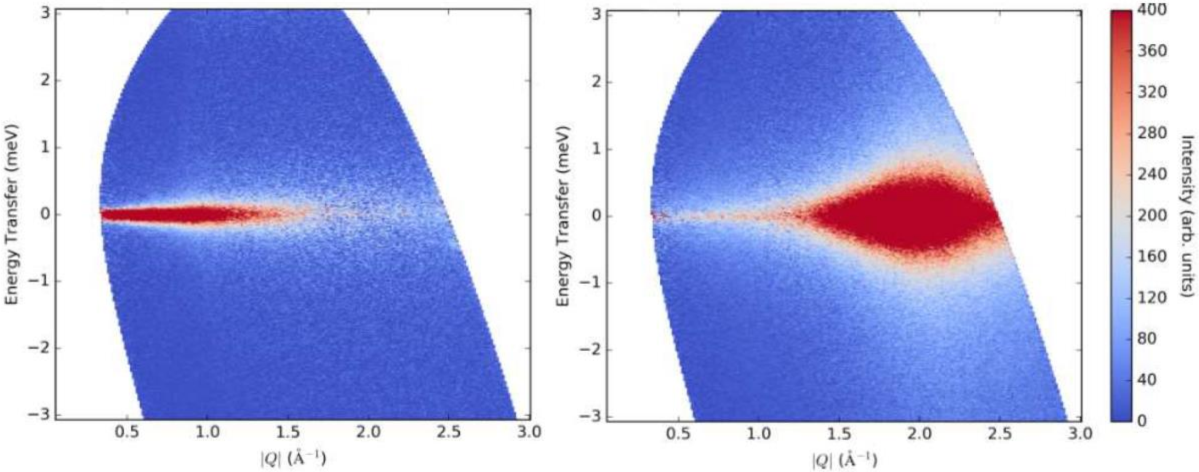
14.3 Spin-resolved scattering of neutrons / Examples

Arbe et al., Phys Rev Res **2**, *022015 (2020)*

Example – Water (D_2O) at 295 K

Measured on LET at ISIS

Single-particle (incoherent) and structural (coherent) dynamics are **separated**



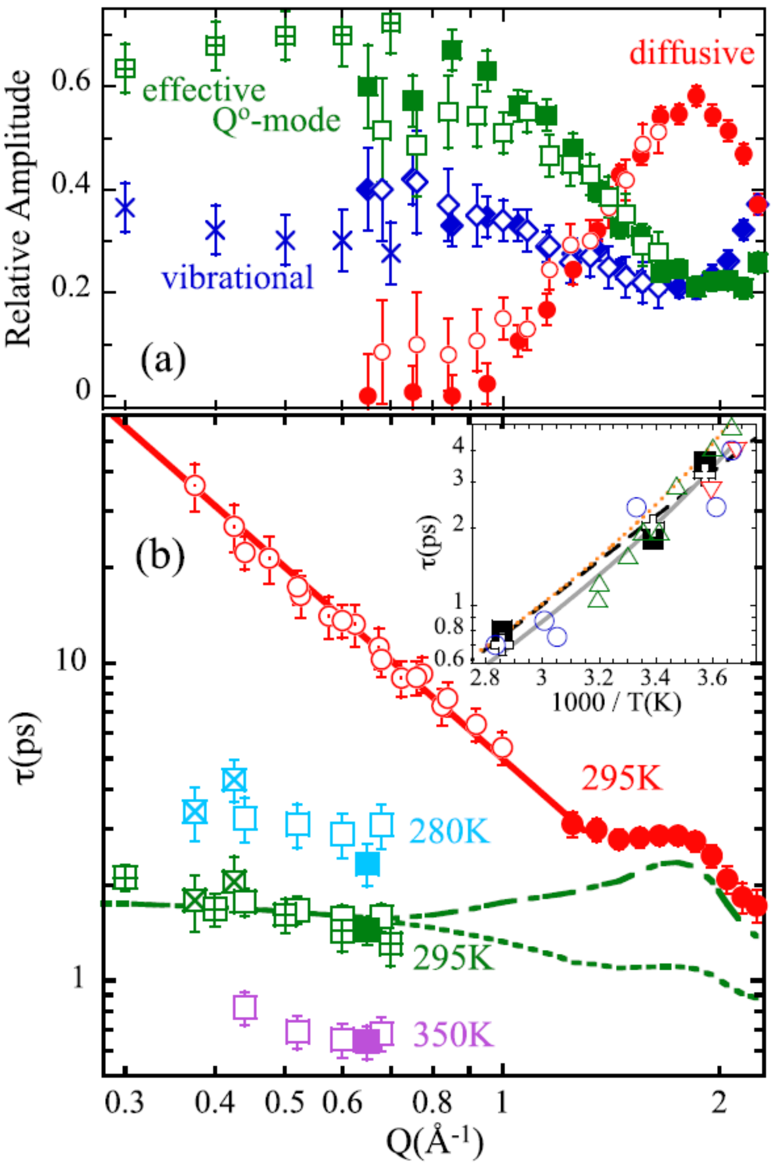
$$\left(\frac{d\sigma}{d\Omega}\right)^{\mathrm{SI}} = \frac{3}{2}\left(\frac{d\sigma}{d\Omega}\right)_{\mathrm{SF}}$$

