OAK RIDGE National Laboratory | HIGH FLUX ISOTOPE REACTOR

Sept 10, 2025, 11 AM - 12 PM

Neutron Polarization (Contrast)

Barry Winn, NNS 2025

AND AN ARMY OF POSTER PRESENTERS!!!!

U.S. DEPARTMENT OF ENERGY

ORNL IS MANAGED BY UT-BATTELLE LLC
FOR THE US DEPARTMENT OF ENERGY

Polarized neutron scattering enables a researcher to answer important questions related to either the nuclear spin or magnetism in materials

Character

Contrast

Configuration

Capability

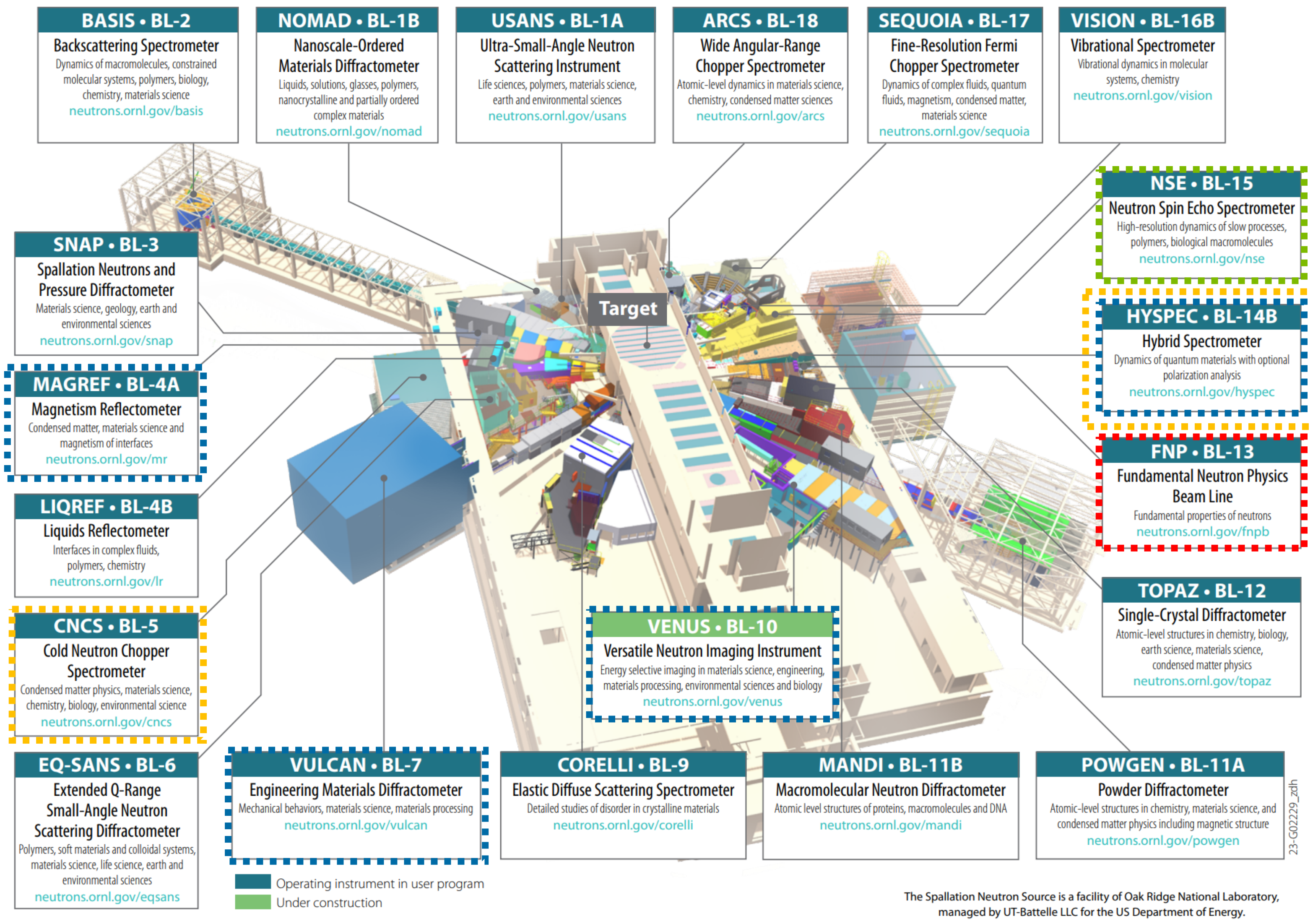
Who uses polarized neutrons at SNS?

