ISIS Neutron and Muon Source

Polarized Neutrons

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Oxford School on Neutron Scattering - 2024

Take-home message

Polarized neutrons can be used to enhance almost any neutron scattering experiment, either by

1. Separating and providing additional information on the **sources of scattering** (nuclear, magnetic, incoherent)

2. Improving the **resolution**

Outline

Definitions

Neutron spin, magnetic moment, precession

Polarization, flipping ratio, polarizers, flippers

Polarized neutron scattering

Polarized neutrons interaction with matter

Separation of sources of scattering

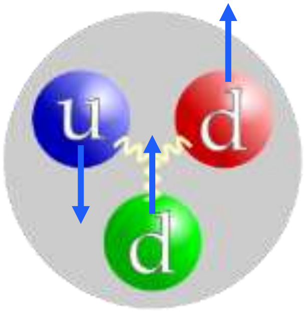
Neutron spin-echo

Principle of NSE - using the neutron spin as measuring tool

Definitions: Neutron magnetic moment

Particles with spin are experimentally observed to possess a magnetic moment

$\vec{\mu} = \gamma \vec{s}$ where, $\vec{s} \equiv \pm s_z = \pm {}^1\!/_2 \hbar$
and $\gamma = -183$ MHz / T for neutrons



Quarks also have s = ½ quantum number, therefore if the up and down quarks are antiparallel, the neutron also has s = ½

The magnetic moment calculation is tricky – but can be measured accurately

Often we see the neutron magnetic moment given in terms of **nuclear magnetons**

$$\mu_n = -1.913 \times \mu_N \quad \text{where,} \quad \mu_N = \frac{e\hbar}{2m_p}$$

What does the minus mean?

Definitions: Neutron spin-1/2

spin-½ particles

s = ½

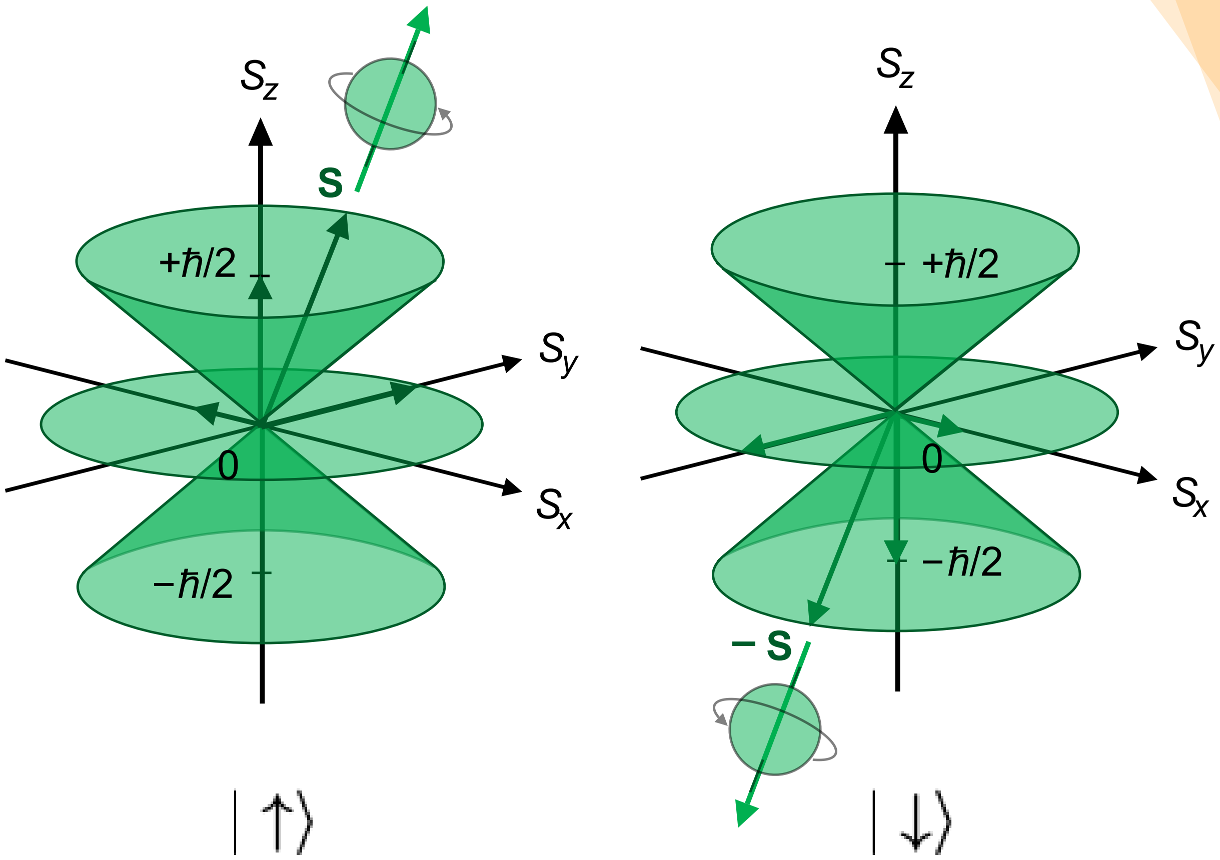
m_s = -s to +s in integer steps

- **only two choices**

Describes an **intrinsic** angular momentum, $\vec{s}$, that the neutron possesses, with

$$|\vec{s}|^2 = s(s+1)\hbar^2 = {}^3/_4\hbar^2$$

$$s_z = m_s\hbar$$



Definitions: Larmor Precession

Magnetic moments in a field experience a **torque** defined as the rate of change of angular momentum

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

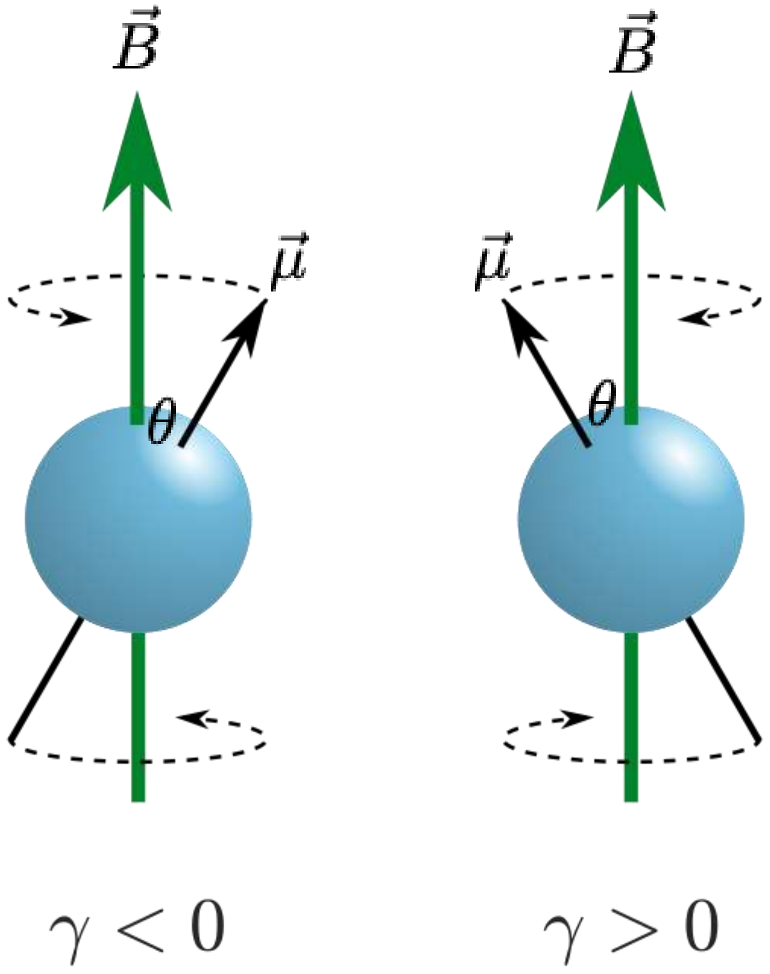
$$\Rightarrow \frac{d\vec{s}}{dt} = \vec{\mu} \times \vec{B}$$

$$\Rightarrow \frac{d\vec{\mu}}{dt} = \gamma\vec{\mu} \times \vec{B}$$

$d\vec{\mu}$ always in direction perpendicular to both $\vec{B}$ and $\vec{\mu}$

therefore, $\vec{\mu}$ precesses around $\vec{B}$ maintaining the angle θ

From definition of the cross product $\frac{|d\vec{\mu}|}{dt} = \gamma \mu B \sin\theta$



Definitions: Larmor precession frequency

The angular frequency of the moment vector is defined as the rate of change of the rotation angle ϕ around the field axis

$$\omega = \frac{d\phi}{dt} \Rightarrow d\phi = \omega dt$$

From the figure, $d\phi$ can also be written as the arc-length $d\vec{\mu}$ divided by component of $\vec{\mu}$ in the plane of rotation

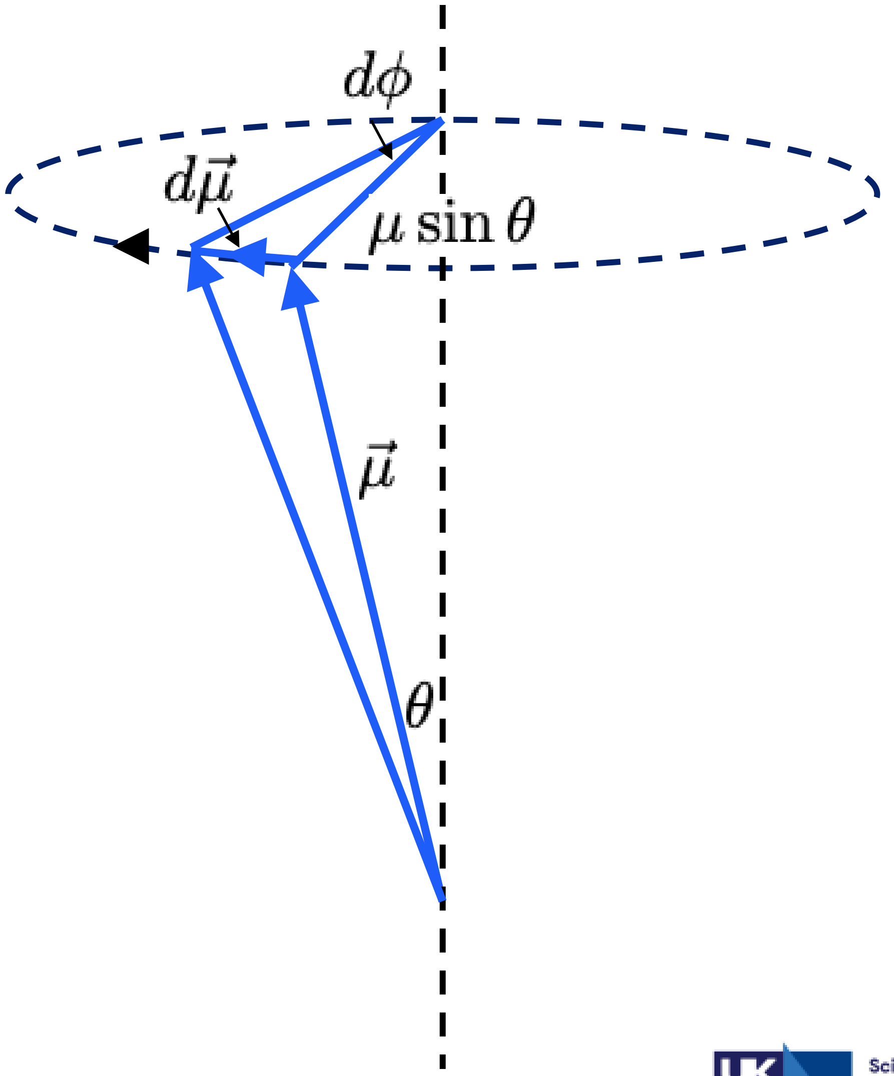
$$d\phi = \frac{|d\vec{\mu}|}{\mu \sin\theta} = \omega dt$$