$$\left(\frac{d\sigma}{d\Omega}\right)_{\mathrm{coh+II}} = \left(\frac{d\sigma}{d\Omega}\right)^{\mathrm{NSF}} - \frac{1}{2}\left(\frac{d\sigma}{d\Omega}\right)^{\mathrm{SF}}$$

	σ_{coh} (b)	σ_{SI} (b)
D	5.59	2.05
O	4.23	~0

14.3 Spin-resolved scattering of neutrons / Examples

Allows to resolve different types of dynamics in water



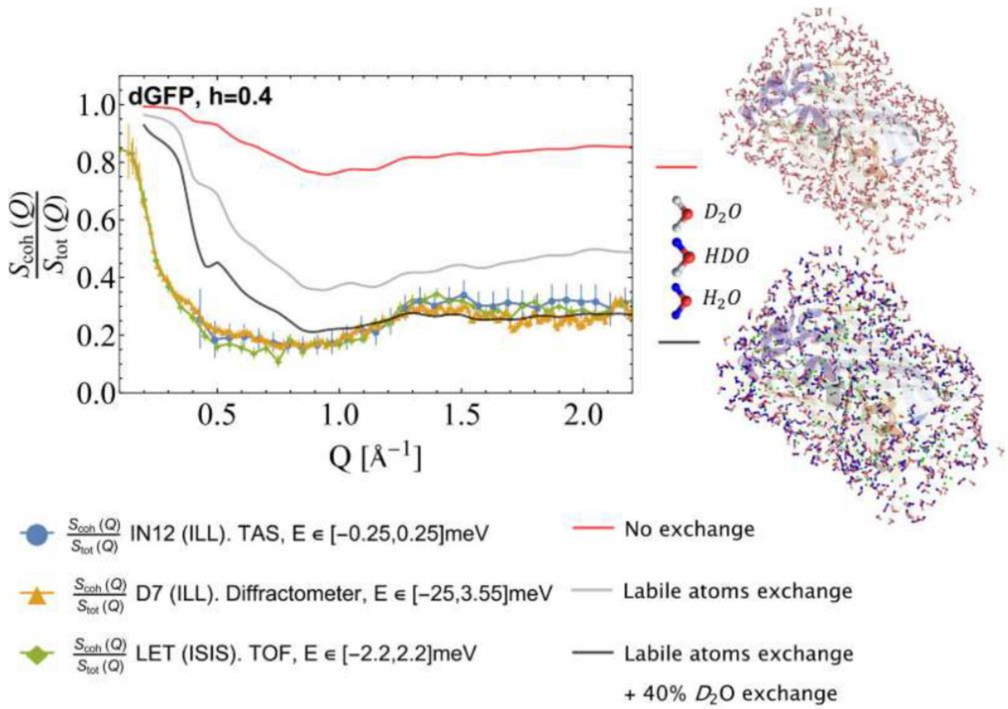
Coherent structural relaxation of water from meso- to intermolecular scales measured using neutron spectroscopy with polarization analysis

