Oak Ridge National Laboratory

Neutron Polarization

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Scope of this lesson

Yes! Utilizing polarized neutrons to *distinguish* different aspects or dimensions (contrast and character) of the "unpolarized" neutron scattering

Just a taste…*Enhance resolution* via Larmor precession of the polarized neutron before and/or after sample

Not in this school: Using polarized neutrons to better understand the *physics of the neutron* itself

Polarization Analysis is NOT a single technique.

You'll learn about several 'configurations' which access and isolate different kinds of intensity variations and concurrent spin reorientations.

A “neutron” by any other name…

Neutrons are NOT neutral

- Doesn’t the term “neutron” imply neutral everything?
  - Electric neutrality, yes
    - Neutrons ignore charge of electrons and protons in atoms
    - Penetrating power!
  - Pesky quarks
    - Neutron **spin**
      - Affects “strong force” interaction
    - Neutron **magnetic dipole moment**
      - Affects magnetic interaction

Spin:
$\sigma_n = ½$

Dipole moment:
$\mu_n = -1.913\ \mu_N$

Nuclear magneton:
$\mu_N = 5.051E-27\ \mathrm{JT}^{-1}$

Which way is ‘up’?
Depends on what you’re using…
Did we really put these on the same diagram with totally different units?
Yes, yes we did…

Now in 3D!

Polarized neutrons might help your research

Science areas (*no, really! Yours, too*)

- Biology
- Soft matter & Polymers
- Materials & Engineering
- Condensed matter & Quantum materials
- Chemistry
- Geology
- Environmental Science

Examples in
mini poster session!

Neutron Scattering Technique (*Instrument*)

- Diffraction
- SANS
- Reflectometry
- Spectroscopy
- Imaging

Instruments with
polarization in
mini poster session!

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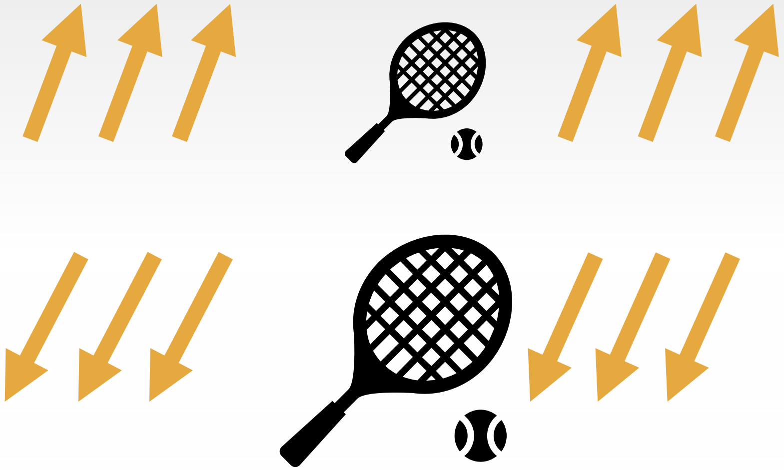
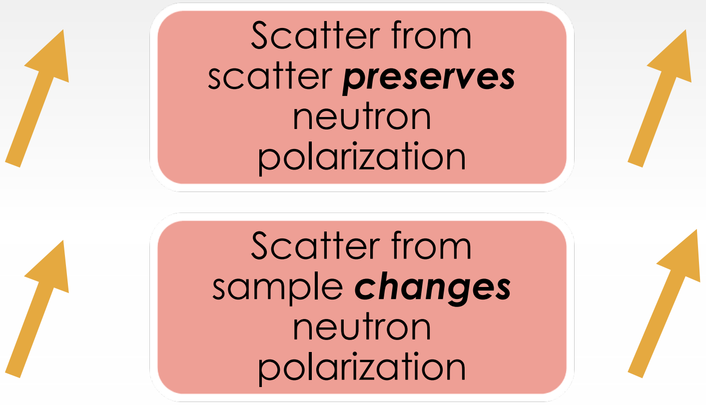
Changes depend on polarization of incident beam

Changes in Scattered Neutron Intensity



Changes in Neutron Polarization State



Key Questions you need to be asking

Q1

Can polarized neutrons help my science?

Not easy to answer. Not just a single Application!

In this presentation we provide a framework for figuring this out

Q2

Are polarized neutrons needed?

Alternative, unpolarized ways to answer same thing?

Q3

Reality check?

A. Available with scattering technique?
B. Time and statistics due to (usually) reduced signal and (often) multiple measurements?
   i. Problematic on high throughput instruments
C. Complications of polarized optics (compatibility with sample conditions, corrections to data, etc.)
D. Ease of reaching results (software tailored for polarization)

Depends on state-of-art, and what's available where

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Q2 Are polarized neutrons needed?

Overlapping information?

- Structure & dynamics in many size and energy scales
  - Sometimes, both at once!
- Nuclei spin-state specific
- Isotope-specific
- Magnetism
- Coherent interference *between* nuclear and magnetic terms!?!

One person's trash is another's treasure

- The lack of coherence of hydrogen scattering makes finding some Bragg peaks *near-impossible*… but that same incoherent scattering is *perfect* for measuring energies of various modes for chemistry

Unclear on directional aspects of your material?

- Even if all your scattering is magnetic, maybe the moments on different atoms point in different directions with different strengths; polarized neutrons can help!