Rearranging this we get

$$\frac{|d\vec{\mu}|}{dt} = \omega\mu\sin\theta = \gamma\mu B\sin\theta$$

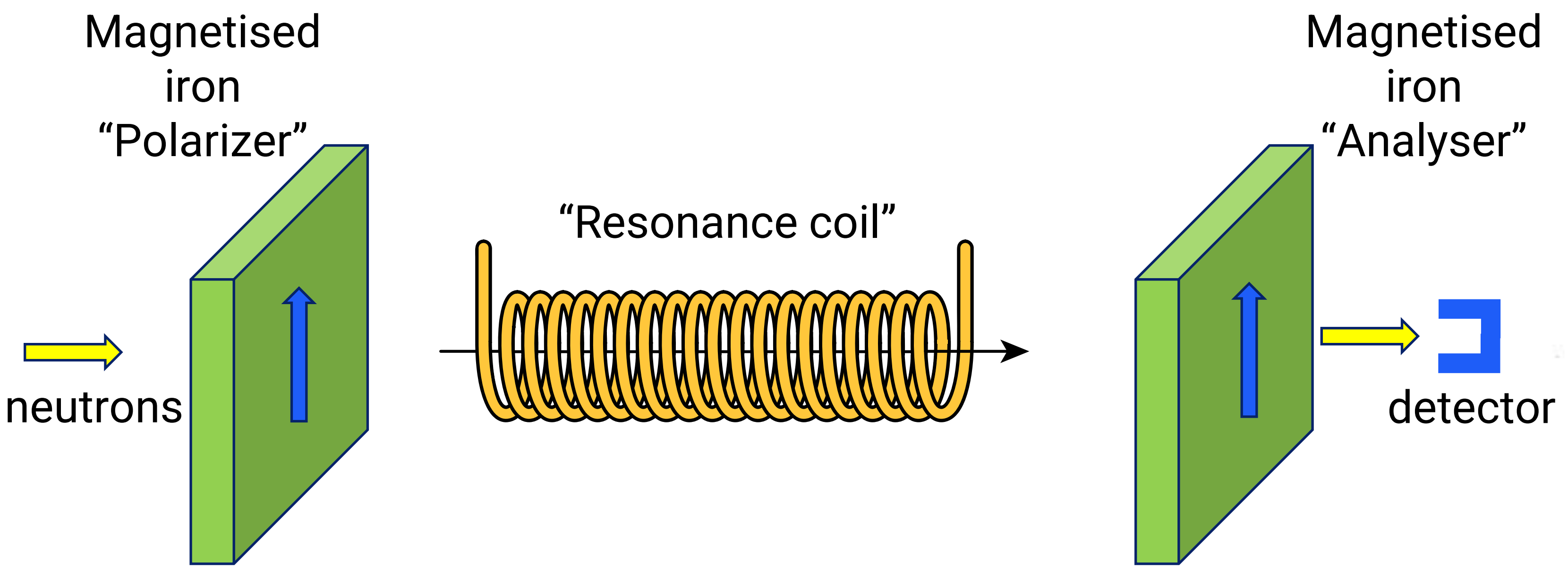
$$\Rightarrow \omega = \gamma B$$

This is the **Larmor precession frequency**, ω_L and γ is known as the **gyromagnetic ratio**



*Alvarez and Bloch, Physical Review **57**, 111 (1940)*

Measuring the neutron magnetic moment: The first ever Neutron Polarization Analysis Experiment



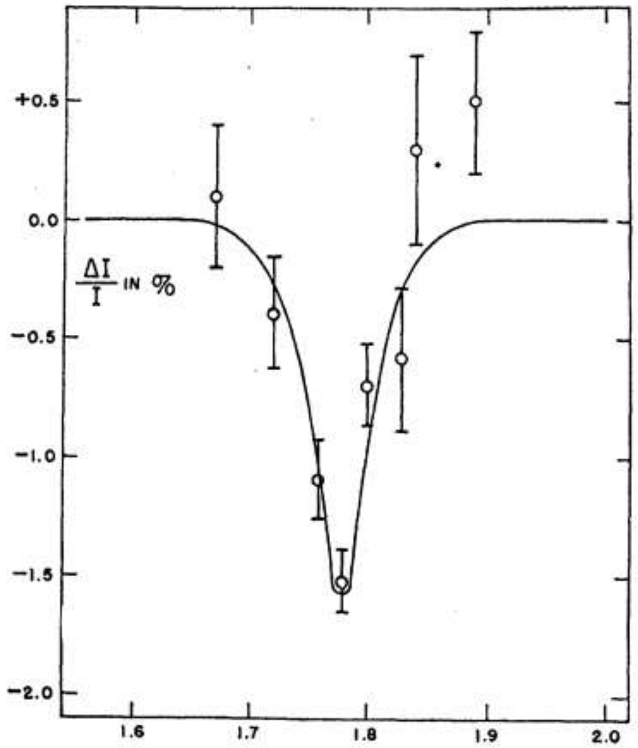


FIG. 5. Neutron resonance dip. The magnet current in arbitrary used is plotted against the fractional change $(\Delta I/I)$ of the intensity of the neutron beam.

$$P = \frac{T_{|\uparrow\rangle} - T_{|\downarrow\rangle}}{T_{|\uparrow\rangle} + T_{|\downarrow\rangle}} = \begin{cases} 1 \text{ for neutrons perfectly polarized \textbf{along} the field} \\ 0 \text{ for unpolarized neutrons} \\ -1 \text{ for neutrons perfectly polarized \textbf{against} the field} \end{cases}$$

Definitions: Flipping Ratio

Instead of "polarization" of the beam, experimentalists often talk in terms of the **neutron flipping ratio**

This can refer to a device – polarizer or analyser – but also to the sample under investigation

$$\Phi = \frac{N_{|\uparrow\rangle}}{N_{|\downarrow\rangle}}$$

where, *N* is the number of neutrons transmitted or scattered.

$$P = \frac{N_{|\uparrow\rangle} - N_{|\downarrow\rangle}}{N_{|\uparrow\rangle} + N_{|\downarrow\rangle}} = \frac{\Delta N}{N} = \frac{\Phi - 1}{\Phi + 1} \quad \text{and} \quad \Phi = \frac{1 + P}{1 - P}$$

This description of a polarized beam is OK for experiments in which a single quantisation axis is defined: **Longitudinal Polarization Analysis**

Worked example: Alvarez and Bloch

In the figure on the right, Alvarez and Bloch plot the polarization of their beam as a function of current in their resonance coil – which then gives the resonant frequency. What was the flipping ratio, and polarizing efficiency of the polarizer and analyser (P_p and P_a) assuming they are the same?

The polarization on resonance is, $P = \Delta I/I = -0.015$

Therefore,

$$\Phi = \frac{1+(-0.015)}{1-(-0.015)} = \frac{0.985}{1.015} \simeq 0.97$$

The measured polarization is just the product of the individual efficiencies

$$P = P_p \times P_a = P_{p/a}^2$$

$$\Rightarrow P_{p/a} = \sqrt{|P|} \simeq 0.122$$

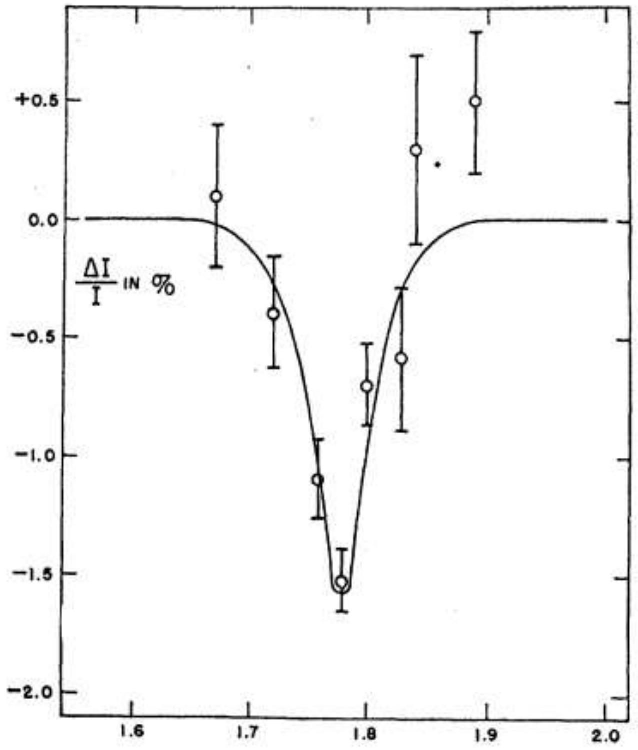
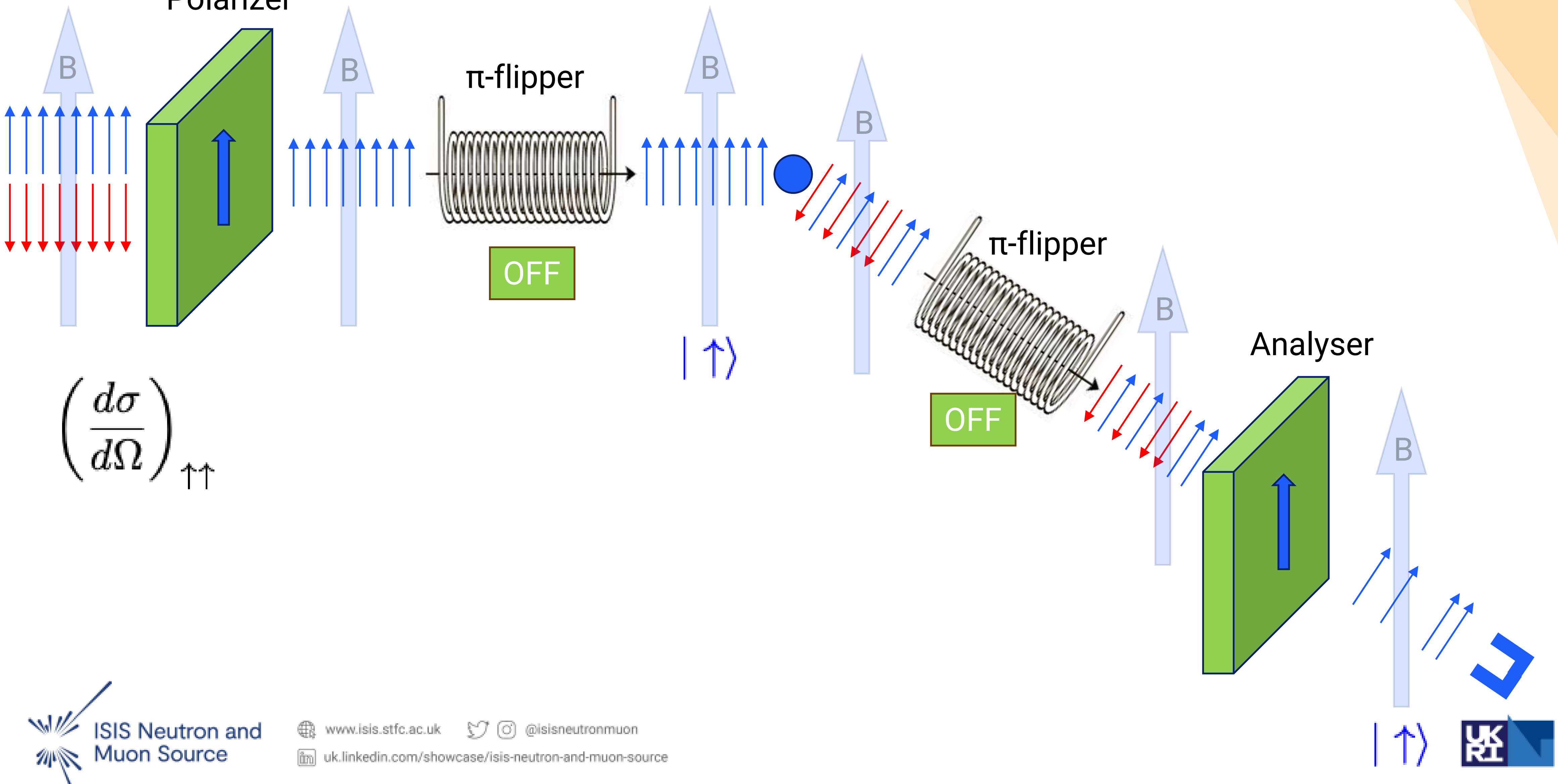