Arbe et al. Phys. Rev. Res. 2, 022015(R) (2020)

14.3 Spin-resolved scattering of neutrons / Examples

Nidriche et al., *PRX Life* **2**, 013005 (2024)

Example – deuterated Green fluorescent protein



New experiments challenging assumptions about "dominant" scattering on deuteration

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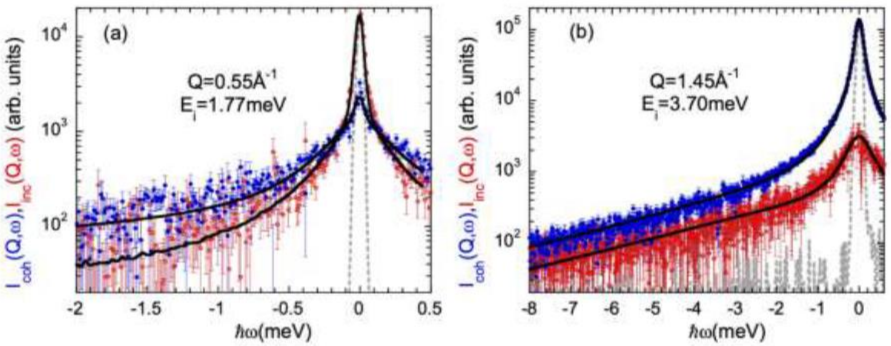
14.3 Spin-resolved scattering of neutrons / Examples

Arbe et al., J. Chem. Phys. ***158*** *(2023) 184502*

Example – dynamics in van der Waals liquid

Tetrahydrofuran – THF, C_4H_8O

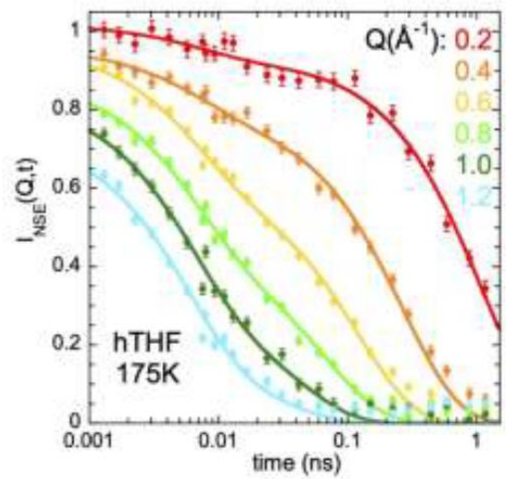
LET at ISIS



Coherent and incoherent scattering in deuterated dTHF

Fit is a model consisting of diffusion (incoherent) and structural relaxation (coherent) – too complicated to disentangle without polarized neutrons – and which requires NSE for the resolution at low Q

WASP at ILL



Mostly incoherent scattering in protonated pTHF

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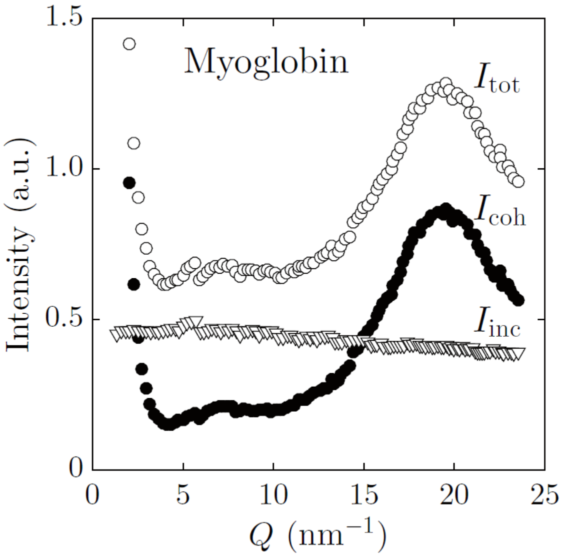
14.4 Spin-resolved scattering of neutrons / Summary