(usually) distinguish even with 'unpolarized' scattering

- Expecting only one kind of scattering
  - Based on system studied
  - Based on where scattering is observed
    - Low momentum transfer Q: magnetic
    - High momentum transfer Q: weak
  - Based on thermodynamic conditions
    - Phase changes (magnetism below T_n…)
    - Compare / contrast / subtract strategies
- MOST neutron scattering experiments leverage unpolarized neutrons!
- But, sometimes, we need to tease contributions apart

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Q1 Clues to how experimentalists utilize polarized neutrons

Somewhere hidden in each publication is a statement that answers this question

- Accounts for the system / material being studied
- Identifies a specific 'capability' leveraging polarized neutron scattering

How to find this statement?

- Find the polarized neutron figure, backtrack to the the text where that figure is referenced, and *voila*!

Sometimes even more context

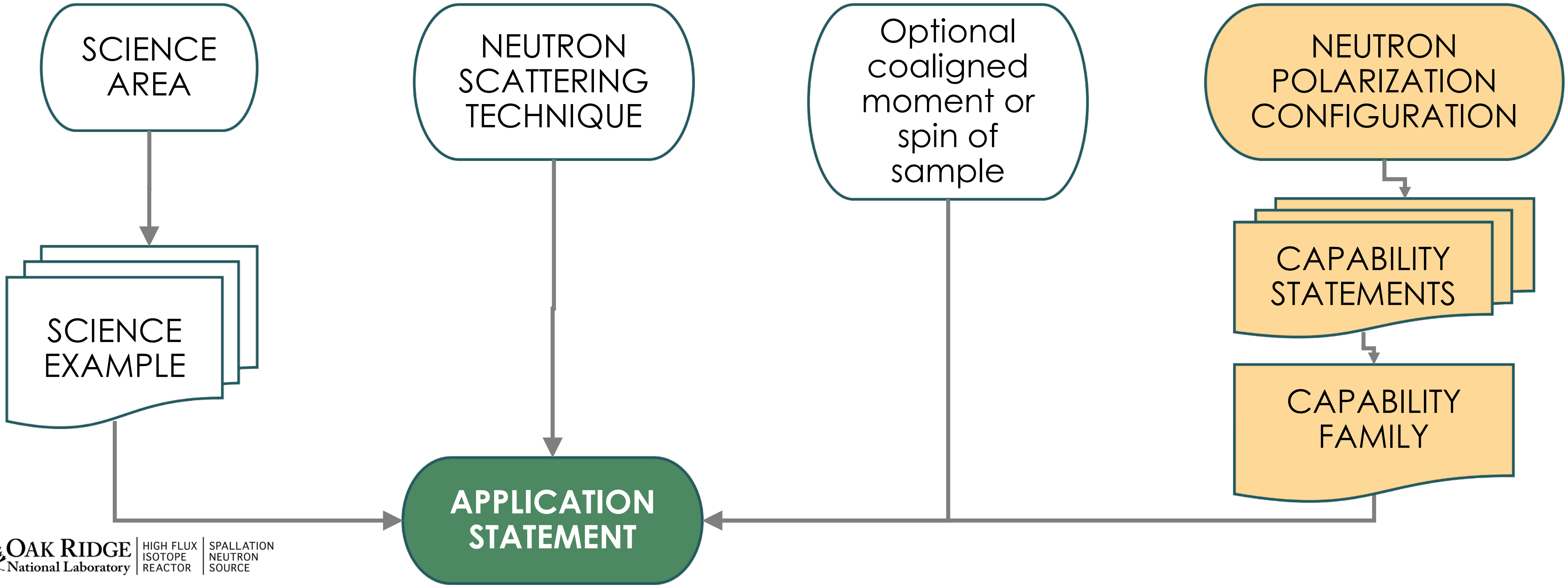
- Often find introductory / explanatory text about polarized neutrons, despite 60-year history

Examples of papers and application statements in mini poster session!

Polarization application statement

Q1 Ingredients for your 'polarized' application statement

As a [***SCIENCE AREA***] neutron scattering experimentalist, I want to [***NEUTRON SCATTERING TECHNIQUE***] so I can [***APPLICATION statement***] for [***SCIENCE EXAMPLE***]



Combine neutron scattering *contrast* and *character*

Reciprocal space ↔ Real space

$N(\mathbf{Q}) = \sum_n b_n e^{i\mathbf{Q}\cdot\mathbf{R}_n}$	Nuclear structure factor
$\mathbf{M}(\mathbf{Q}) = \sum_n \mathbf{M}_n e^{i\mathbf{Q}\cdot\mathbf{R}_n}$	Fourier transform of magnetic moments / magnetic structure factor

	Incoherent	Coherent	Absorption
Spin / Nuclear	I_N & I_S ⇔	$N(\mathbf{Q}, E)$	σ_{abs}
Magnetic	☹	$\mathbf{M}(\mathbf{Q}, E)$	☹