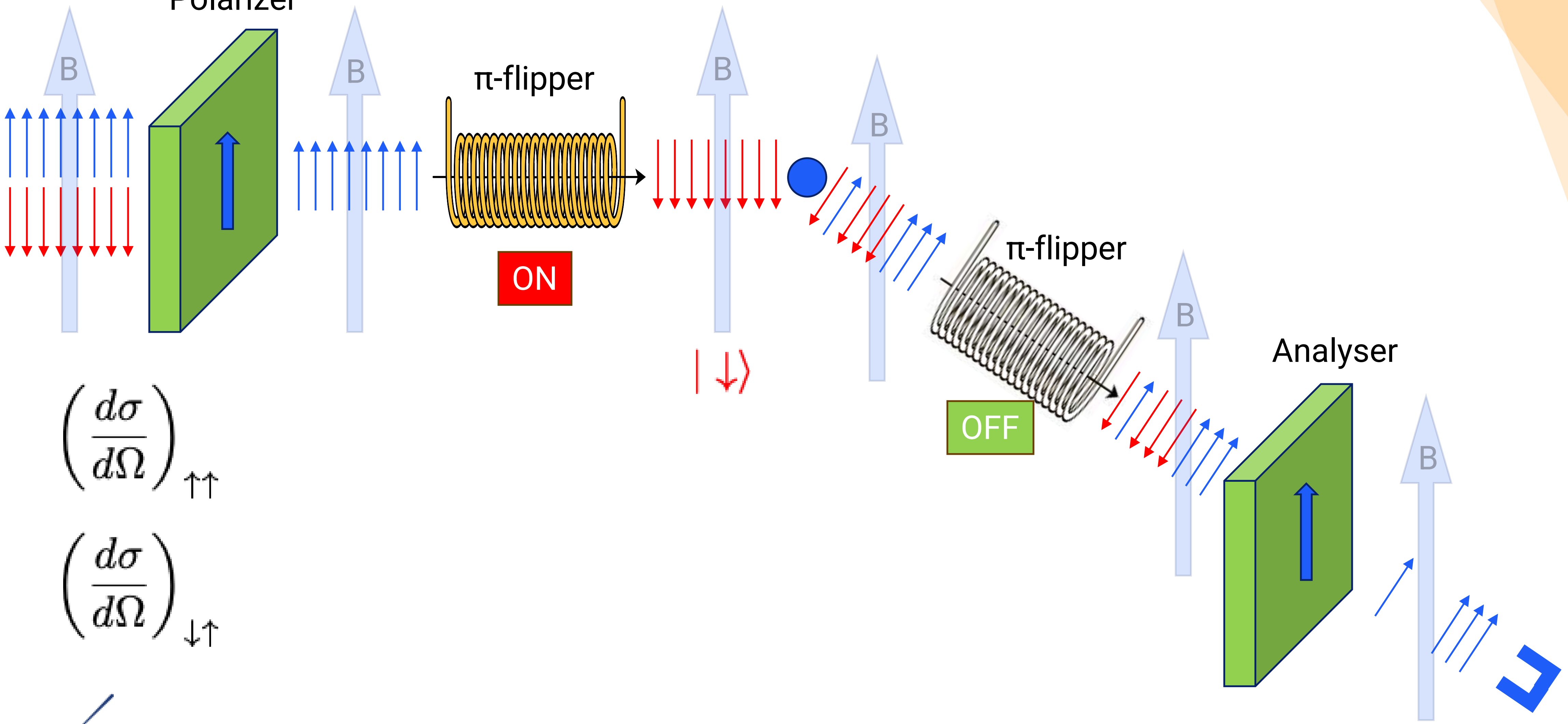
FIG. 5. Neutron resonance dip. The magnet current in arbitrary used is plotted against the fractional change ($\Delta I/I$) of the intensity of the neutron beam.

Longitudinal Neutron Polarization Analysis Experiment



$$\left(\frac{d\sigma}{d\Omega}\right)_{\uparrow\uparrow}$$

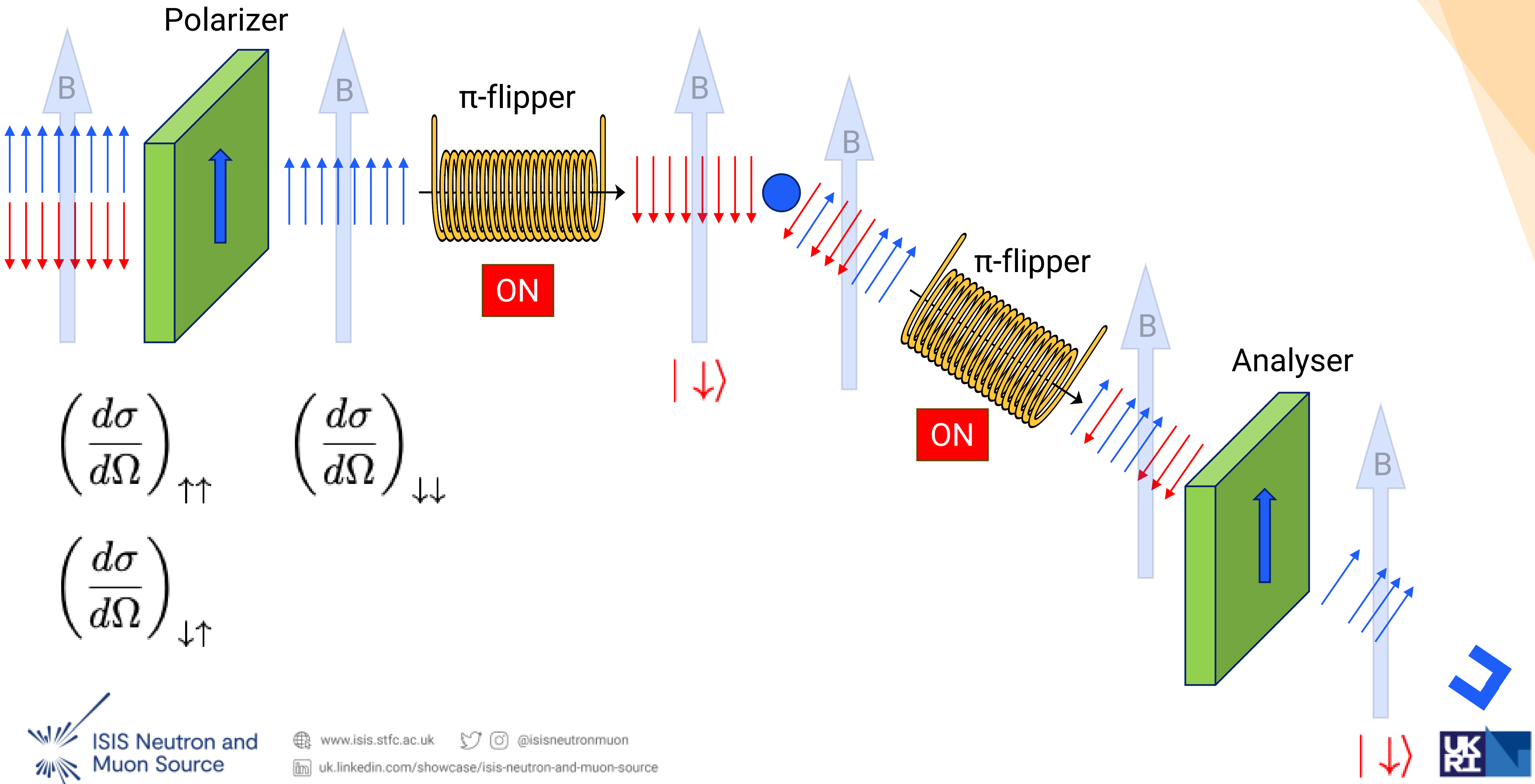
Longitudinal Neutron Polarization Analysis Experiment



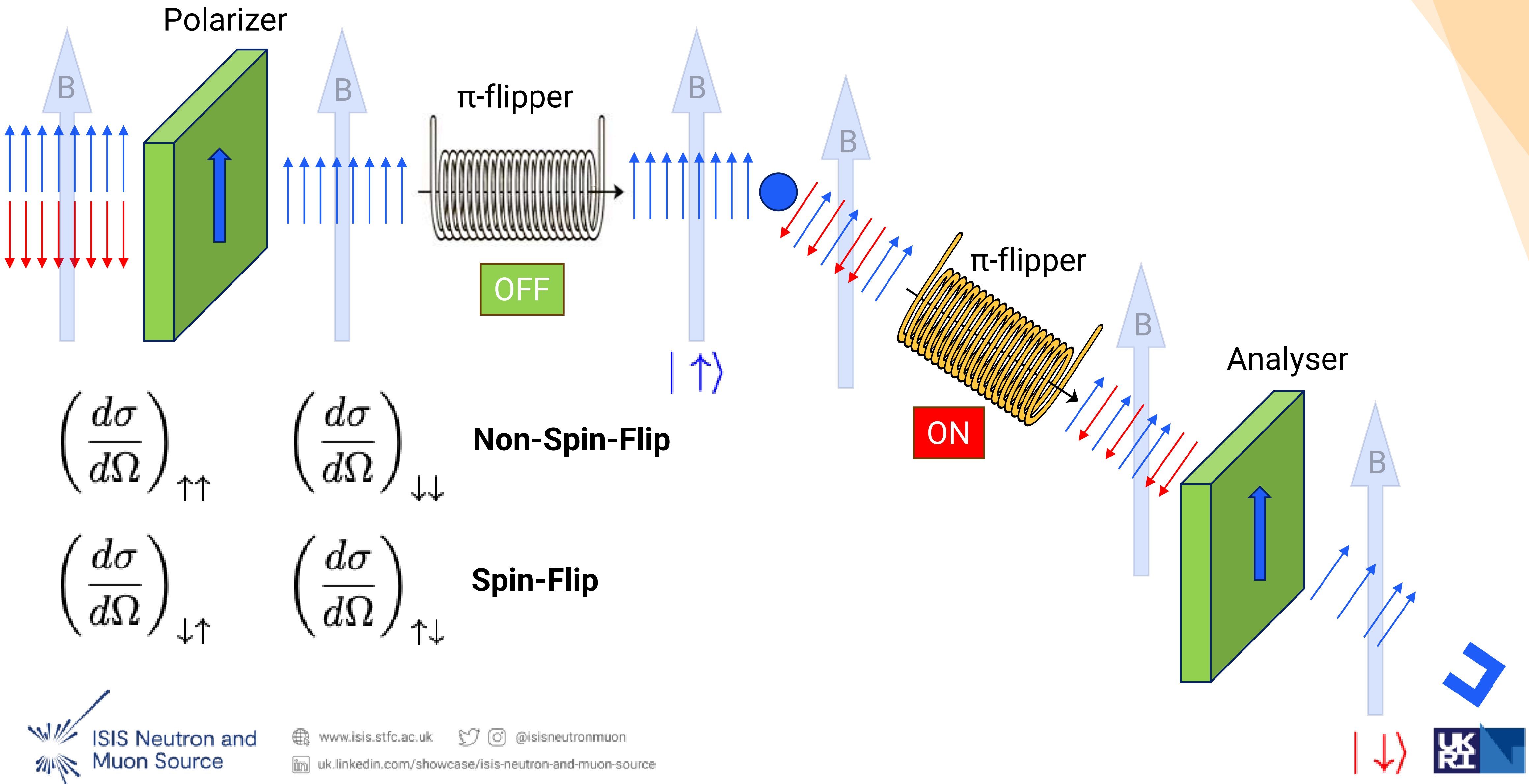
$$\left(\frac{d\sigma}{d\Omega}\right)_{\uparrow\uparrow}$$