See Boothroyd, p.125 / summary / Ross Stewart

Remember that "normally" (i.e. without polarization analysis)
the inc and coh scattering is "always on top of each other" and cannot be separated
(even if 1H is employed and sigma_inc dominates,
we do not have sigma_coh = 0 !)
Spin-resolved scattering helps to separate the contributions



1) Nuclear coh and isotopic inc scattering are both NSF
2) nuclear spin inc scattering is 1/3 NSF and 2/3 SF

3) With magnetization M and spin polarization P:
   Magnetic scattering only “sees” M_perp, the component of M perpendicular to Q
   components of M_perp along P give NSF
   components of M_perp perpendicular to P give SF
   When P is parallel to Q, electronic magnetic scattering is entirely SF

14.5 Spin-resolved scattering of neutrons / References

Moon, Riste and Koehler, Physical Review 181, 920 (1969)

Ross Stewart, Oxford School on Neutron Scattering - 2024

Andrew T. Boothroyd
Principles of Neutron Scattering from Condensed Matter
Oxford University Press 2020
Sec 4.4 (p 110)
Sec 4.5.1 (p 112)

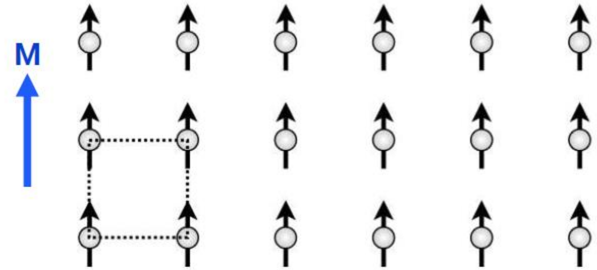
Arbe et al., Phys Rev Res 2, 022015 (2020)
Arbe et al., J. Chem. Phys. 158, 184502 (2023)
Morbidini et al., J. Chem. Phys. 159, 221103 (2023)
Nidriche et al., PRX Life 2, 013005 (2024)

Addendum: Polarization of neutron beams

Scattering from Ferromagnets

Boothroyd – Sec 7.3.2 (p 233)

Assuming no spin-incoherent scattering in a ferromagnetic material, and assuming that the magnetization is along the polarization direction – we only need to look at the $U^{\uparrow\uparrow}$ and $U^{\downarrow\downarrow}$ amplitudes



$$|U^{\uparrow\uparrow}|^2 = b^2(Q) + p^2 M_\perp^2(Q) - 2b(Q)pM_\perp(Q)$$
$$|U^{\downarrow\downarrow}|^2 = b^2(Q) + p^2 M_\perp^2(Q) + 2b(Q)pM_\perp(Q)$$

Writing this in terms of cross-sections and structure factors

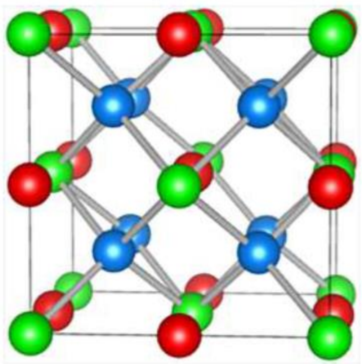
$$\left(\frac{d\sigma}{d\Omega}\right)^{\uparrow\uparrow} \propto |F_N - F_M|^2$$
$$\left(\frac{d\sigma}{d\Omega}\right)^{\downarrow\downarrow} \propto |F_N + F_M|^2$$

Leading to a flipping ratio of

$$\Phi = \left(\frac{1-\phi}{1+\phi}\right)^2 \quad \text{where,} \quad \phi = \frac{F_M}{F_N}$$

Addendum: Polarization of neutron beams

Example – Heusler alloy, Cu_2MnAl



- Cubic ferromagnet
- Used as a neutron polarizer

If the (111) Bragg peak from Cu_2MnAl produces a polarization, P = -0.99, what is the ratio of the magnetic and nuclear (111) structure factors?