Vector convention: boldface $\mathbf{Q}$ instead of $\vec{Q}$

Absorption never measured in scattered signal

Meet the "Vector" family

$\overrightarrow{\boldsymbol{R_n}}$		Coordinates of one atom in unit cell for crystal	Real space
$\overrightarrow{\boldsymbol{M_n}}$		Which way and how strong a magnetic moment of an *ATOM* points	
$\vec{\boldsymbol{P}}$	Polarization	A measure of how 'polarized' the incident beam is, and average orientation of those neutrons' spin (or magnetic moment) at sample position $\vec{P} = 2\langle\overrightarrow{\sigma_s}\rangle$	
$\overrightarrow{\boldsymbol{P^1}}$		The new polarization of the scattered neutrons	
$\vec{\boldsymbol{Q}}$	Momentum transfer	Incident neutron momentum minus final neutron momentum $\overrightarrow{\boldsymbol{Q_{lab}}} = \overrightarrow{\boldsymbol{k_i}} - \overrightarrow{\boldsymbol{k_f}}$	Reciprocal space
$\overrightarrow{\boldsymbol{M(Q)}}$	Magnetic structure factor	Fourier transform of $\overrightarrow{\boldsymbol{M_n}}$	
$\overrightarrow{\boldsymbol{M_\perp}}$	"M perp"	The component of the Magnetic structure factor perpendicular to the momentum transfer $\vec{\boldsymbol{Q}}$	

Polarization Configurations access Intensity and/or *Polarization State*

$N(\boldsymbol{Q}) = \sum_n b_n e^{i\boldsymbol{Q}\cdot\boldsymbol{R}_n}$	Nuclear structure factor
$\boldsymbol{M}_\perp = \boldsymbol{e_Q} \times \boldsymbol{M}(\boldsymbol{Q}) \times \boldsymbol{e_Q}$	"M perpendicular"
$\boldsymbol{M}(\boldsymbol{Q}) = \sum_n \boldsymbol{M}_n e^{i\boldsymbol{Q}\cdot\boldsymbol{R}_n}$	Fourier transform of magnetic moments / magnetic structure factor
$\boldsymbol{e_Q} = \boldsymbol{Q}/\lvert\boldsymbol{Q}\rvert$	Unit vector along momentum transfer **Q**
I_{si}	Spin incoherent scattered intensity
$\boldsymbol{P}, \boldsymbol{P}'$	Initial and final polarization

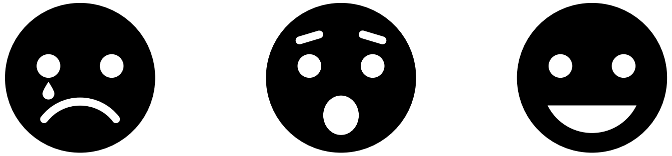
POLARIZATION CONFIGURATION	Impacts the scattered neutron	Optics
Half Polarized Dynamic Nuclear Polarization Solve Phase Problem	Intensity	1 filter 1 flipper
Longitudinal Analysis I Larmor	Polarization State	2 filters 1 flipper
Longitudinal Analysis II Spherical Neutron Polarimetry	Both	2 filters 2 flippers

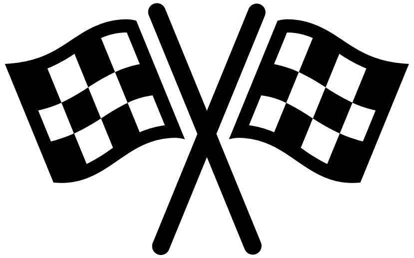
$$I = I_n + N^\dagger N + I_{si} + \boldsymbol{M}_\perp^\dagger \boldsymbol{M}_\perp + \boldsymbol{P}\cdot\boldsymbol{M}_\perp^\dagger N + \boldsymbol{P}\cdot\boldsymbol{M}_\perp N^\dagger + i\boldsymbol{P}\cdot\left(\boldsymbol{M}_\perp^\dagger \times \boldsymbol{M}_\perp\right)$$

$$\boldsymbol{P}'I = \boldsymbol{P}\left(I_n + N^\dagger N - \frac{1}{3}I_{si}\right) + (\boldsymbol{P}\cdot\boldsymbol{M}_\perp^\dagger)\boldsymbol{M}_\perp + (\boldsymbol{P}\cdot\boldsymbol{M}_\perp)\boldsymbol{M}_\perp^\dagger - \boldsymbol{P}\left(\boldsymbol{M}_\perp^\dagger\boldsymbol{M}_\perp\right) + iN\left(\boldsymbol{P}\times\boldsymbol{M}_\perp^\dagger\right) - iN^\dagger(\boldsymbol{P}\times\boldsymbol{M}_\perp) + N\boldsymbol{M}_\perp^\dagger + N^\dagger\boldsymbol{M}_\perp - i\left(\boldsymbol{M}_\perp^\dagger\times\boldsymbol{M}_\perp\right)$$

[1]S. V. **Maleev,** V. G. Bar'yaktar, and R. A. Suris, The scattering of slow neutrons by complex magnetic structures Sov. Phys. Solid State 4, 2533 (1963)
[2]M. **Blume**, Polarization effects in the magnetic elastic scattering of slow neutrons, Phys. Rev. 130, 1670 (1963).