$$\left(\frac{d\sigma}{d\Omega}\right)_{\downarrow\uparrow}$$

Longitudinal Neutron Polarization Analysis Experiment



Longitudinal Neutron Polarization Analysis Experiment



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

Non-Spin-Flip

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

Spin-Flip

Nuclear Spin-Dependent Scattering

Nuclear scattering

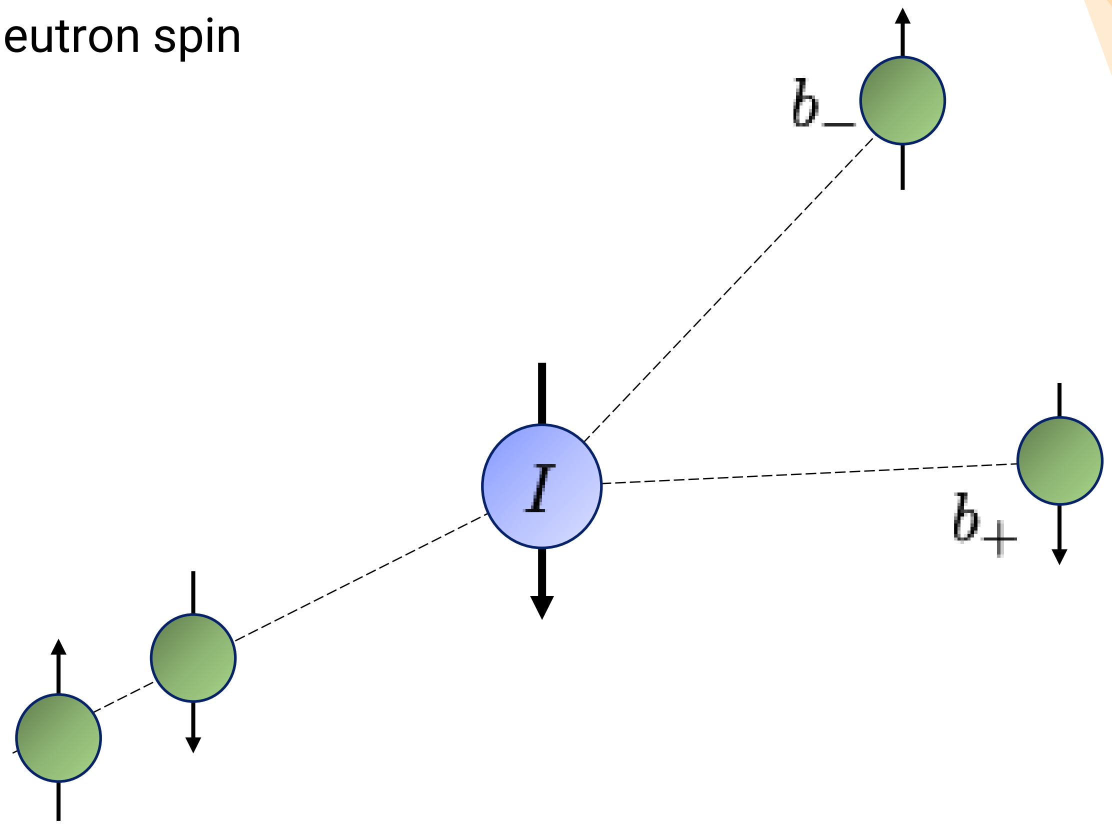
The scattering length depends on the whether the neutron spin is parallel or antiparallel to the nuclear spin

b_+ - neutron/nuclear spins add

b_- - neutron/nuclear spins subtract

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

$$b_{\text{inc}} = \sqrt{\overline{b^2} - \bar{b}^2} = \frac{b_+ - b_-}{2I+1}\sqrt{(I(I+1))}$$



Reminder: Magnetic scattering

Magnetic scattering

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

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

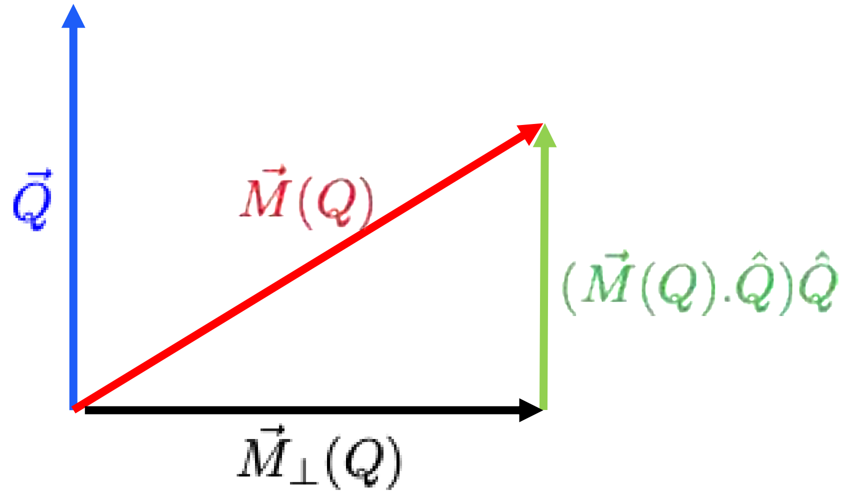
$$\Rightarrow \nabla.\vec{B}(\vec{r}) = \frac{1}{\sqrt{2\pi}^3}\int i\vec{Q}.\vec{B}(\vec{Q})\exp(i\vec{Q}.\vec{r})d\vec{Q} = 0$$

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

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

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

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



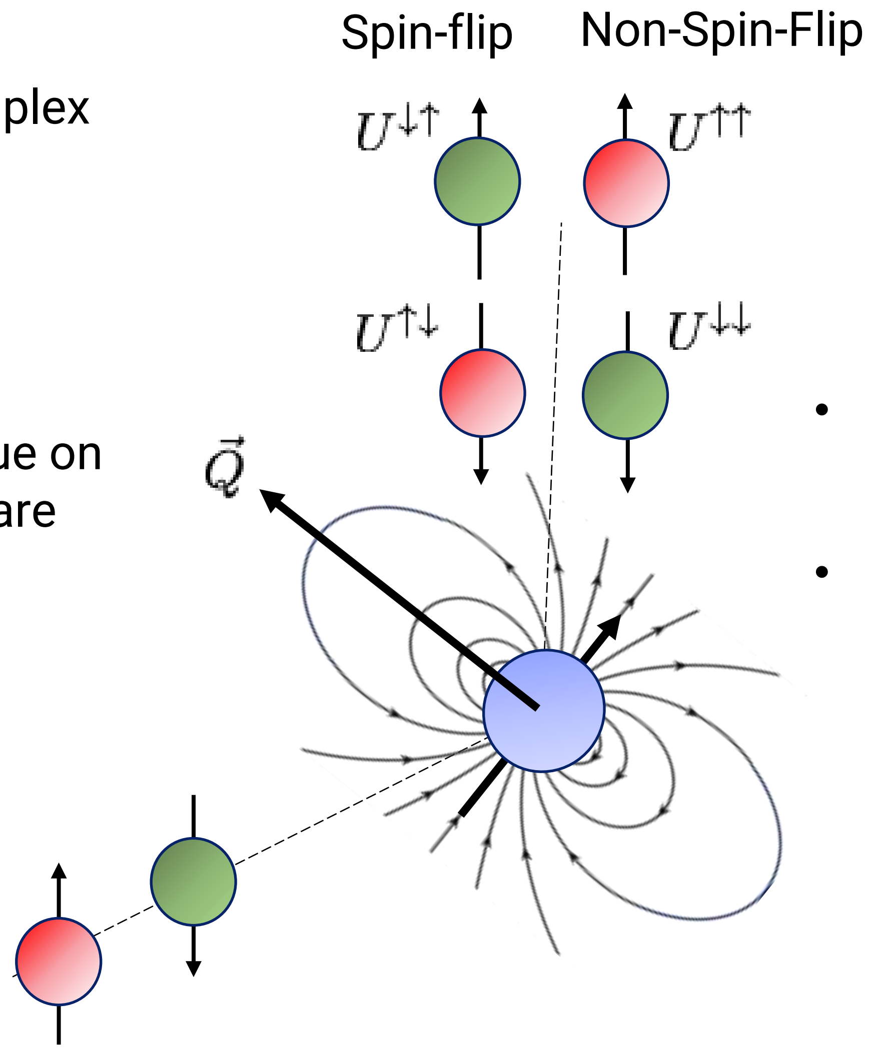
Neutron probes component of the magnetization perpendicular to Q

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

Polarized neutron scattering

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

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

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

Coherent (nuclear) Scattering

Assuming no magnetism in the sample – we can work out the **coherent** (see A Boothroyd lectures) nuclear scattering, just by taking the average of the amplitudes

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

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

Incoherent (nuclear) Scattering

Again, assuming no magnetism we can work out the **incoherent** scattering which (from A Boothroyd's lectures), 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 $\boxed{\overline{b^2} - \overline{b}^2} + \boxed{\overline{B^2 I_z^2}}$ **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 $I_x^2 = I_y^2 = I_z^2 = 1/3\ I(I+1)$

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

Boothroyd – Sec 4.5.1 (p 112)

Incoherent (nuclear) Scattering

Again, assuming no magnetism we can work out the **incoherent** scattering which (from A Boothroyd's lectures), 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 the scattered polarization is preserved
- if the scattering is fully spin-incoherent then,