Magnetic Moment Contrast

Nuclear Spin Contrast

Enhanced Resolution via ‘Larmor’ Techniques

Studies of the neutron itself

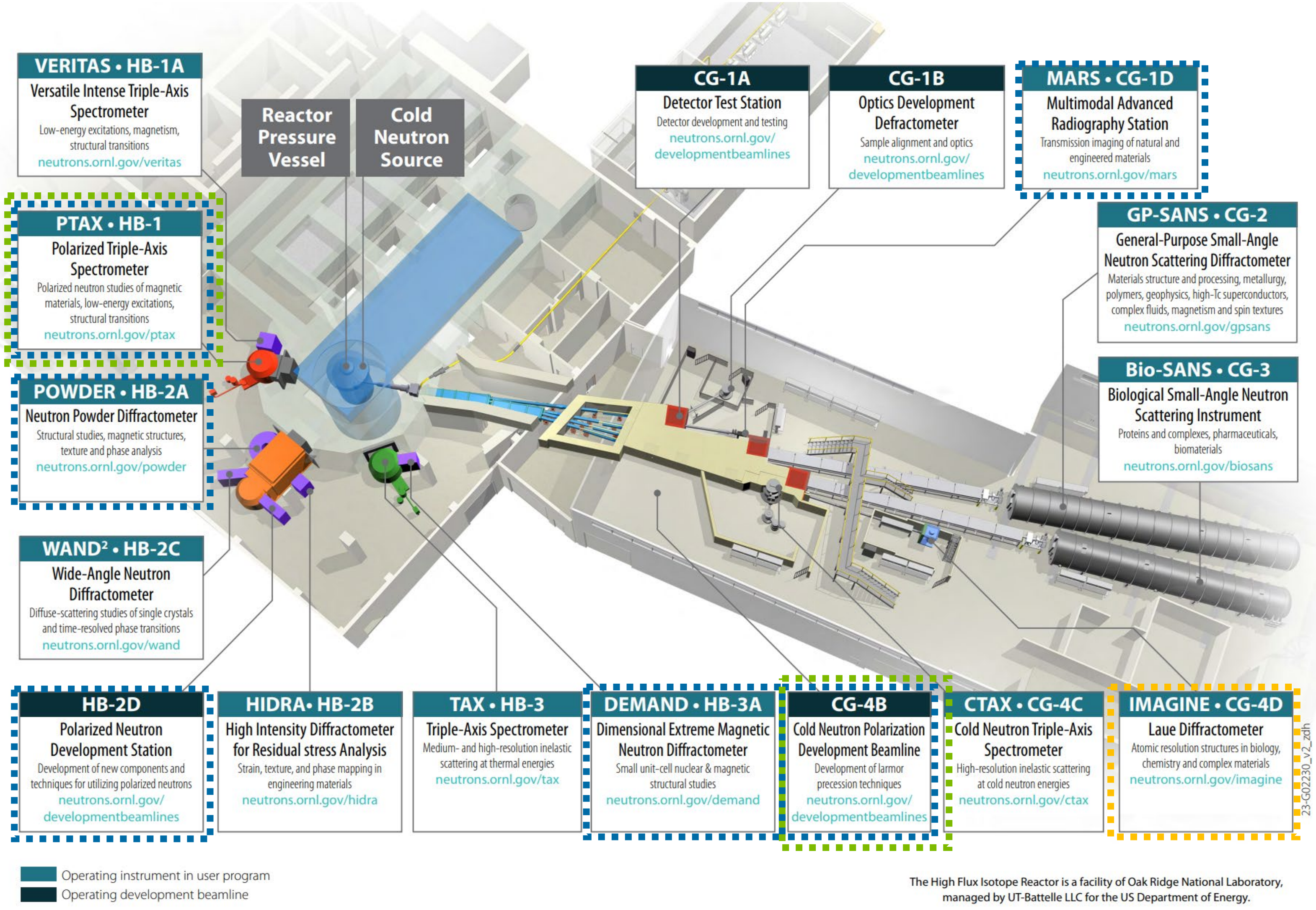


Who uses polarized neutrons at HFIR?