Yes, the Maleev-Blume equations are VERY busy





- Leverage *personality flaw* found in some scientists
  A. *Make assumptions* about the system you are studying
  B. Eliminate terms
  C. Simplify / Streamline the math

- Linear algebra
  - *N* equations & *N* unknowns → solvable problem
- Let’s call the solutions to the streamlined equations “Capabilities”
  - Think word problems in reverse…

Configurations, Capabilities and Capability Families

- "Configurations"
  - Combine specific polarization optics
  - Access different Maleev-Blume equations
- "Capabilities" are specific solutions to streamlined Linear algebra problems
  - Assume certain terms in Maleev-Blume equations aren't present
  - Vector: Polarization-state 'equation' is really several equations
- "Capability families" are intuitive groupings of those specific solutions

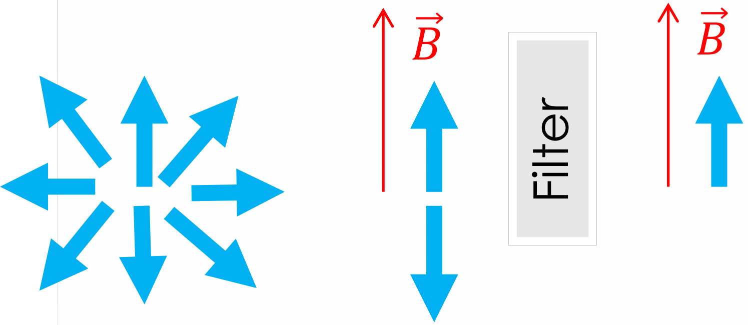
Capability Families

Isolate nuclear scattering	N & I_N
Isolate spin-incoherent scattering	I_{si}
Leverage dynamic nuclear polarization	$N \leftrightarrow I_{si}$
Solve Phase Problem	N & $\boldsymbol{M}_\perp$
Explore magnetic scattering	$\boldsymbol{M}_\perp$
Explore coinciding of nuclear and magnetic scattering	N with $\boldsymbol{M}_\perp$
Explore magnetic chirality	$\boldsymbol{M}_\perp$ cross terms

Polarization optics: ingredients for P. Configurations

Filters

- 'Quantum' has its advantages…
  - Unpolarized classical has arrows pointing everywhere
  - In ambient field, though, a quantum superposition of 'up' & 'down'
  - A filter can achieve up to* 50% transmission



*Actual transmission varies widely…

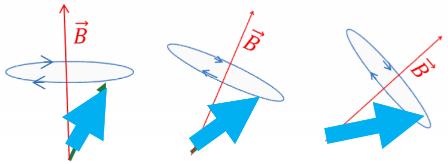
Guide fields and nutators

- Larmor precession, via torque $\vec{\tau}$ on neutron magnetic moment $\vec{\mu}$ by applied magnetic field $\vec{B}$

$$\vec{\tau} = \vec{\mu} \times \vec{B},\ \omega = -\gamma B$$

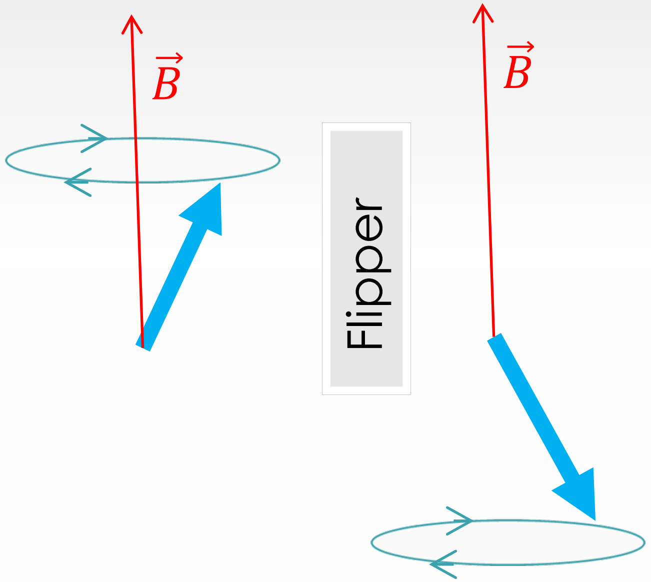
γ = -1.833E4 rad/Gauss-sec

- Frequency ω is INDEPENDENT of polar angle φ between applied field and moment
- Magnetic 'guide' fields keep $\vec{\mu}$ either aligned or anti-aligned with respect to $\vec{B}$
  - Keeps ω fast while changing direction of $\vec{B}$ slowly



Flippers

- Optionally invert the neutron spin-state with respect to the ambient guide field