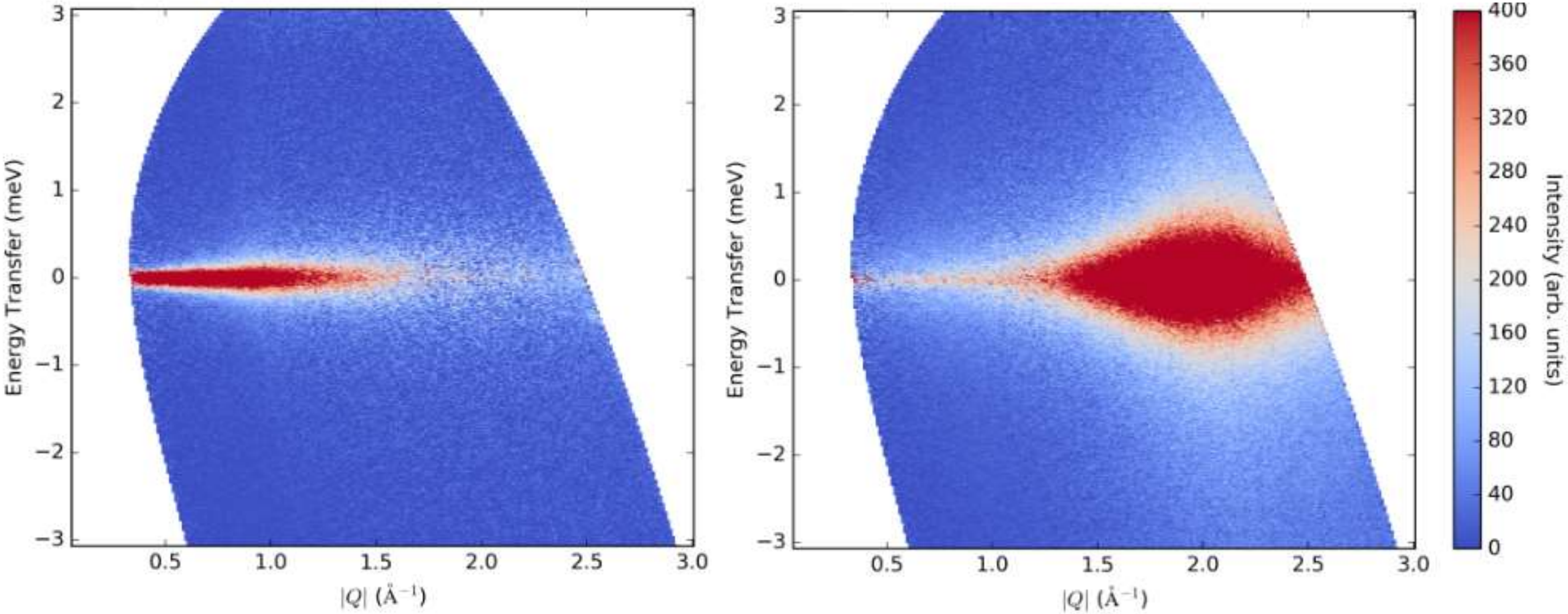
$$\vec{P}' = -{}^{1}\!/_{3}\vec{P}$$

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

Example 1 – Water (D_2O) at 295 K

Measured on LET at ISIS

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



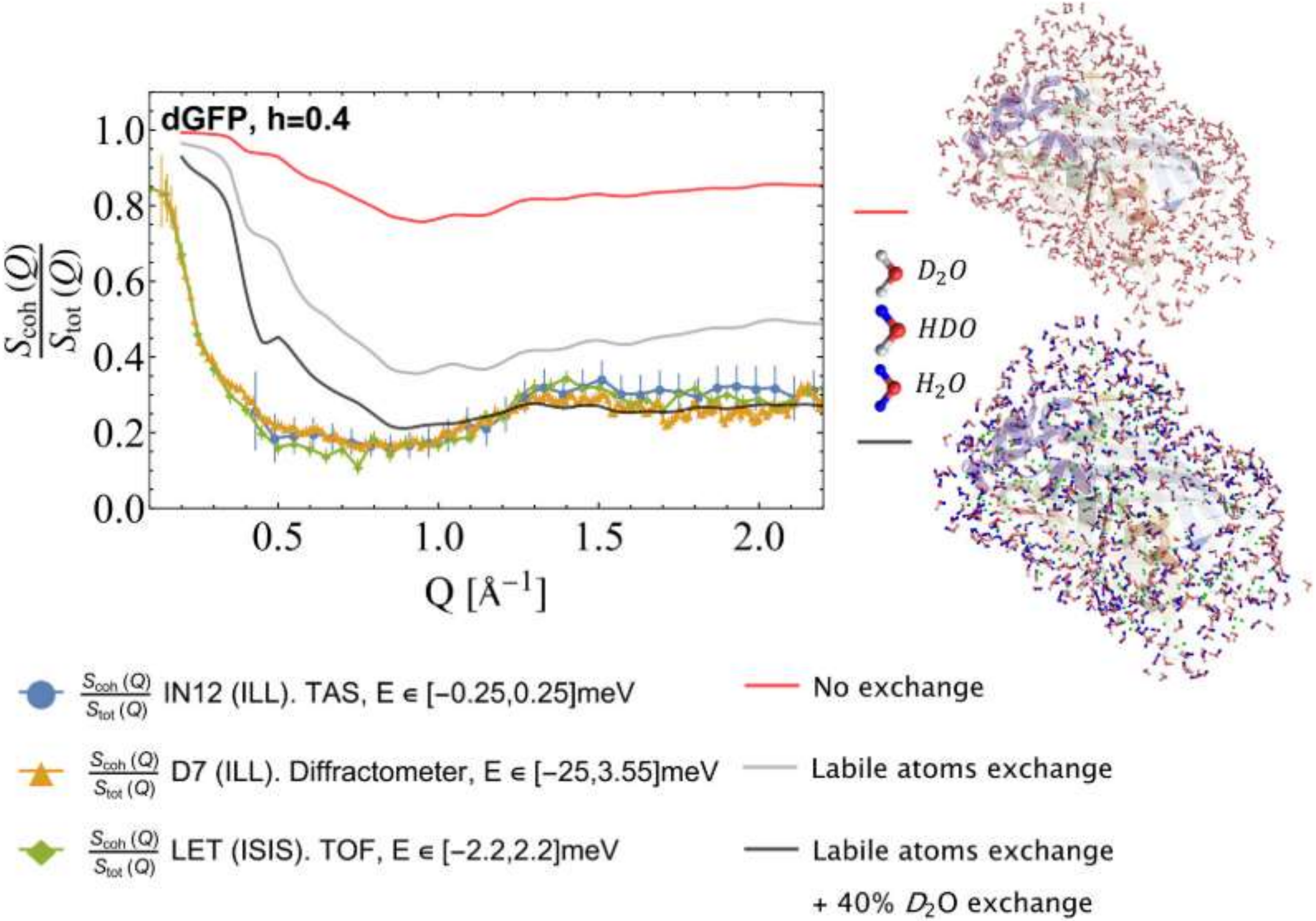
$$\left(\frac{d\sigma}{d\Omega}\right)^{\mathrm{SI}} = \frac{3}{2}\left(\frac{d\sigma}{d\Omega}\right)_{\mathrm{SF}}$$

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

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

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

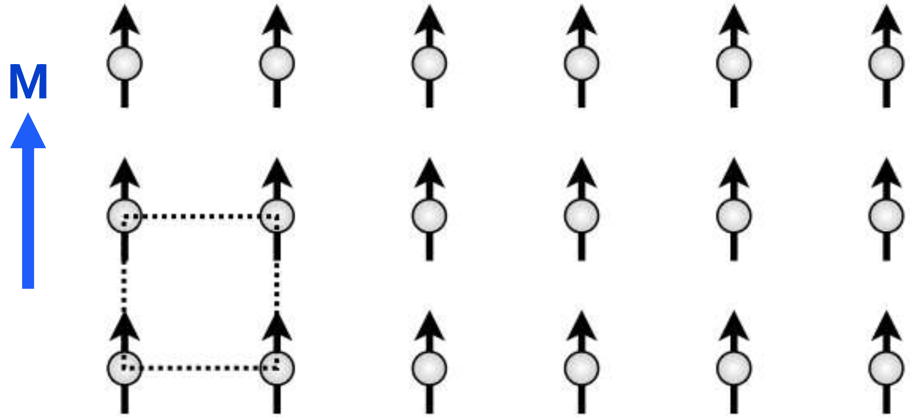
Example 2 – deuterated Green fluorescent protein



New experiments challenging assumptions about “dominant” scattering on deuteration

Scattering from Ferromagnets

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



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

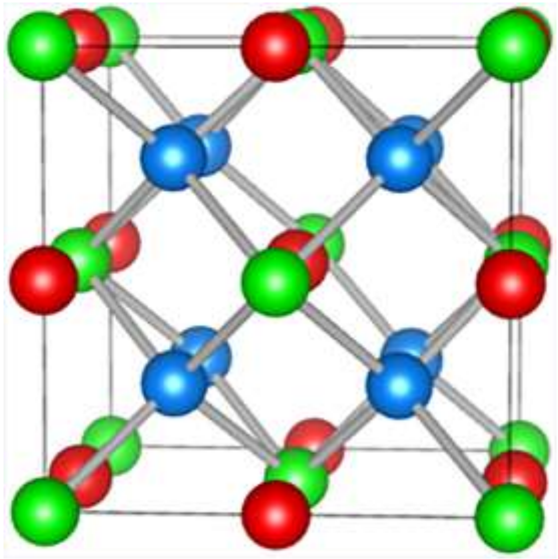
Writing this in terms of cross-sections and structure factors

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

Leading to a flipping ratio of

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

Example 3 – 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, $\Phi = \frac{1+(-0.99)}{1-(-0.99)} \simeq 0.005$

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

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

Example 4 – nickel

In nickel, the ratio of the magnetic and nuclear structure factors for the (400) Bragg peak is $\phi = 6 \times 10^{-4}$. What is the flipping ratio? Compare that with the extra magnetic intensity which would be seen in an unpolarized experiment

$$\phi = 6 \times 10^{-4} \Rightarrow \Phi = \left(\frac{1 - 6 \times 10^{-4}}{1 + 6 \times 10^{-4}} \right)^2 = 0.997$$

The ratio of the magnetic and nuclear intensities in an unpolarized experiment is

$$\frac{F_M^2}{F_N^2} = \phi^2 = 3.6 \times 10^{-7} \Rightarrow \frac{\Delta I}{I} = \frac{F_N^2 + F_M^2}{F_N^2} = 1 + \phi^2 = 1.00000036$$

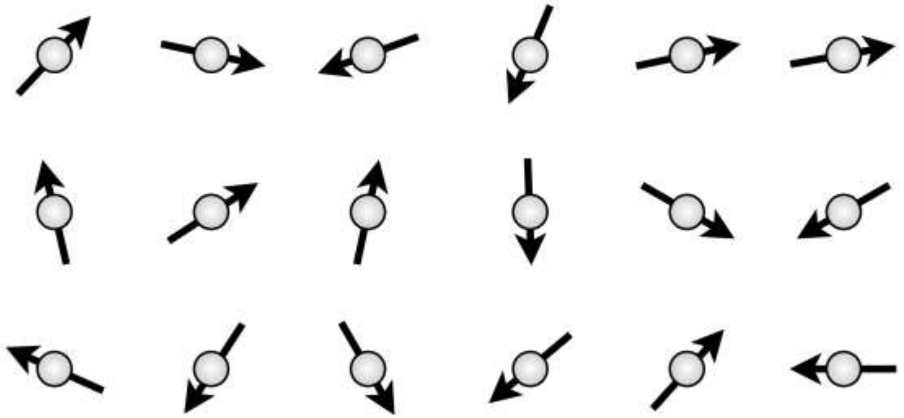
So – magnetic structure factors much easier to measure using polarized neutrons (also, much less sensitive to systematic errors)

Halpern and Johnson, Phys. Rev. ***15****, 898 (1939)*

Squires – Sec 9.3 (p 179)

Scattering from disordered magnets

Paramagnetic scattering



M = 0

$$\left(\frac{d\sigma}{d\Omega}\right)^{\mathrm{NSF}} = \frac{1}{2}\left[1-\left(\hat{P}\cdot\hat{Q}\right)^2\right]\left(\frac{d\sigma}{d\Omega}\right)_{\mathrm{mag}}$$

$$\left(\frac{d\sigma}{d\Omega}\right)^{\mathrm{SF}} = \frac{1}{2}\left[1+\left(\hat{P}\cdot\hat{Q}\right)^2\right]\left(\frac{d\sigma}{d\Omega}\right)_{\mathrm{mag}}$$

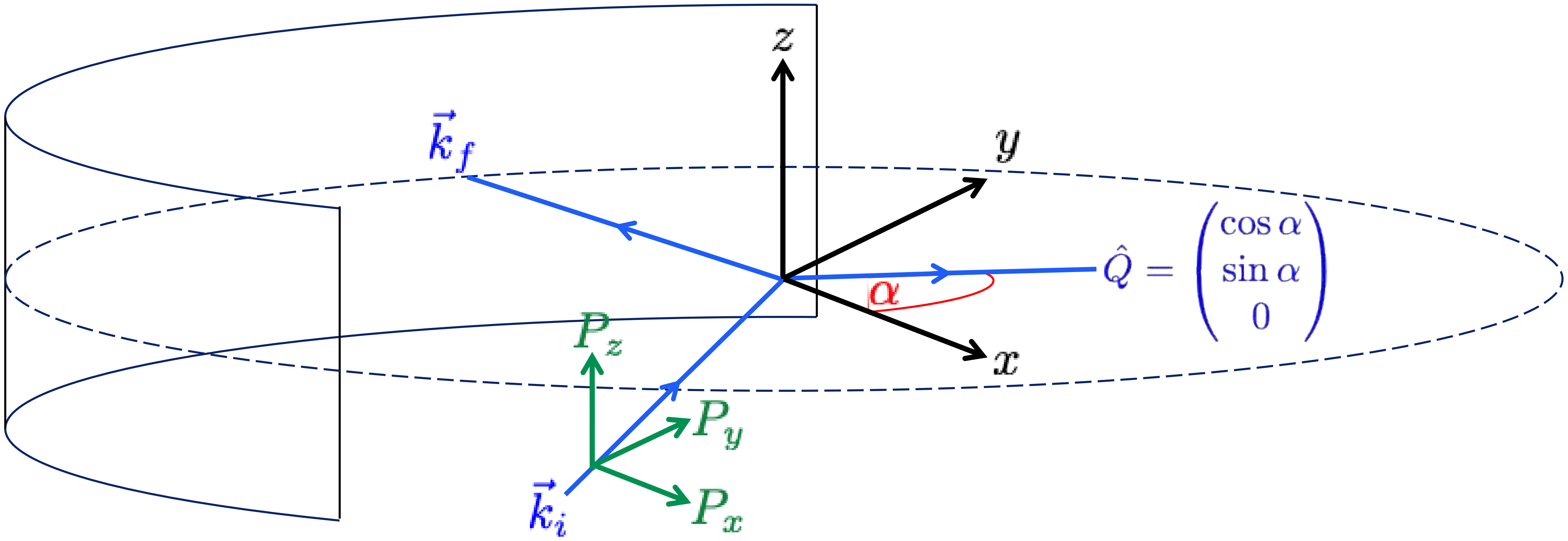
We can therefore write the polarization as $P = \dfrac{\left[1-\left(\hat{P}\cdot\hat{Q}\right)^2\right]-\left[1+\left(\hat{P}\cdot\hat{Q}\right)^2\right]}{\left[1-\left(\hat{P}\cdot\hat{Q}\right)^2\right]+\left[1+\left(\hat{P}\cdot\hat{Q}\right)^2\right]}$

This is easily simplified to give **the Halpern-Johnson Equation** $\vec{P}' = -\left(\vec{P}\cdot\hat{Q}\right)\hat{Q}$