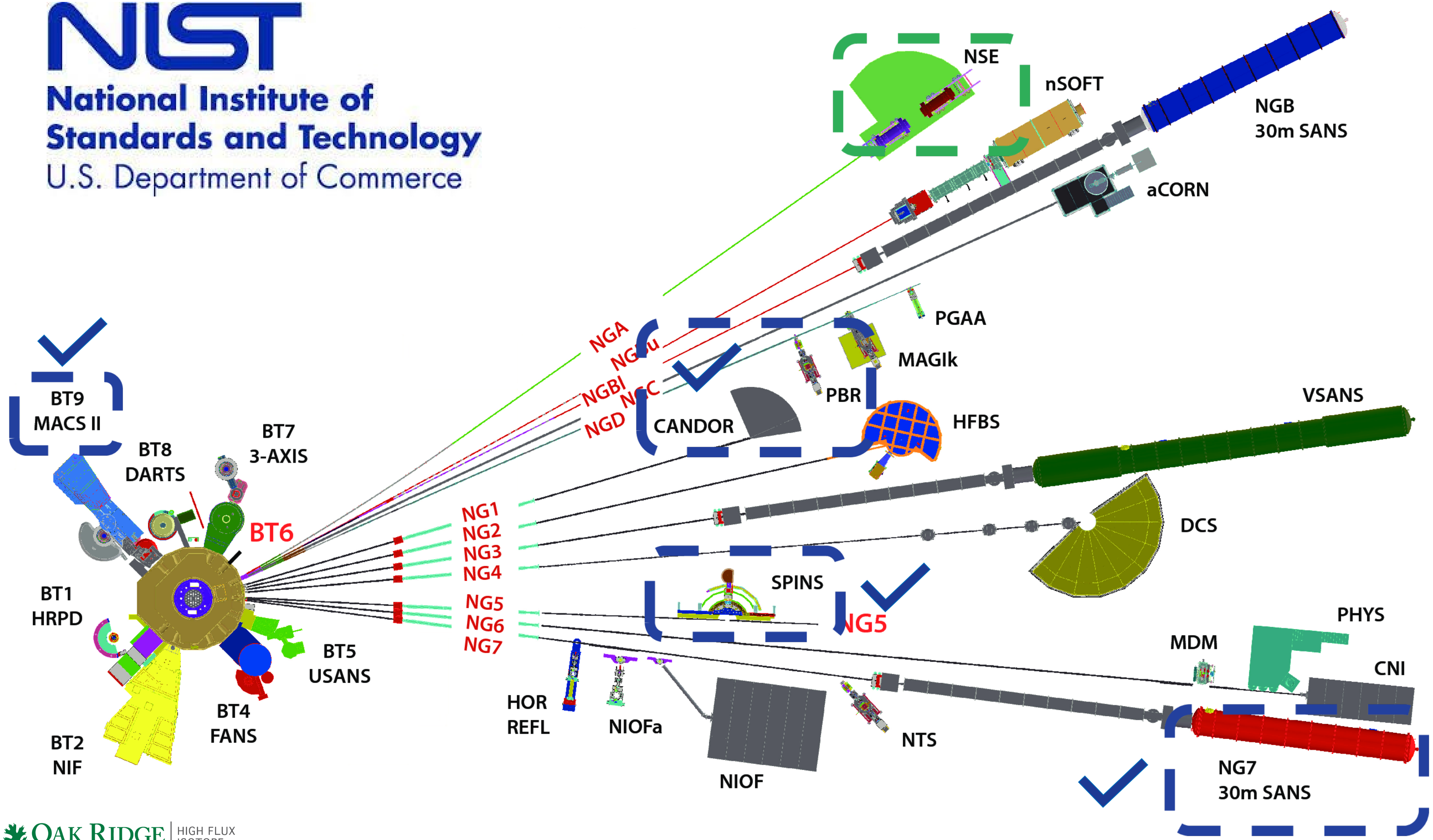
Magnetic Moment Contrast

Nuclear Spin Contrast

Enhanced resolution via 'Larmor' techniques

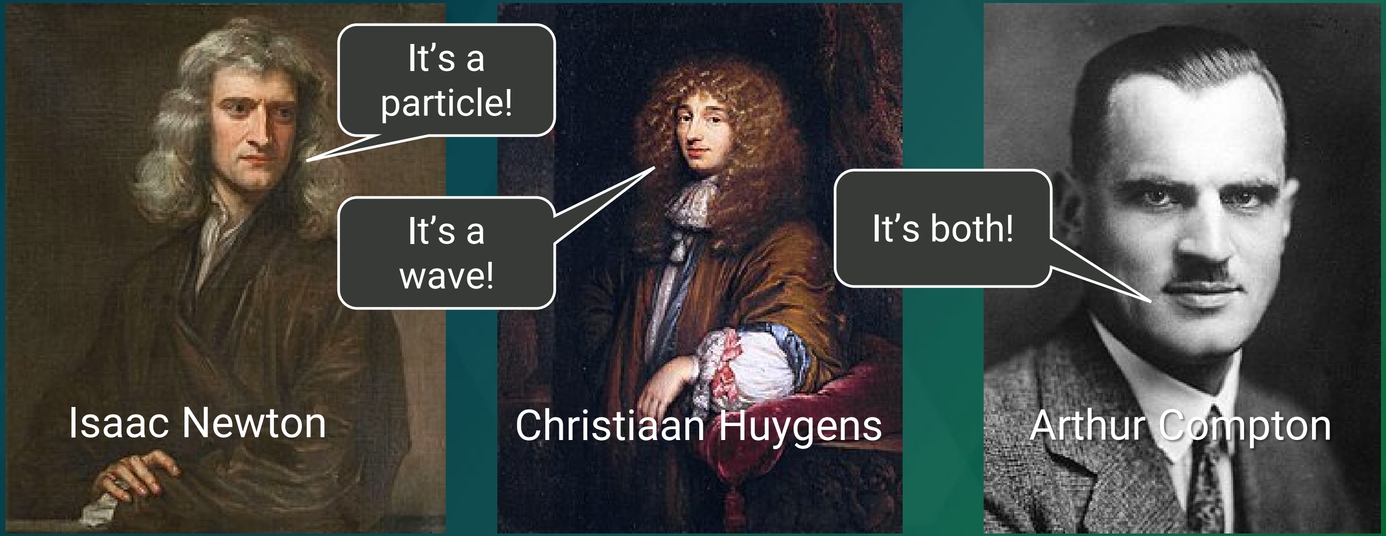


NIST
National Institute of Standards and Technology
U.S. Department of Commerce



OAK RIDGE National Laboratory | HIGH FLUX ISOTOPE REACTOR

CHARACTER:
Neutrons sometimes behave as particles, and sometimes as waves



Confusion about Light

"Solved" with
Quantum Mechanics

Neutrons Too!