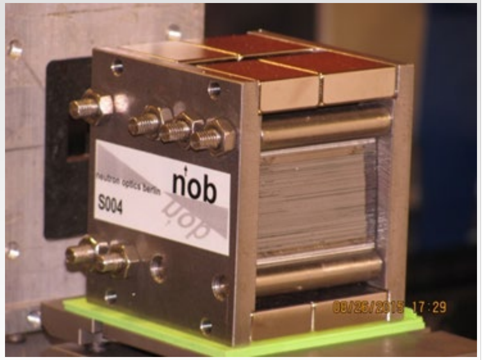


Polarization optics: ingredients for P. Configurations

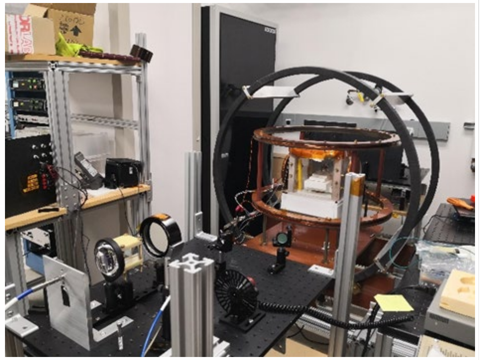
Filters

Heusler crystal

Polarizing Supermirror



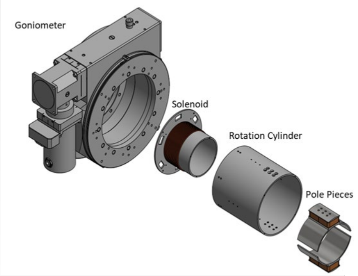
Nuclear-polarized ^{3}He



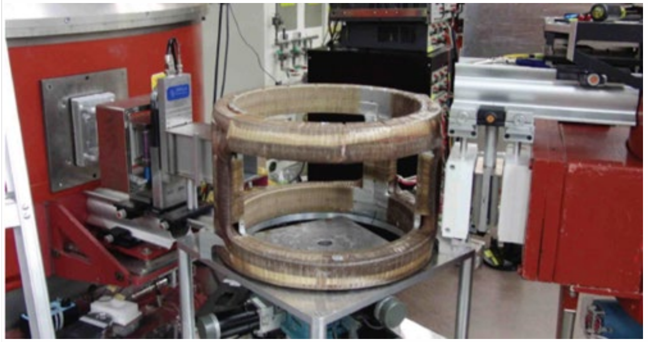
Guide fields and nutators

Permanent Magnet Yoked Assemblies

Rotatable nutator

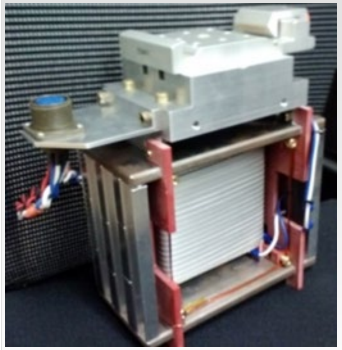


3D Coils



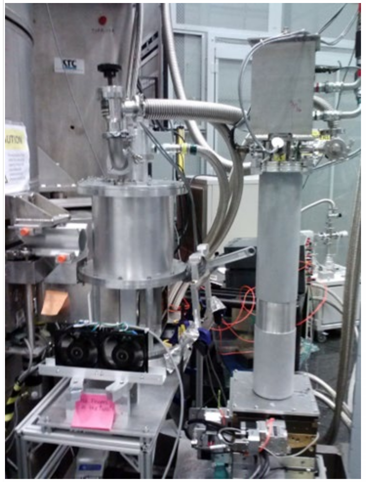
Flippers

Mezei



Radio-Frequency

Cryogenic (Meissner screen)