“Planar multidetector” – XYZ Polarization Analysis

Paramagnetic scattering

$$\left(\frac{d\sigma}{d\Omega}\right)^{\mathrm{NSF}} = \frac{1}{2}\left[1-\left(\hat{P}\cdot\hat{Q}\right)^2\right]\left(\frac{d\sigma}{d\Omega}\right)_{\mathrm{mag}} \qquad \left(\frac{d\sigma}{d\Omega}\right)^{\mathrm{SF}} = \frac{1}{2}\left[1+\left(\hat{P}\cdot\hat{Q}\right)^2\right]\left(\frac{d\sigma}{d\Omega}\right)_{\mathrm{mag}}$$



XYZ polarization analysis – paramagnetic scattering

Polarization along x-direction:

$$\left(\hat{P}_x \cdot \hat{Q}\right)^2 = \left[\begin{pmatrix}1\\0\\0\end{pmatrix} \cdot \begin{pmatrix}\cos\alpha\\ \sin\alpha\\ 0\end{pmatrix}\right]^2 = \cos^2\alpha \begin{cases} \Rightarrow \left(\dfrac{d\sigma}{d\Omega}\right)_x^{\mathrm{NSF}} = \dfrac{1-\cos^2\alpha}{2}\left(\dfrac{d\sigma}{d\Omega}\right)_{\mathrm{mag}} = \dfrac{\sin^2\alpha}{2}\left(\dfrac{d\sigma}{d\Omega}\right)_{\mathrm{mag}} \\ \Rightarrow \left(\dfrac{d\sigma}{d\Omega}\right)_x^{\mathrm{SF}} = \dfrac{1+\cos^2\alpha}{2}\left(\dfrac{d\sigma}{d\Omega}\right)_{\mathrm{mag}} \end{cases}$$

Polarization along y-direction:

$$\left(\hat{P}_y \cdot \hat{Q}\right)^2 = \left[\begin{pmatrix}0\\1\\0\end{pmatrix} \cdot \begin{pmatrix}\cos\alpha\\ \sin\alpha\\ 0\end{pmatrix}\right]^2 = \sin^2\alpha \begin{cases} \Rightarrow \left(\dfrac{d\sigma}{d\Omega}\right)_y^{\mathrm{NSF}} = \dfrac{1-\sin^2\alpha}{2}\left(\dfrac{d\sigma}{d\Omega}\right)_{\mathrm{mag}} = \dfrac{\cos^2\alpha}{2}\left(\dfrac{d\sigma}{d\Omega}\right)_{\mathrm{mag}} \\ \Rightarrow \left(\dfrac{d\sigma}{d\Omega}\right)_y^{\mathrm{SF}} = \dfrac{1+\sin^2\alpha}{2}\left(\dfrac{d\sigma}{d\Omega}\right)_{\mathrm{mag}} \end{cases}$$

Polarization along z-direction:

$$\left(\hat{P}_y \cdot \hat{Q}\right)^2 = \left[\begin{pmatrix}0\\0\\1\end{pmatrix} \cdot \begin{pmatrix}\cos\alpha\\ \sin\alpha\\ 0\end{pmatrix}\right]^2 = 0 \begin{cases} \Rightarrow \left(\dfrac{d\sigma}{d\Omega}\right)_z^{\mathrm{NSF}} = \dfrac{1}{2}\left(\dfrac{d\sigma}{d\Omega}\right)_{\mathrm{mag}} \\ \Rightarrow \left(\dfrac{d\sigma}{d\Omega}\right)_z^{\mathrm{SF}} = \dfrac{1}{2}\left(\dfrac{d\sigma}{d\Omega}\right)_{\mathrm{mag}} \end{cases}$$

Schärpf and Capellmann, Phys. Stat. Sol. (a) **135** 359 (1993)

Boothroyd – Sec 4.6 (p 118)

XYZ Polarization analysis – Schärpf Equations

$$\left(\frac{d\sigma}{d\Omega}\right)_x^{\mathrm{NSF}} = \left(\frac{d\sigma}{d\Omega}\right)_{\mathrm{coh+II}} + \frac{1}{3}\left(\frac{d\sigma}{d\Omega}\right)_{\mathrm{SI}} + \frac{\sin^2\alpha}{2}\left(\frac{d\sigma}{d\Omega}\right)_{\mathrm{mag}}$$

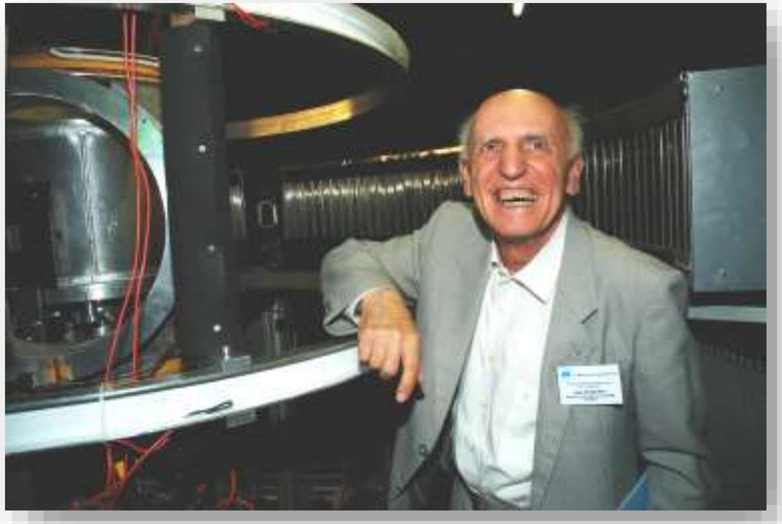
$$\left(\frac{d\sigma}{d\Omega}\right)_y^{\mathrm{NSF}} = \left(\frac{d\sigma}{d\Omega}\right)_{\mathrm{coh+II}} + \frac{1}{3}\left(\frac{d\sigma}{d\Omega}\right)_{\mathrm{SI}} + \frac{\cos^2\alpha}{2}\left(\frac{d\sigma}{d\Omega}\right)_{\mathrm{mag}}$$

$$\left(\frac{d\sigma}{d\Omega}\right)_z^{\mathrm{NSF}} = \left(\frac{d\sigma}{d\Omega}\right)_{\mathrm{coh+II}} + \frac{1}{3}\left(\frac{d\sigma}{d\Omega}\right)_{\mathrm{SI}} + \frac{1}{2}\left(\frac{d\sigma}{d\Omega}\right)_{\mathrm{mag}}$$

$$\left(\frac{d\sigma}{d\Omega}\right)_x^{\mathrm{SF}} = \frac{2}{3}\left(\frac{d\sigma}{d\Omega}\right)_{\mathrm{SI}} + \frac{1+\cos^2\alpha}{2}\left(\frac{d\sigma}{d\Omega}\right)_{\mathrm{mag}}$$

$$\left(\frac{d\sigma}{d\Omega}\right)_y^{\mathrm{SF}} = \frac{2}{3}\left(\frac{d\sigma}{d\Omega}\right)_{\mathrm{SI}} + \frac{1+\sin^2\alpha}{2}\left(\frac{d\sigma}{d\Omega}\right)_{\mathrm{mag}}$$

$$\left(\frac{d\sigma}{d\Omega}\right)_z^{\mathrm{SF}} = \frac{2}{3}\left(\frac{d\sigma}{d\Omega}\right)_{\mathrm{SI}} + \frac{1}{2}\left(\frac{d\sigma}{d\Omega}\right)_{\mathrm{mag}}$$



Otto Schärpf (1929-2019)

- 6 equations
- 4 unknowns
- α known as the **Schärpf Angle**

XYZ Polarization analysis – Schärpf Equations

Coherent (+II) nuclear scattering

$$\left(\frac{d\sigma}{d\Omega}\right)_{\mathrm{coh+II}} = \frac{1}{6}\left[2\left(\frac{d\sigma}{d\Omega}\right)^{\mathrm{TNSF}} - \left(\frac{d\sigma}{d\Omega}\right)^{\mathrm{TSF}}\right]$$

where TNSF and TSF refer to the total non-spin-flip and spin-flip scattering respectively

Magnetic scattering – can be independently calculated in two ways

$$\left(\frac{d\sigma}{d\Omega}\right)_{\mathrm{mag}} = 2\left(\frac{d\sigma}{d\Omega}\right)_x^{\mathrm{SF}} + 2\left(\frac{d\sigma}{d\Omega}\right)_y^{\mathrm{SF}} - 4\left(\frac{d\sigma}{d\Omega}\right)_z^{\mathrm{SF}}$$

$$\left(\frac{d\sigma}{d\Omega}\right)_{\mathrm{mag}} = 4\left(\frac{d\sigma}{d\Omega}\right)_z^{\mathrm{NSF}} - 2\left(\frac{d\sigma}{d\Omega}\right)_x^{\mathrm{NSF}} - 2\left(\frac{d\sigma}{d\Omega}\right)_y^{\mathrm{NSF}}$$