We can write the ratio of the structure factors, ϕ, as a function of the flipping ratio

$$\Phi = \frac{1+P}{1-P} = \left(\frac{1-\phi}{1+\phi}\right)^2$$

$$\Rightarrow \phi = \frac{1-\sqrt{\Phi}}{1+\sqrt{\Phi}}$$

The flipping ratio is, $\Phi = \dfrac{1+(-0.99)}{1-(-0.99)} \simeq 0.005$

Therefore $\phi = \dfrac{1-0.071}{1+0.071} \simeq 0.87$

So F_N and F_M don't have to be that close to get a good polarization

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Addendum: Magnetic neutron scattering

Reminder: Magnetic scattering

Boothroyd – Sec 4.2 (p 103)

Magnetic scattering

The magnetic scattering is a vector interaction – $V_m = -\vec{\mu}_n.\vec{B}(r)$

Since the magnetic field in the sample is divergence-free ($\nabla.\vec{B}(r) = 0$) after taking the Fourier transform we get,

$$\vec{B}(\vec{r}) = \frac{1}{\sqrt{2\pi}^3}\int \vec{B}(\vec{Q})\exp(i\vec{Q}.\vec{r})d\vec{Q}$$

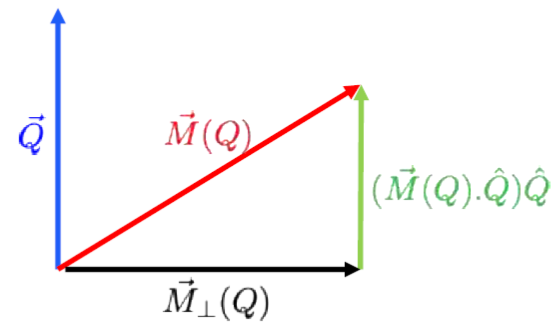
$$\Rightarrow \nabla.\vec{B}(\vec{r}) = \frac{1}{\sqrt{2\pi}^3}\int i\vec{Q}.\vec{B}(\vec{Q})\exp(i\vec{Q}.\vec{r})d\vec{Q} = 0$$

$$\Rightarrow \vec{Q}.\vec{B}(\vec{Q}) = 0$$

$$V_m(Q) = -\vec{\mu_n}.\vec{B}_\perp(Q)$$

$$= -\mu_0\vec{\mu_n}.\vec{M}_\perp(Q)$$

where, $\vec{M}_\perp(Q) = \vec{M}(Q) - (\vec{M}(Q).\hat{Q})\hat{Q}$



Neutron probes component of the magnetization perpendicular to Q

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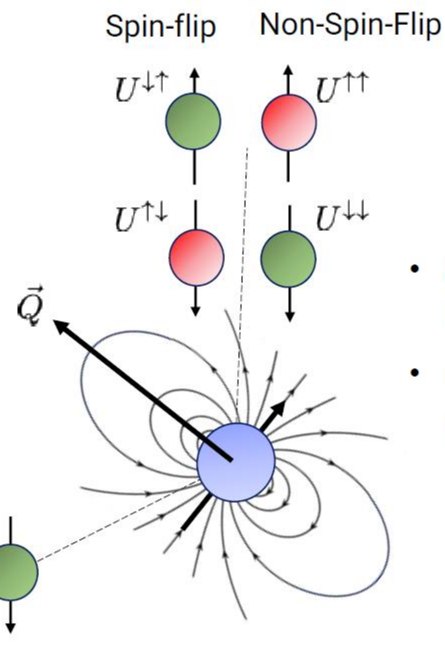
Addendum: Magnetic neutron scattering

Magnetic Spin-dependent Scattering (classical)

Magnetic scattering has complex spin-dependence

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

There will be a classical torque on the neutron moment if there are components of the field perpendicular to it



- if $\vec{\mu}$ parallel to $\vec{B}$
  No torque – so all scattering is non-spin-flip
- if $\vec{\mu}$ perpendicular to $\vec{B}$
  Neutron spin can precess in the field – spin-flip scattering