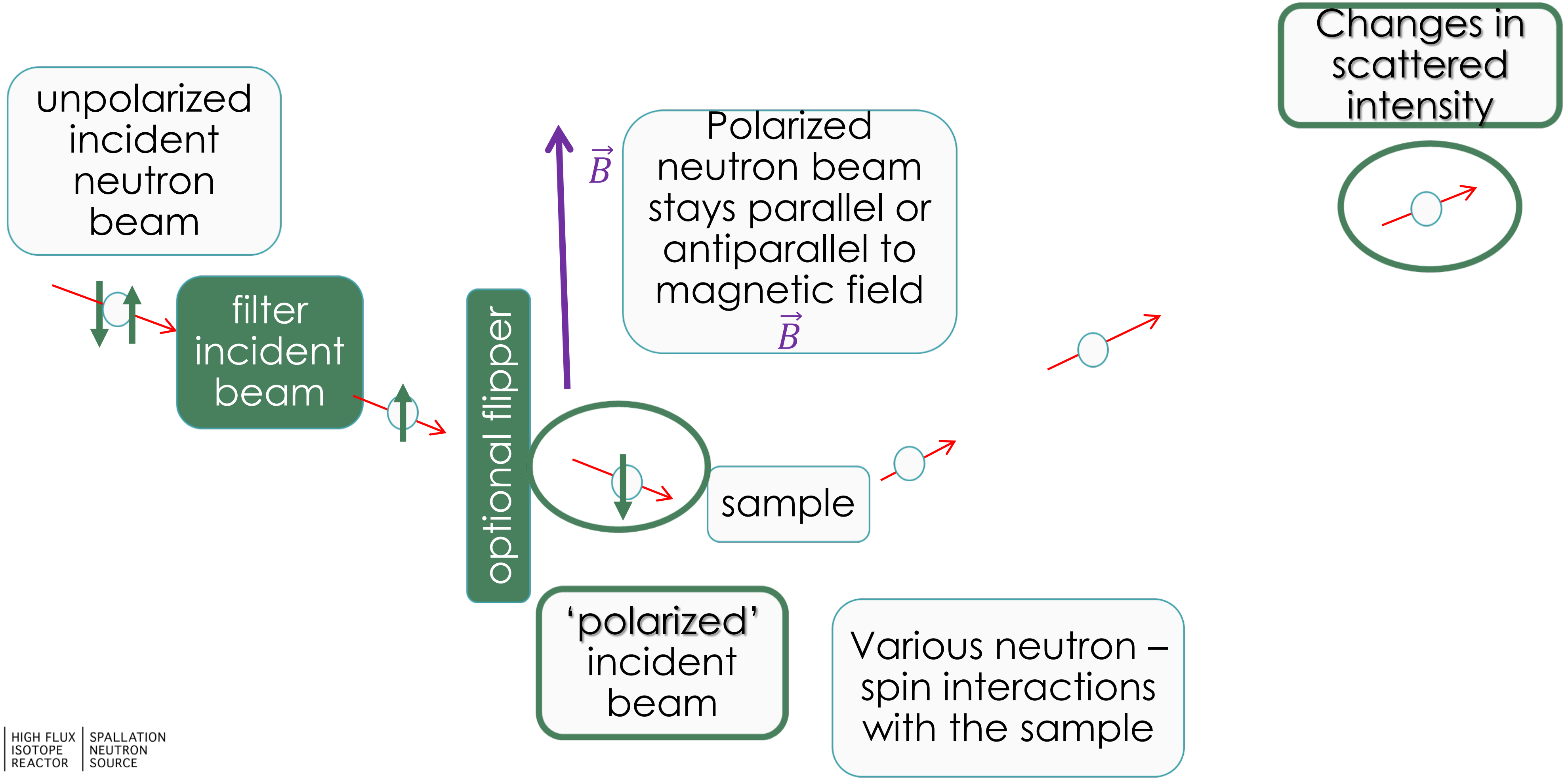


Adiabatic Fast Passage /w ^{3}He

Configuration: Half Polarized

$$I = N^{\dagger}N + I_{si} + \boldsymbol{M}_{\perp}^{\dagger}\boldsymbol{M}_{\perp} + \boldsymbol{P}\cdot\boldsymbol{M}_{\perp}^{\dagger}N + \boldsymbol{P}\cdot\boldsymbol{M}_{\perp}N^{\dagger} + i\boldsymbol{P}\cdot\left(\boldsymbol{M}_{\perp}^{\dagger}\times\boldsymbol{M}_{\perp}\right)$$

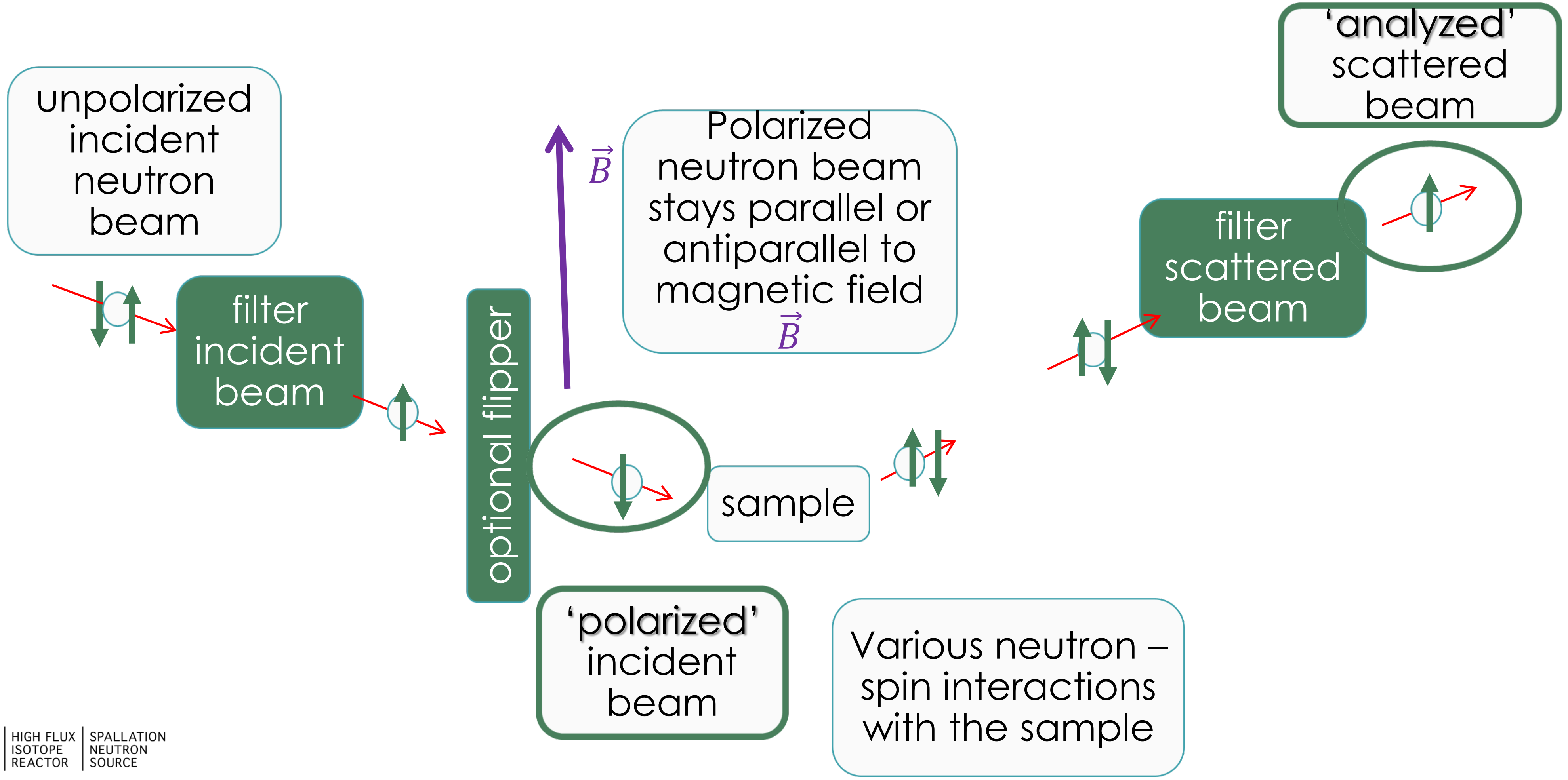
$$\boldsymbol{P}^{\prime}I = \boldsymbol{P}\left(N^{\dagger}N - \frac{1}{3}I_{si}\right) + (\boldsymbol{P}\cdot\boldsymbol{M}_{\perp}^{\dagger})\boldsymbol{M}_{\perp} + (\boldsymbol{P}\cdot\boldsymbol{M}_{\perp})\boldsymbol{M}_{\perp}^{\dagger} - \boldsymbol{P}(\boldsymbol{M}_{\perp}^{\dagger}\boldsymbol{M}_{\perp}) + iN(\boldsymbol{P}\times\boldsymbol{M}_{\perp}^{\dagger}) - iN^{\dagger}(\boldsymbol{P}\times\boldsymbol{M}_{\perp}) + N\boldsymbol{M}_{\perp}^{\dagger} + N^{\dagger}\boldsymbol{M}_{\perp} - i(\boldsymbol{M}_{\perp}^{\dagger}\times\boldsymbol{M}_{\perp})$$