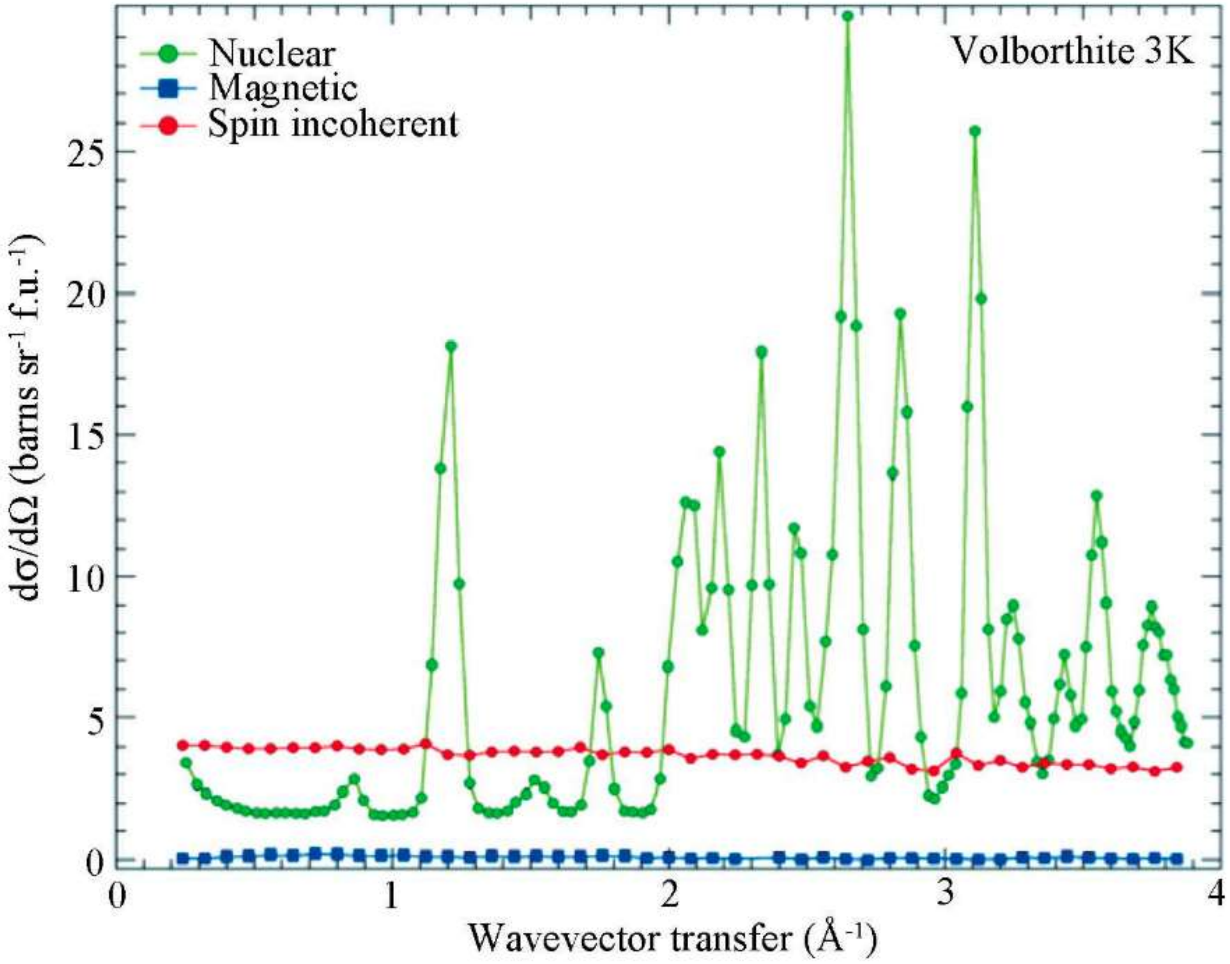
can take the average of these

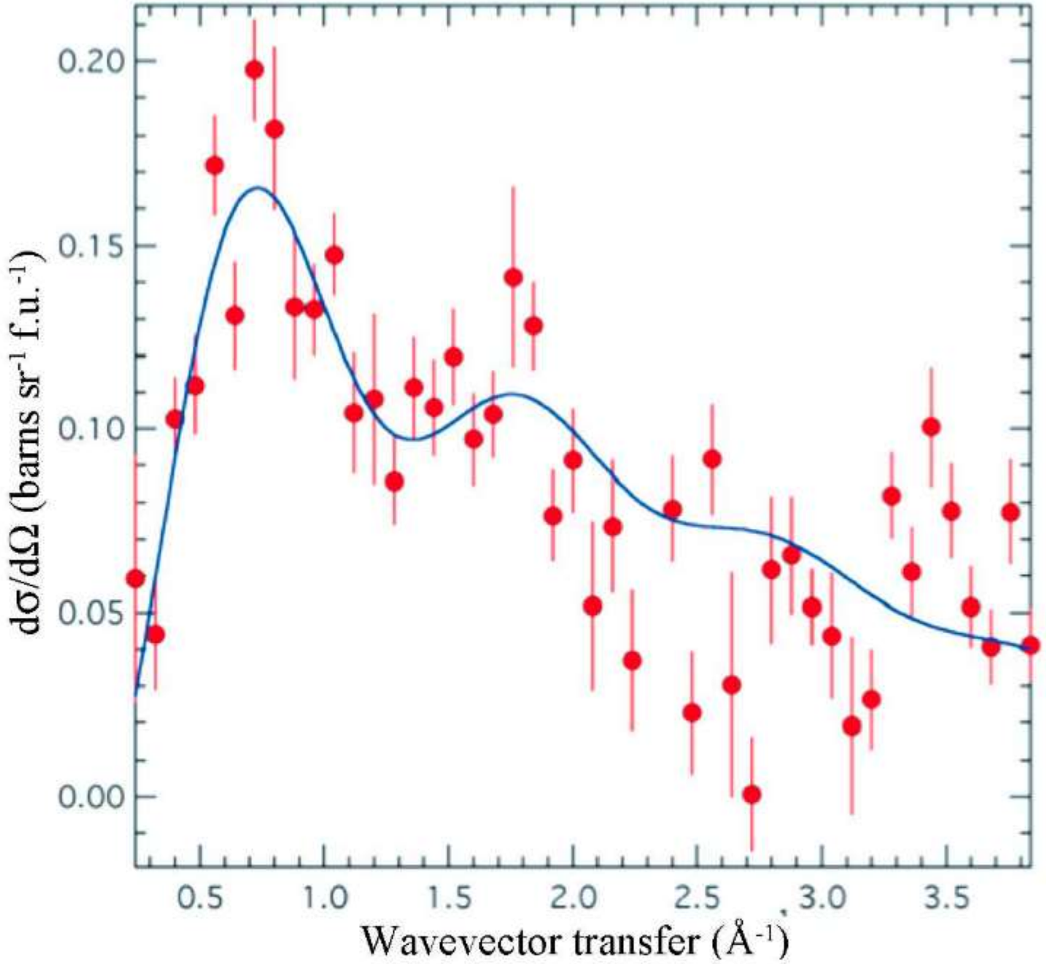
Spin-incoherent scattering

$$\left(\frac{d\sigma}{d\Omega}\right)_{\mathrm{SI}} = \frac{1}{2}\left(\frac{d\sigma}{d\Omega}\right)^{\mathrm{TSF}} - \left(\frac{d\sigma}{d\Omega}\right)_{\mathrm{mag}}$$

Stewart, et al., *J. Appl. Phys* **42**, 69 (2009)

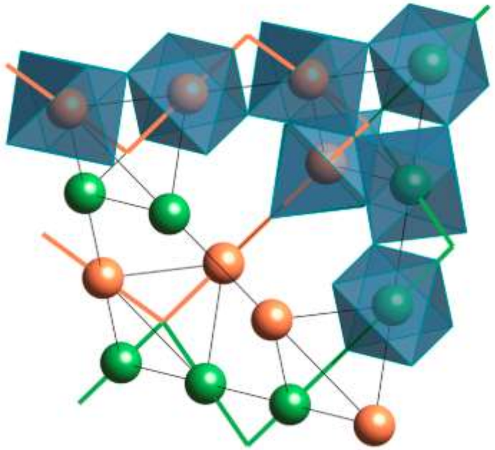
Why is this necessary?



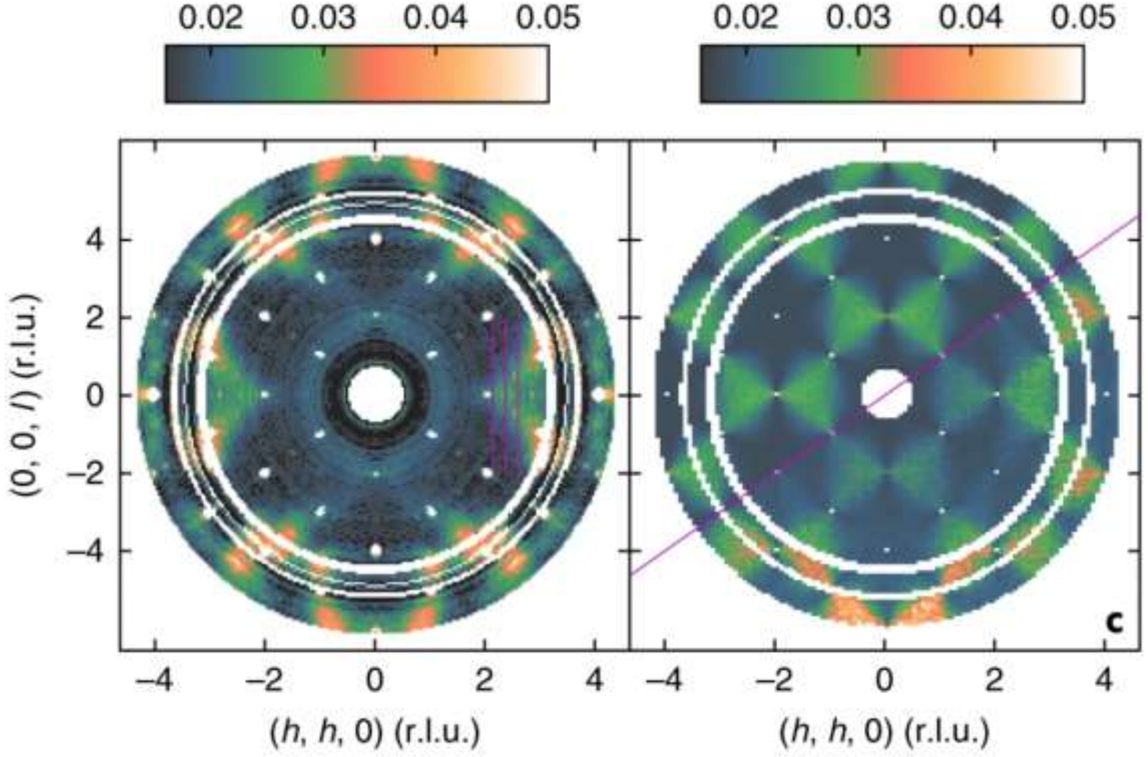


Fennell, et al., *Nature Phys.* **15** (2019) 60-66

Example 5 – correlated disorder in $CsNiCrF_6$

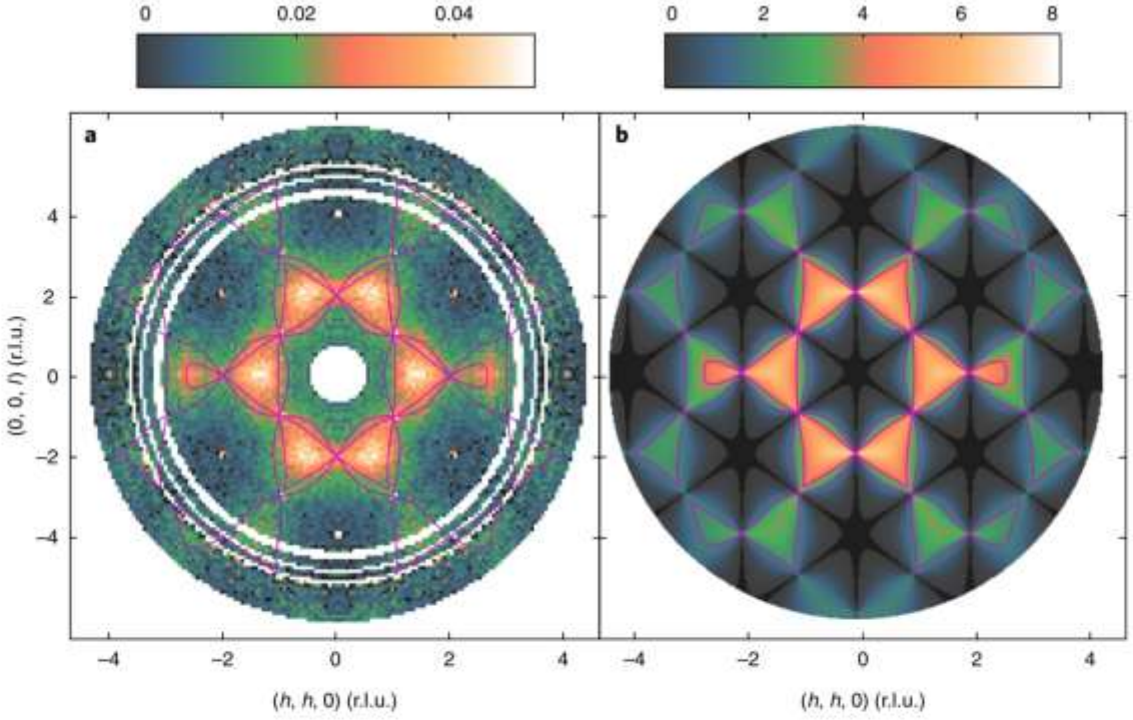


Nuclear scattering



Experiment Calculation

Magnetic scattering



Experiment Calculation

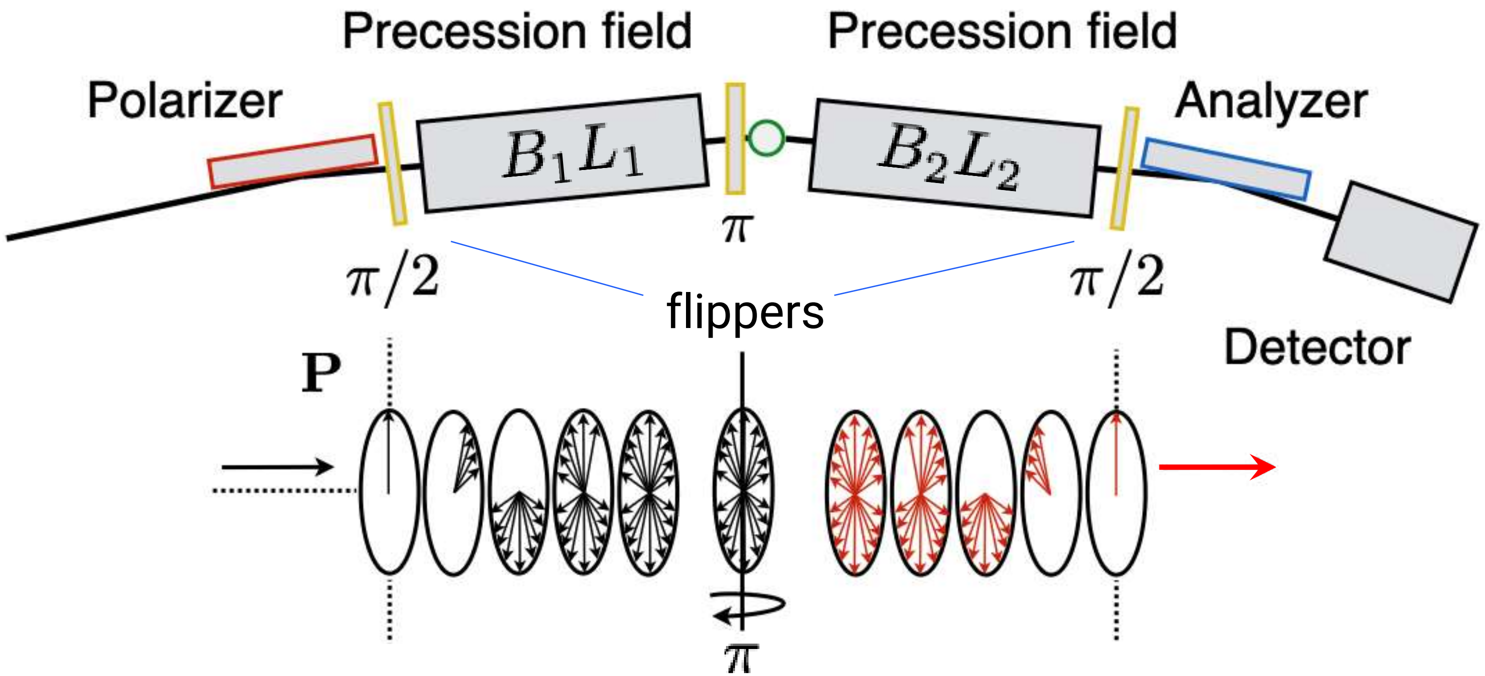
Reminder – Rules for Polarized Neutron Scattering