CHARACTER:
Neutrons sometimes behave as particles, and sometimes as waves

Scatter like a wave

"**Coherent**" scattering

"Feels" more of a volume all at once,
Scattering VERY direction dependent

Examples of coherent scattering:
Diffraction (feels adjacent scatter planes)
Phonons (feels collective wiggles)
Index of refraction (feels density)

Scatter like a particle

"**Incoherent**" scattering

Single point of contact,
scatters in random directions

Loses 'coherence' via:
Random isotopes
Random nuclear spin orientations
Suppression of coherent scattering

CONTRAST: Neutrons scatter via 2 different forces, too

Nuclear Strong force

Interaction with nuclei of atoms
Depends on the *isotope*
Depends on *spin of the nuclei*
Depends on *nuclear resonances*

“*Sees*” lattice structure via nuclei location
“*Sees*” phonons & vibrational modes

Includes both scattering and absorption
(absorption is a nuclear reaction,
creating a new isotope
with an additional neutron)

Magnetic force

Interaction with the *magnetic field*
in a region about atoms

“*Sees*” magnetic structure
“*Sees*” magnetic excitations

Think “*Contrast*” of the scattering neutron

Combine Contrast & Character; or Particles, Waves & Forces

Absorption	^{10}B, ^{3}He, ^{6}Li, Gd, Cd

Character: Coherent ↕ Incoherent

Coherent & Strong
- Deuterium (^{2}H)
- Nuclear atomic structure
- Phonons
- Many others…

Coherent cross-talk or interference

C herent & netic
- Ferromagnetic structure
- Magnetic multilayer structure
- Skyrmion structure
- Superconductor, structure & spin waves
- Quantum Materials

Incoherent & Strong
- Hydrogen (^{1}H)
- Vanadium
- TiZr

Incoherent & Magnetic
- Paramagnons in gaseous state

Strong force ← **Contrast** → Magnetism

OAK RIDGE National Laboratory | HIGH FLUX ISOTOPE REACTOR

CONTRAST: Vector-ing from the perspective of the 2 forces

Strong force

Magnetic force

Spin:
$\sigma_n = \frac{1}{2}$

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

Nuclear magneton:
$\mu_N = 5.051E-27\ \mathrm{JT}^{-1}$
$\mu_N = 3.15E-5\ \mathrm{meV/T}$

Quantum weirdness

Enrico Fermi

-- interacting with ---

Relative ...pins of atomic nuclii

Relative orien...aterials

--- leads to changes in ---

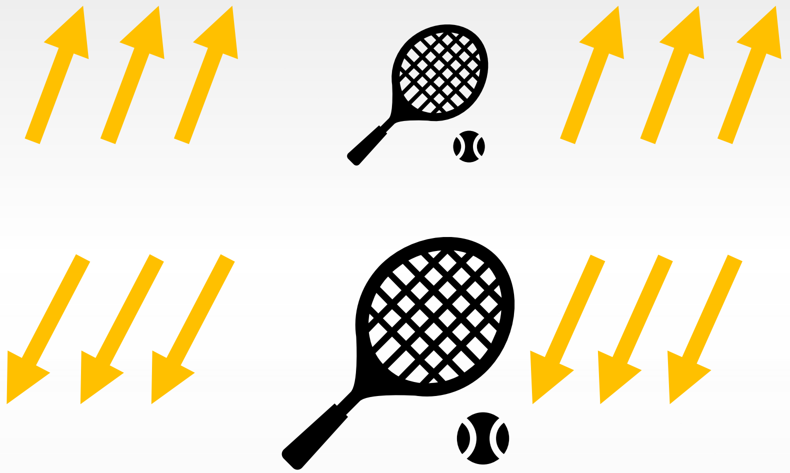
Scattered intensity

Reorientation of the spin or magnetic moment of the neutron

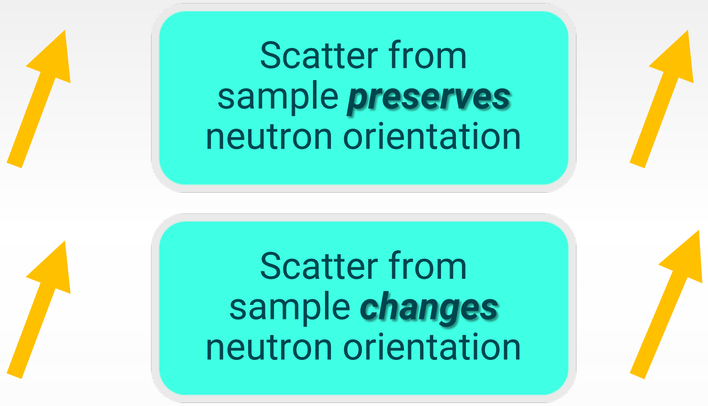
3 charged quarks dancing inside each neutron