Configuration: Longitudinal 1

$$I = N^{\dagger}N + I_{si} + \boldsymbol{M}_{\perp}^{\dagger}\boldsymbol{M}_{\perp} + \boldsymbol{P}\cdot\boldsymbol{M}_{\perp}^{\dagger}N + \boldsymbol{P}\cdot\boldsymbol{M}_{\perp}N^{\dagger} + i\boldsymbol{P}\cdot\left(\boldsymbol{M}_{\perp}^{\dagger}\times\boldsymbol{M}_{\perp}\right)$$

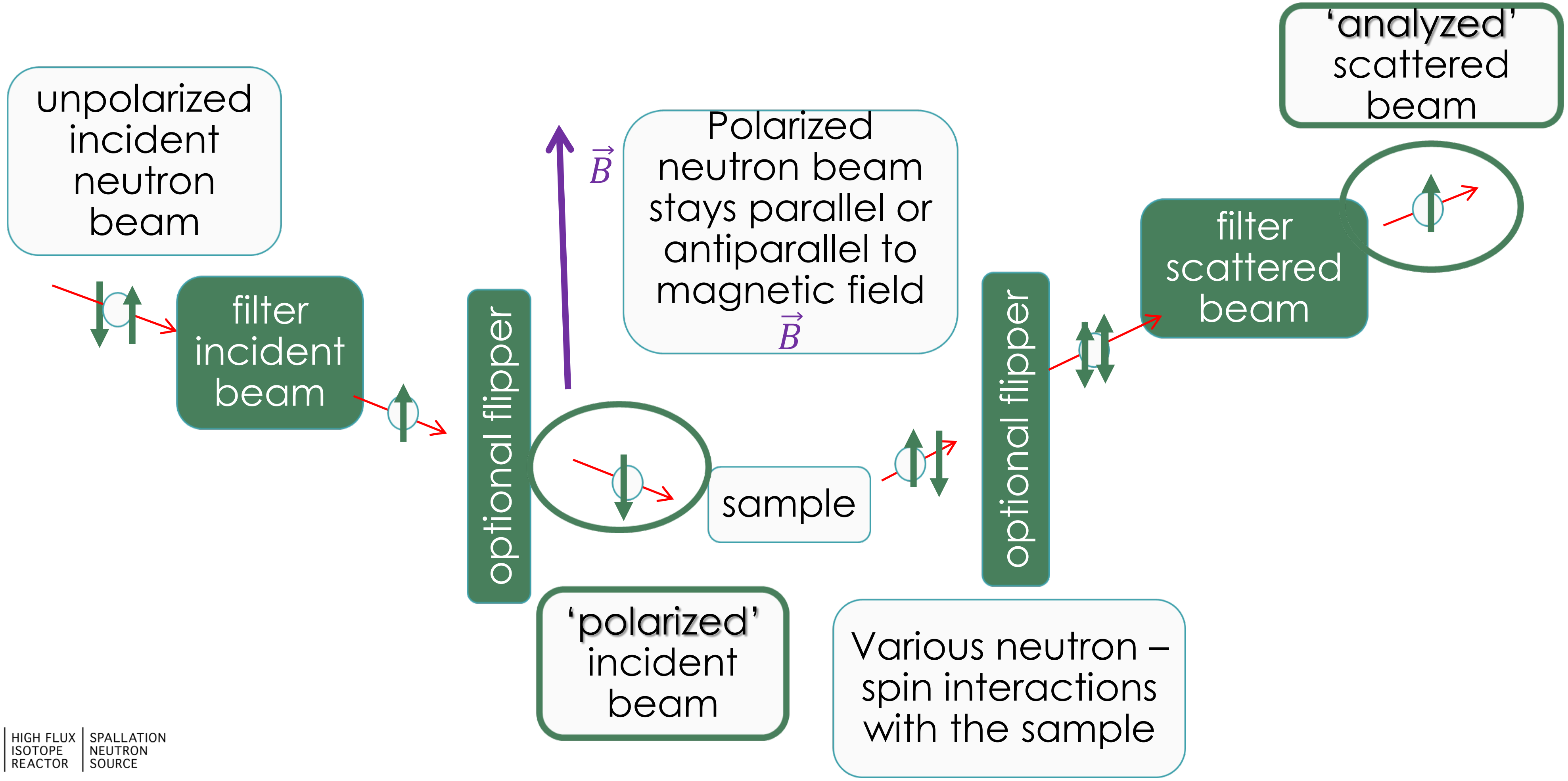
$$\boldsymbol{P}'I = \boldsymbol{P}\left(N^{\dagger}N - \frac{1}{3}I_{si}\right) + (\boldsymbol{P}\cdot\boldsymbol{M}_{\perp}^{\dagger})\boldsymbol{M}_{\perp} + (\boldsymbol{P}\cdot\boldsymbol{M}_{\perp})\boldsymbol{M}_{\perp}^{\dagger} - \boldsymbol{P}(\boldsymbol{M}_{\perp}^{\dagger}\boldsymbol{M}_{\perp}) + iN(\boldsymbol{P}\times\boldsymbol{M}_{\perp}^{\dagger}) - iN^{\dagger}(\boldsymbol{P}\times\boldsymbol{M}_{\perp}) + N\boldsymbol{M}_{\perp}^{\dagger} + N^{\dagger}\boldsymbol{M}_{\perp} - i(\boldsymbol{M}_{\perp}^{\dagger}\times\boldsymbol{M}_{\perp})$$