1. The nuclear coherent and isotope incoherent scattering is always NSF

2. The spin-incoherent scattering is always 1/3 NSF and 2/3 SF

3. Magnetism: must be in a direction perpendicular to $\vec{Q}$ and:
   - NSF if parallel to $\vec{P}$
   - SF if perpendicular to $\vec{P}$

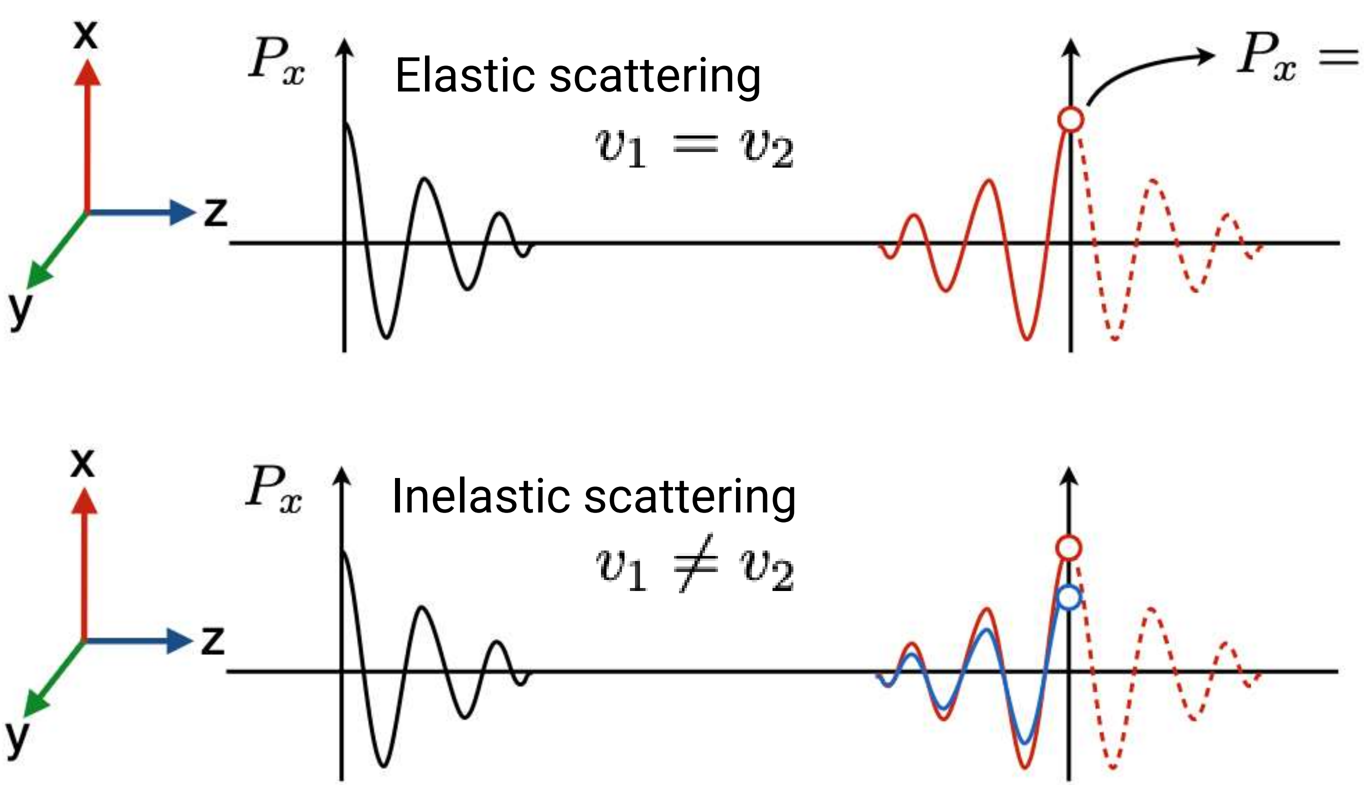
Neutron Spin-Echo

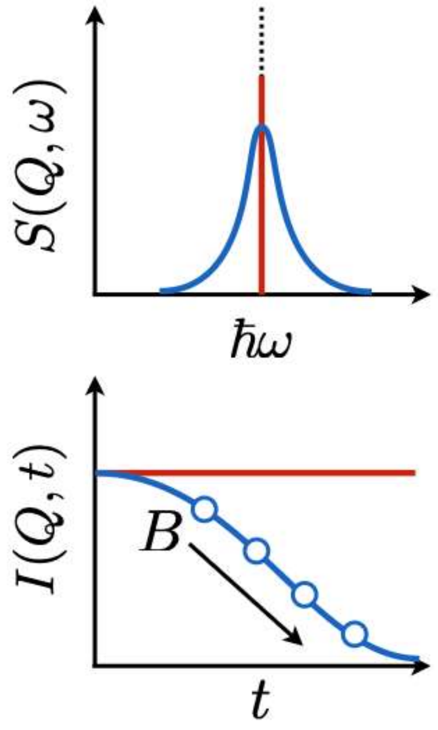


Number of radians precessed in each arm: $\phi_L = \omega t = \omega \times \frac{L}{v} = \frac{\gamma BL}{v}$

If $B_1L_1 = B_2L_2$, and $v_1 = v_2$ then the neutron spins will all re-align: $\Delta\phi_L = \frac{\gamma B_1L_1}{v_1} - \frac{\gamma B_2L_2}{v_2} = 0$

Neutron Spin-Echo





(assumes that the sample doesn't depolarize the beam)

NSE Resolution – Spin-Echo Time

Neutron energy is $E = \frac{1}{2} m_n v^2 \Rightarrow \Delta E = m_n v \Delta v$

In NSE we measure a phase shift $\phi = \frac{\gamma BL}{v} \Rightarrow \Delta\phi = \frac{\gamma BL}{v^2}\Delta v = \frac{\gamma BL \Delta E}{m_n v^3}$

Since we know that $\Delta E = \hbar\omega$ and that the phase shift $\phi = \omega t$ we can identify the Spin-Echo time

$$t = \frac{\gamma BL\hbar}{m_n v^3} = \frac{\gamma BL m_n^2 \lambda^3}{2\pi h^2}$$

Putting in numbers: $BL = 0.27$ Tm on WASP at ILL, and $\lambda = 1$ nm we find a Spin-Echo time, $t = 18$ ns

This is equivalent to $\omega = 2\pi/t = 0.35$ GHz, or 0.08 µeV

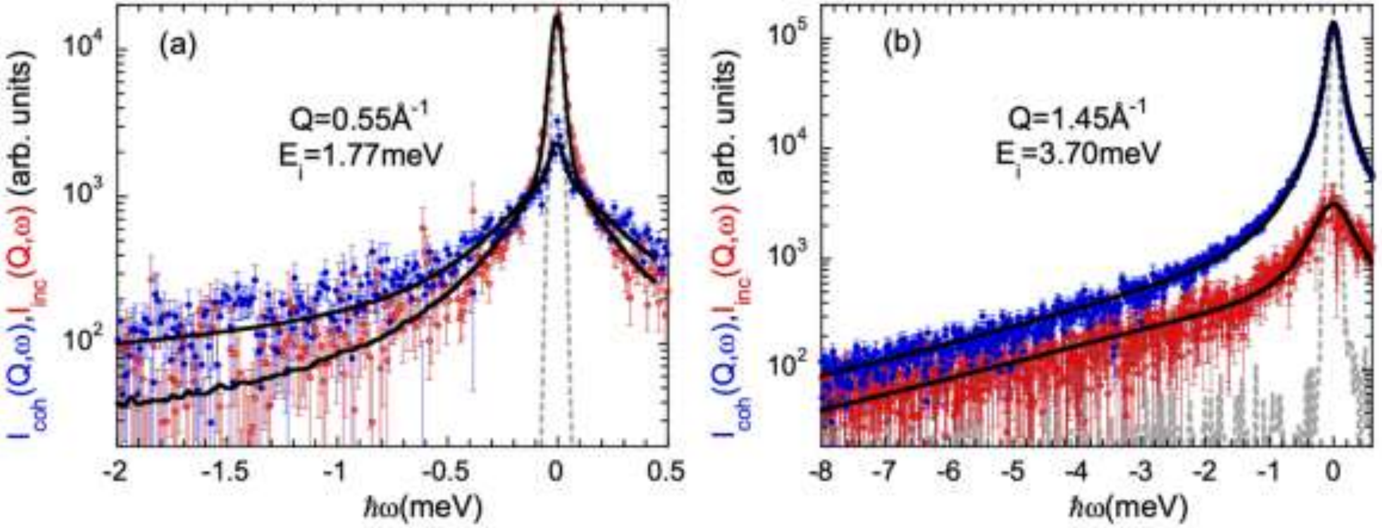
Much higher energy resolution than on a conventional spectrometer

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

Example 6 – dynamics in van der Waals liquid

Tetrahydrofuran – THF, C_4H_8O

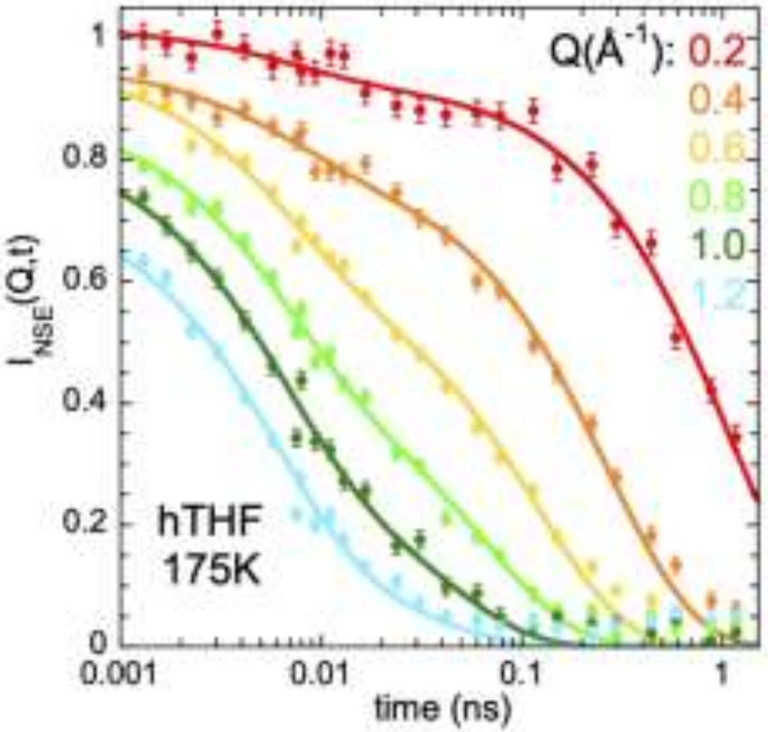
LET at ISIS



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

Take-home message

Polarized neutrons can be used to enhance almost any neutron scattering experiment, either by

1. Separating and providing additional information on the **sources of scattering** (nuclear, magnetic, incoherent)

2. Improving the **resolution**