Changes depend on polarization of incident beam

Changes in Scattered Neutron Intensity

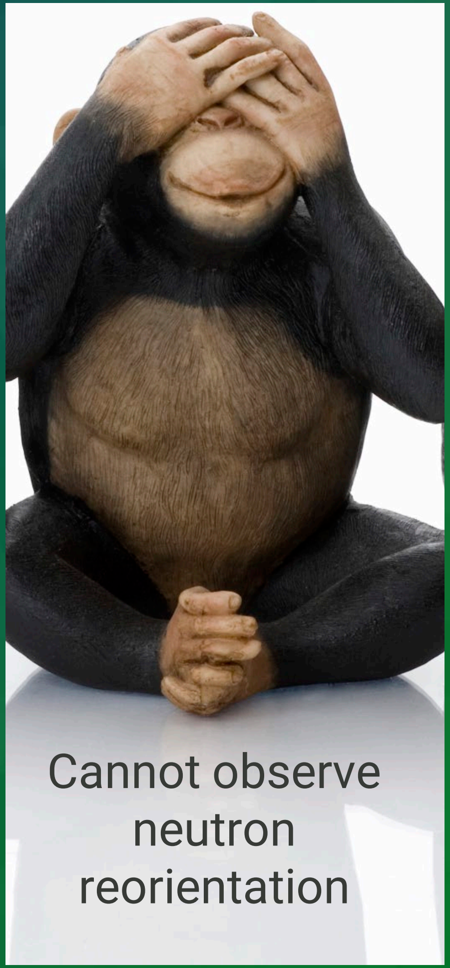


Changes in Neutron Orientation



Yet, with unpolarized neutron scattering alone…

Scattered intensity



Reorientation of the spin or magnetic moment of the neutron

If only we had a way to filter and play with

the neutron spin or magnetic moment…

We could isolate different features

We could reveal different dimensions

We could answer new questions
(that we'll call '<u>CAPABILITIES</u>')

Oak Ridge National Laboratory | HIGH FLUX ISOTOPE REACTOR

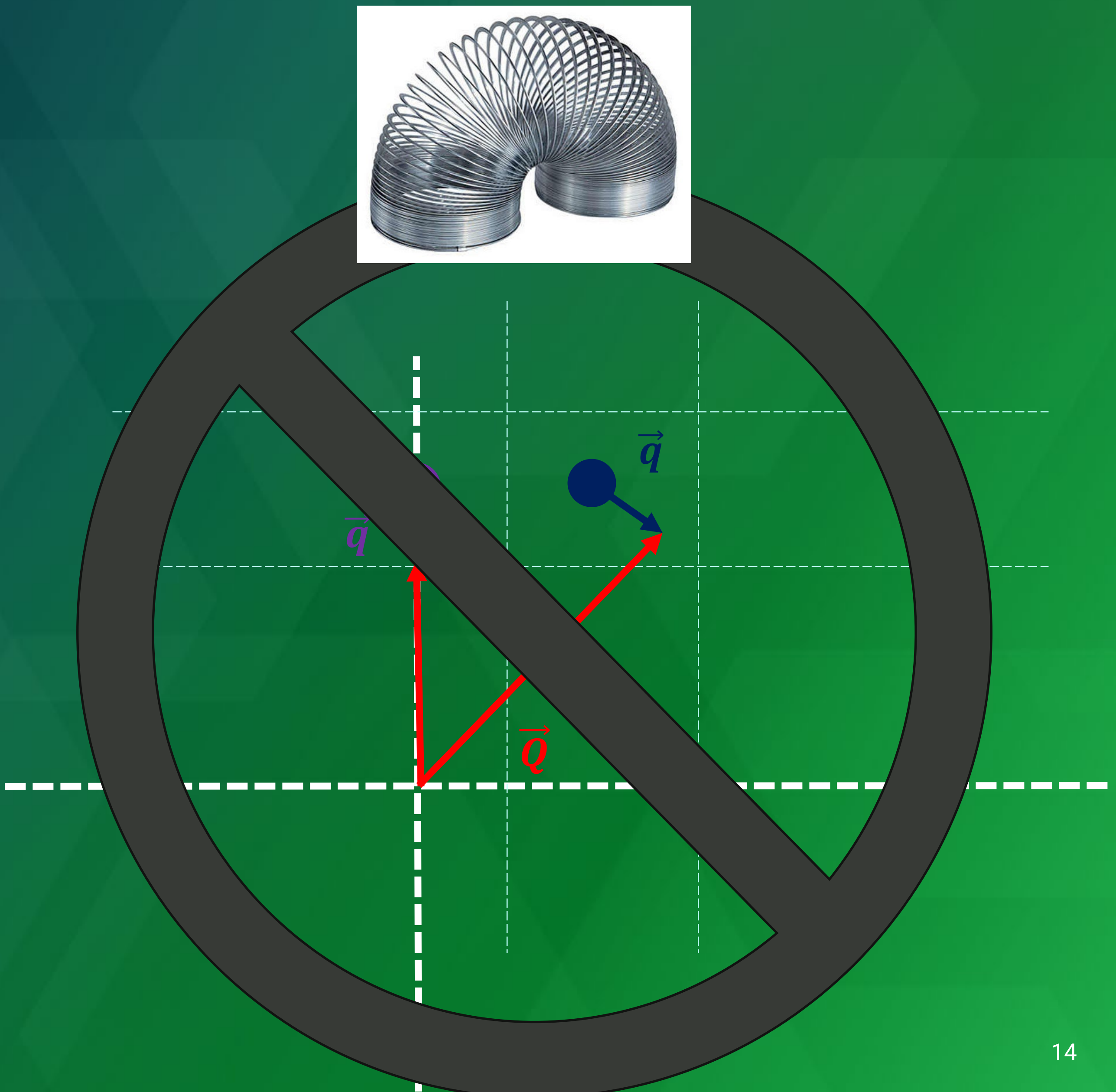
But beware, ‘polarization’ has 4 meanings for neutron scattering