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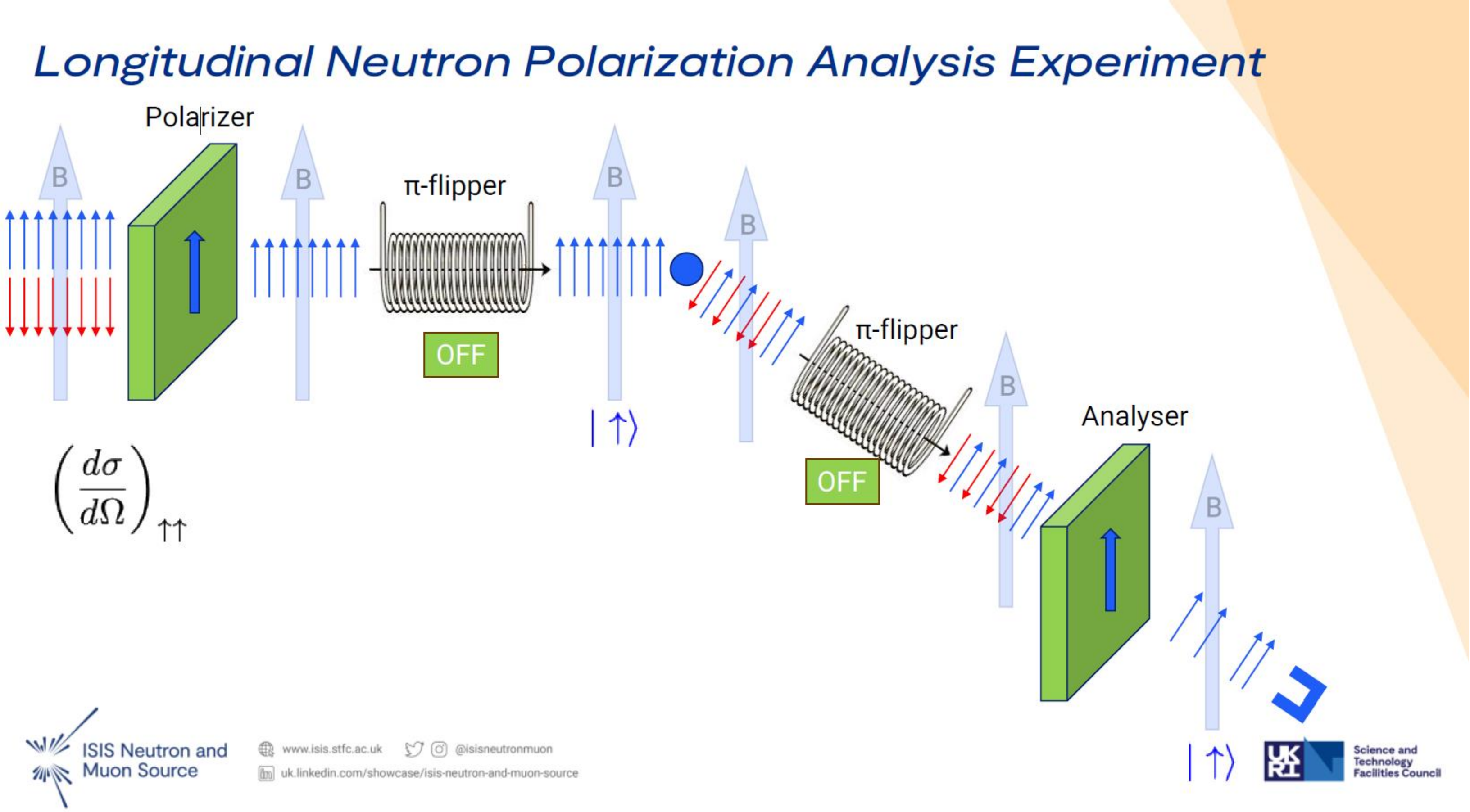
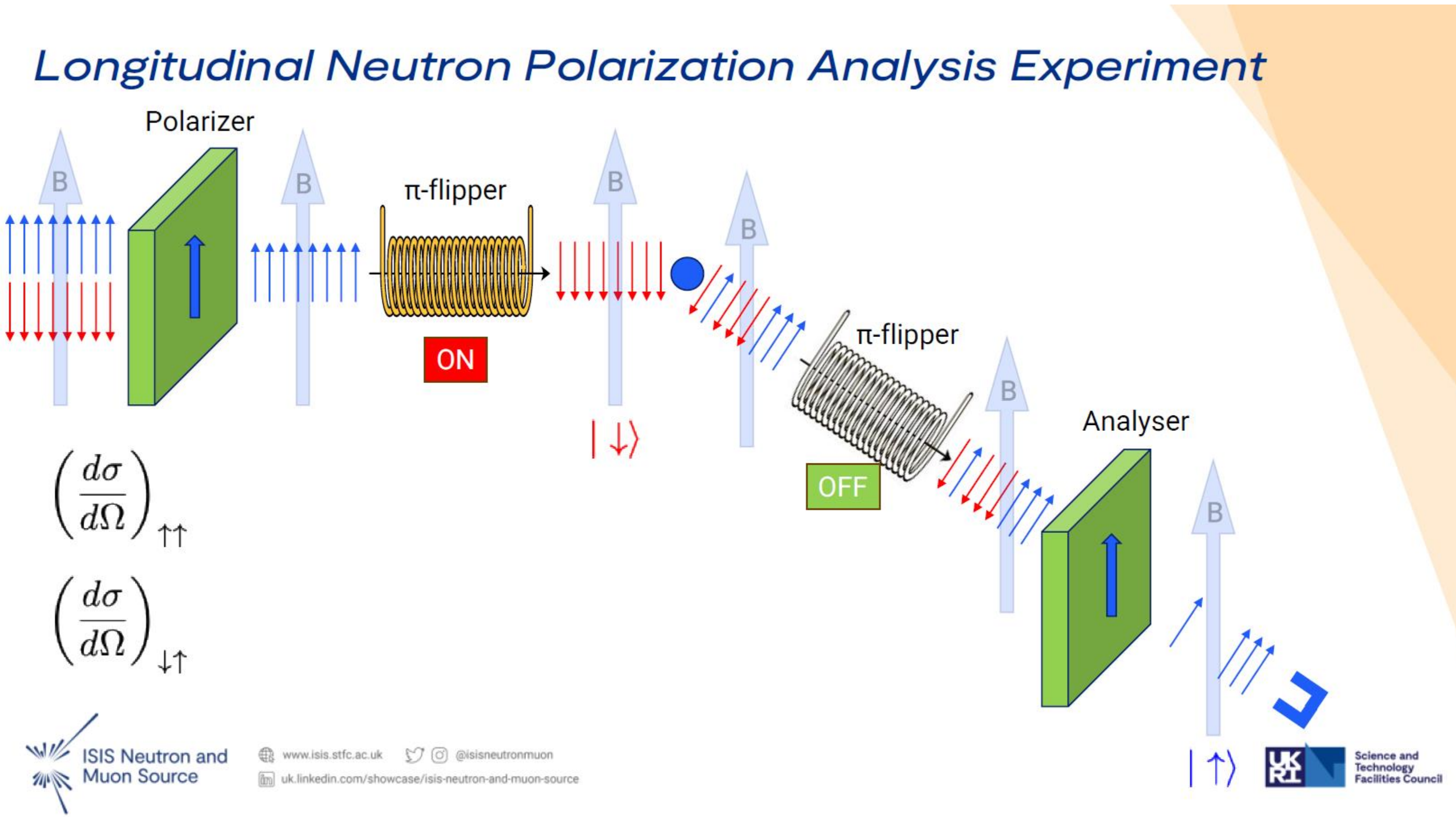