Configuration: Longitudinal 2

$$I = N^{\dagger}N + I_{si} + \boldsymbol{M}_{\perp}^{\dagger}\boldsymbol{M}_{\perp} + \boldsymbol{P}\cdot\boldsymbol{M}_{\perp}^{\dagger}N + \boldsymbol{P}\cdot\boldsymbol{M}_{\perp}N^{\dagger} + i\boldsymbol{P}\cdot\left(\boldsymbol{M}_{\perp}^{\dagger}\times\boldsymbol{M}_{\perp}\right)$$

$$\boldsymbol{P}'I = \boldsymbol{P}\left(N^{\dagger}N - \frac{1}{3}I_{si}\right) + (\boldsymbol{P}\cdot\boldsymbol{M}_{\perp}^{\dagger})\boldsymbol{M}_{\perp} + (\boldsymbol{P}\cdot\boldsymbol{M}_{\perp})\boldsymbol{M}_{\perp}^{\dagger} - \boldsymbol{P}(\boldsymbol{M}_{\perp}^{\dagger}\boldsymbol{M}_{\perp}) + iN(\boldsymbol{P}\times\boldsymbol{M}_{\perp}^{\dagger}) - iN^{\dagger}(\boldsymbol{P}\times\boldsymbol{M}_{\perp}) + N\boldsymbol{M}_{\perp}^{\dagger} + N^{\dagger}\boldsymbol{M}_{\perp} - i(\boldsymbol{M}_{\perp}^{\dagger}\times\boldsymbol{M}_{\perp})$$



Complementarity between polarized neutron scattering -&- X-ray magnetic circular dichroism

- In addition to the other pro's & con's comparing neutrons & x-rays…

Polarized neutrons	X-ray dichroism
polarized diffraction goes beyond element specificity to lattice-site-specific moment measurements	Element specificity near absorption edges, & small sample sensitivity due to resonant enhancement
Not element specific in general when it comes to magnetism	Access to magnetism when x-rays excite an electron that contributes to magnetism (transition metals –d electrons →L x-ray edges)
Relatively direct measurement of magnetism	Calculation gymnastics
Indirectly could leverage neutron isotope specificity, possibly with coherent interference effects	Potentially separate magnetism into orbital and spin moments

See Poster after this lecture

Coming at neutron spin from another angle…

- Enhanced resolution via Larmor techniques
  - Enhanced diffraction
  - Enhanced spectroscopy
  - Enhanced in weird directions in Q-E space

How to prepare for a polarized neutron experiment

- Reach out to polarized instrument staff
  - For help preparing your ‘polarization application statement’
  - For identifying configuration
  - For differences compared to unpolarized experiments (longer, increased # of measurements, etc.)
  - For preparing your proposal
  - For sample preparation (may need a smaller sample, well centered, etc.)

Explore further during NXS

Demonstration experiment **N2** leverages the **Longitudinal 1** configuration at HYSPEC

Demonstration experiment **N20** leverages the **Longitudinal 2** configuration at the Magnetism Reflectometer

For future reading

- Several dissertations
  - See instrument-specific publication lists
- Various online slide decks and tutorials
  - Kathryn Krycka, 'Neutron Polarization' slides & video at https://neutrons.ornl.gov/nxs/2021/lectures
  - Ross Stewart, https://www.oxfordneutronschool.org/2011/lectures/osns_stewart_polarised_2011.pdf
  - Werner Schweika, https://juser.fz-juelich.de/record/20415/files/C6_Schweika.pdf
- Books / chapters
  - Tapan Chatterji (ed.), *Neutron Scattering from Magnetic Materials* (2006) / several chapters
  - Stephen W Lovesey, *Theory of Neutorn Scatteirng from Condensed Matter V2* (1984) / ch 10
  - G. Shirane, SM Shapiro, JM Tranquada, *Neutron Scattering with a Triple Axis Spectrometer* (2002) / ch 8

Active development and community

- Semi annual meetings / proceedings of PNCMI (polarized neutrons for condensed matter investigations)
  - Proceedings from 2016: https://iopscience.iop.org/issue/1742-6596/862/1
  - Proceedings from 2018: https://iopscience.iop.org/issue/1742-6596/1316/1
  - Proceedings from 2022: https://iopscience.iop.org/issue/1742-6596/2481/1
- Aspirations & new directions at ORNL & NCNR
  - Just ask!
- Actively building user community via training workshops

Conclusion

Now go out to the poster session and discover how your specific research might benefit!