1

2

$$-1 \geq P \geq 1$$

3



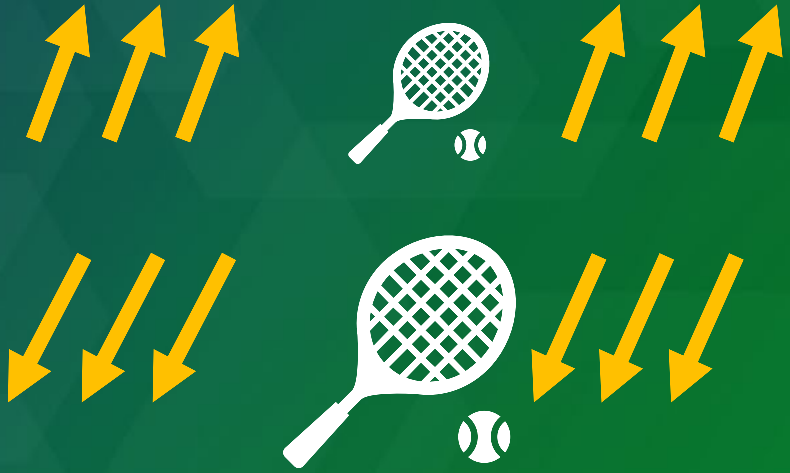
What? ANOTHER meaning for polarization?

4

This time, we're NOT referring to polarization of the neutron
INSTEAD, we're co-aligning either ATOMIC NUCLEI spins or magnetic moments inside of some material

In this case, the MATERIAL is 'polarized' instead of the neutron!