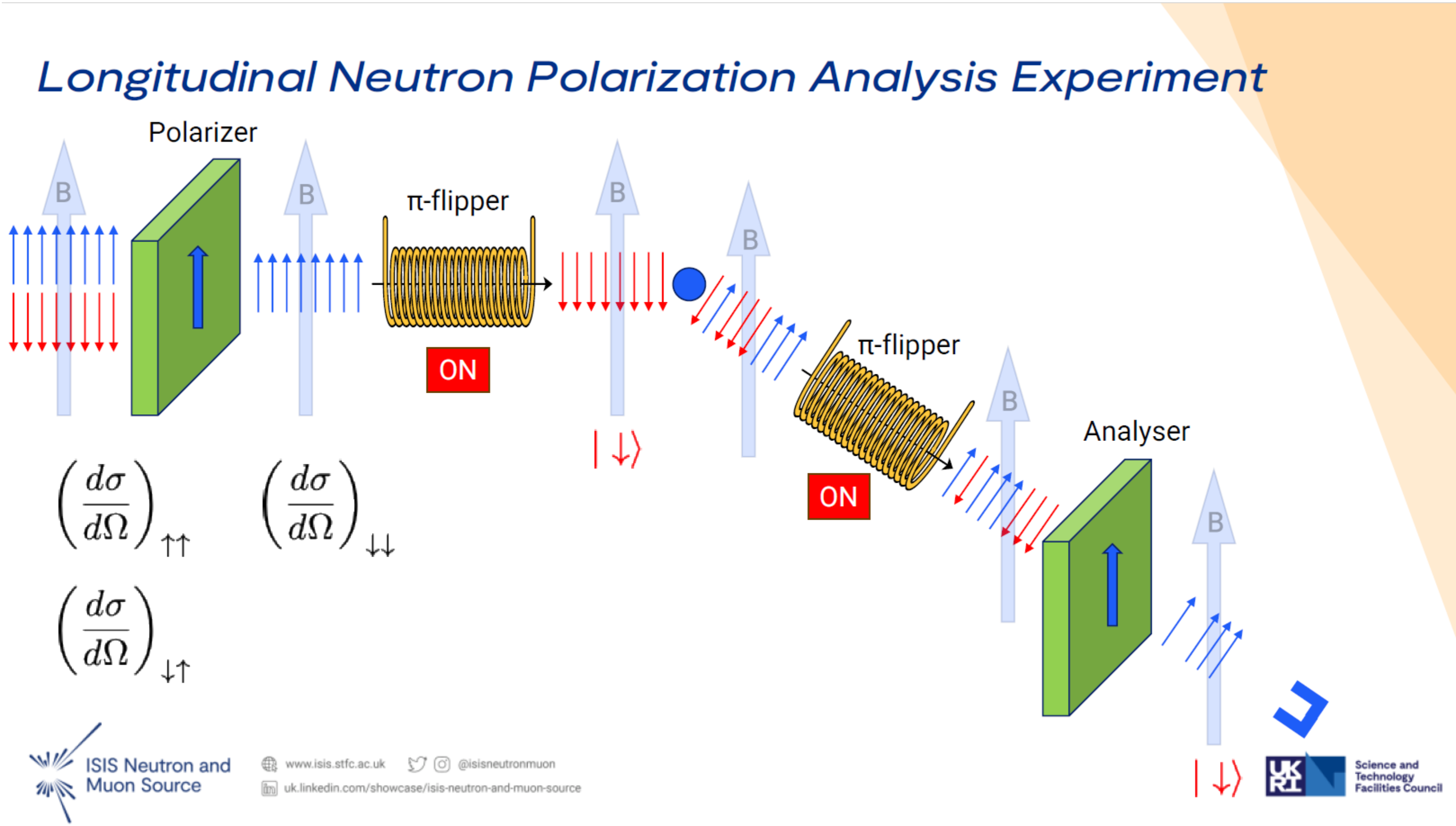
Addendum: Magnetic neutron scattering / Experimental



Addendum: Magnetic neutron scattering / Experimental



Addendum: Magnetic neutron scattering / Experimental



Addendum: Magnetic neutron scattering / Experimental