Polarized materials can change scattered intensity of polarized neutrons



OAK RIDGE National Laboratory | HIGH FLUX ISOTOPE REACTOR

Ingredients for CONFIGURATIONS: Polarization Optics

Guide fields, Flippers, and Filters

Guide fields & Larmor precession

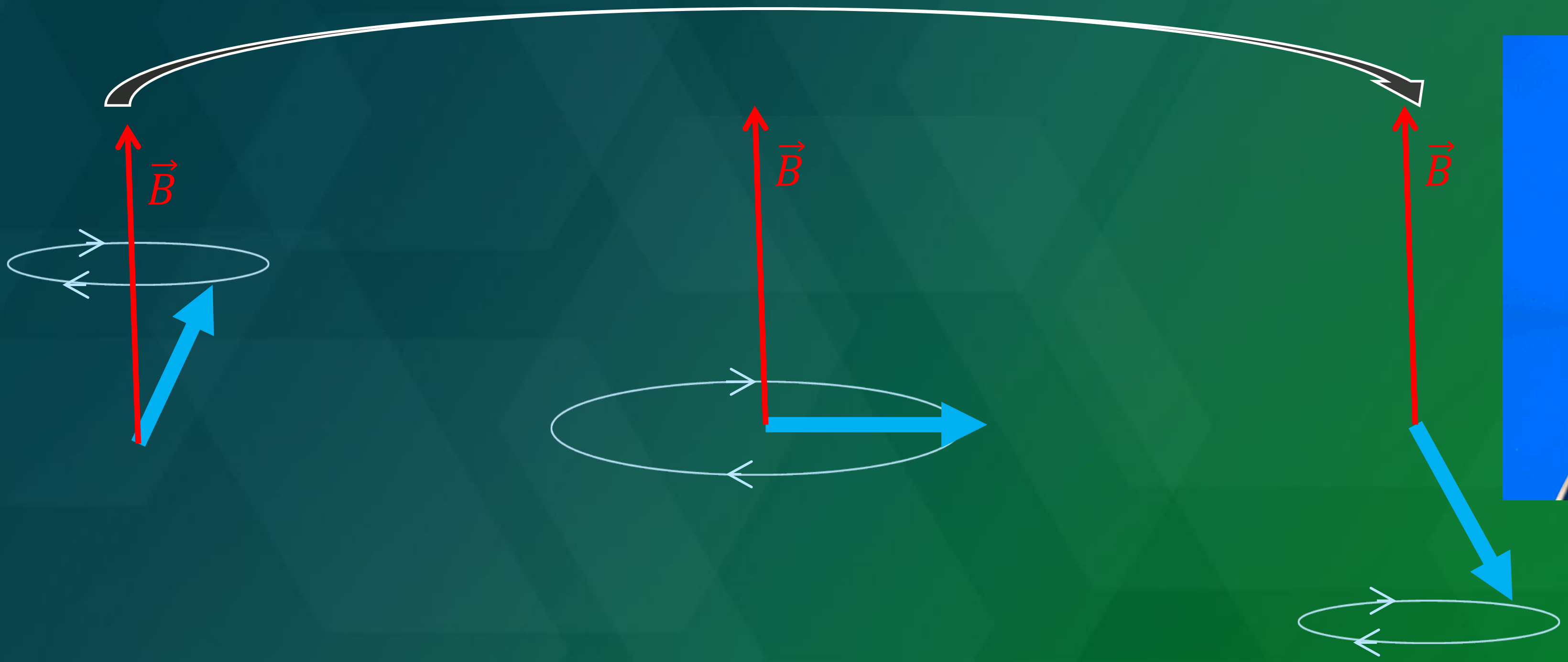
Ice skater

Break dancer

Rope dancer

Guide fields & Larmor precession

$$\vec{\omega} = k\vec{B}$$



(mostly) parallel

P~1

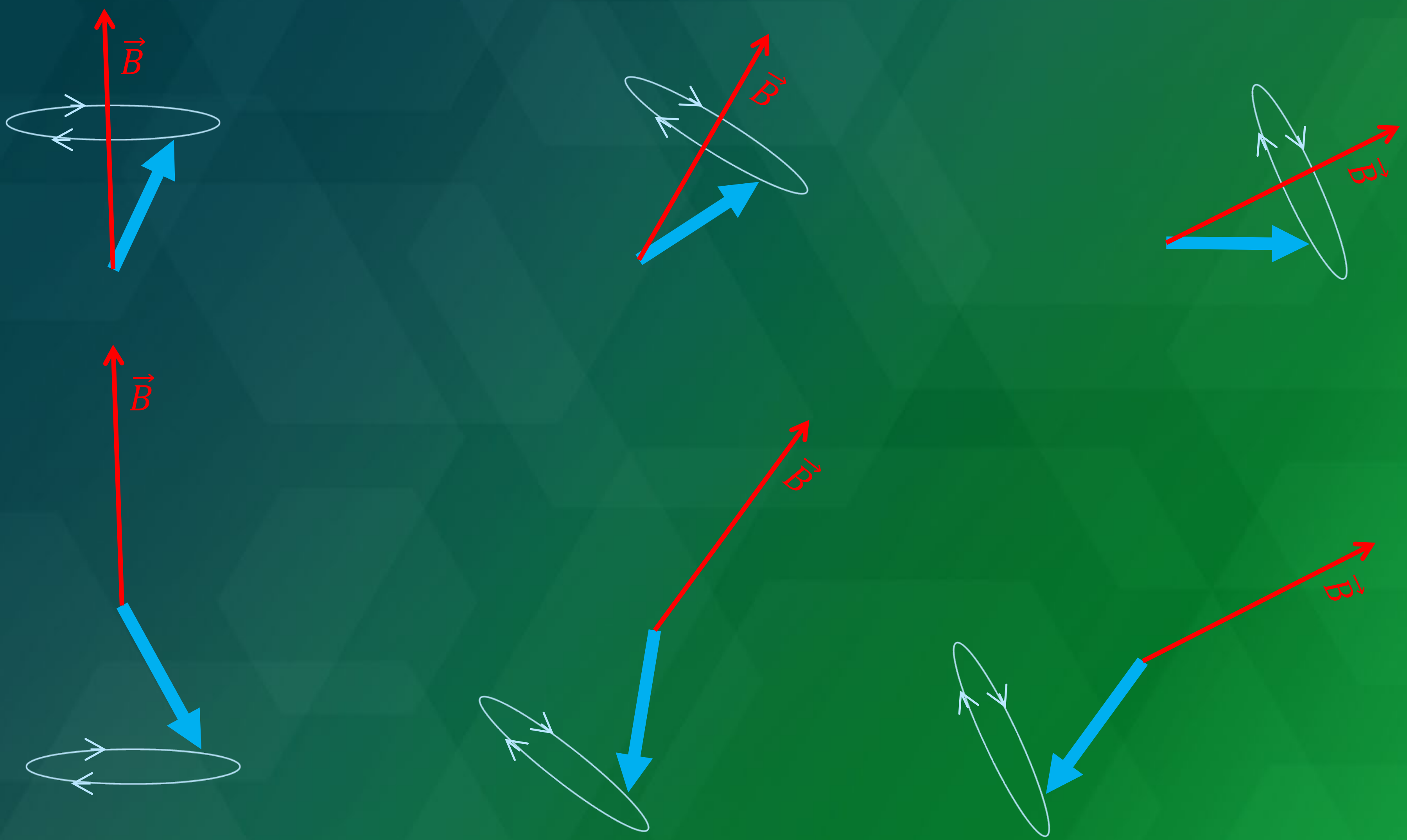
Right angle

P~0

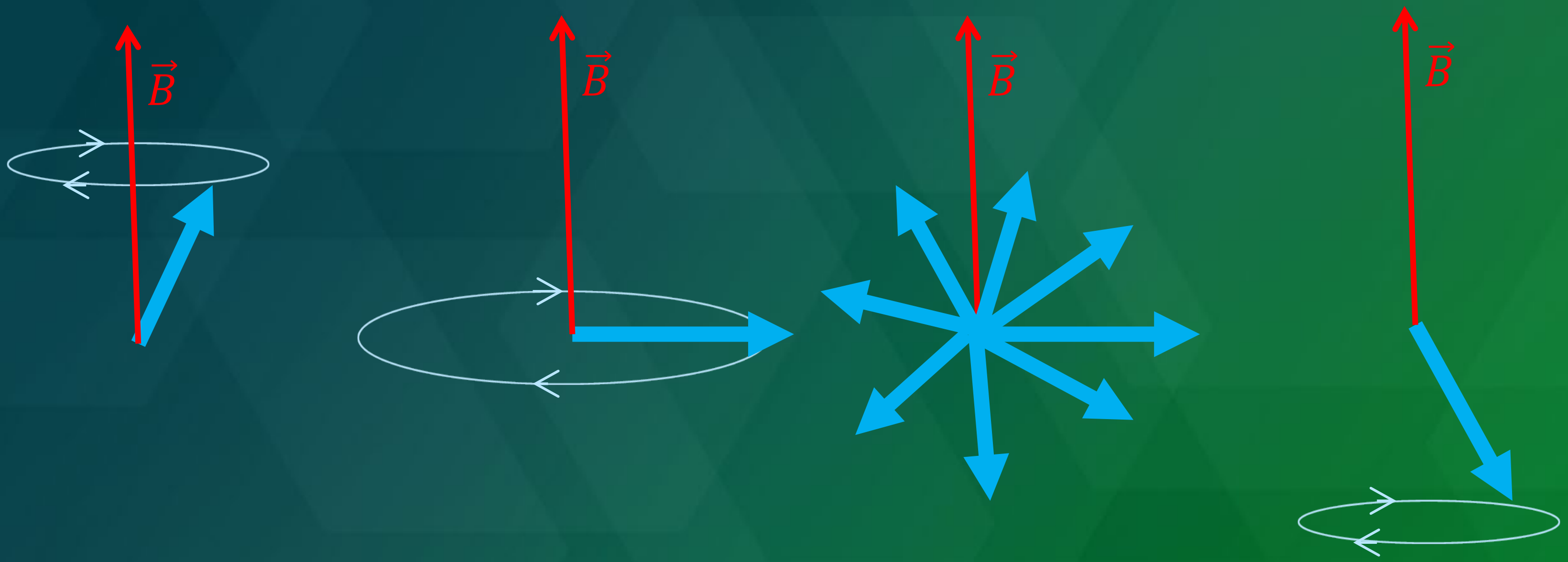
(mostly) antiparallel

P~-1

Guide fields as ‘nutators’
Steering neutron moment while flying is possible
-IF- we precess fast enough to track the change in field direction



A **Quantum** perspective for Larmor Precession helps to figure how FILTERS work



Classical

Quantum

So, if we could FILTER while the neutron is experiencing an external magnetic field, we could pass through up to half the neutrons!?!

Taking changes in scattered intensity to the EXTREME: From 'unpolarized' random directions in a neutron beam to HALF having single direction

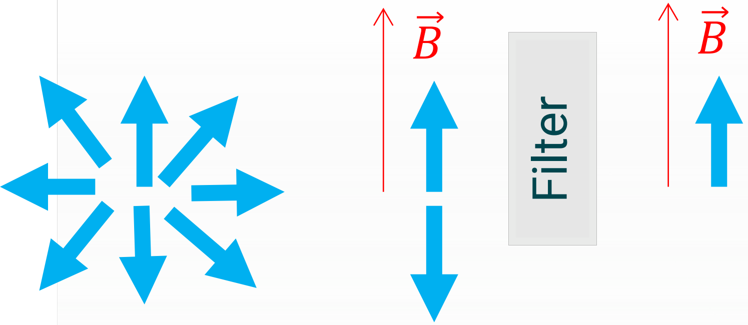
Polarized neutron developers have, over time, found and developed awesome materials that scatter or absorb selectively just one neutron state

These EXTREME systems are now optics we use as polarization FILTERS

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…

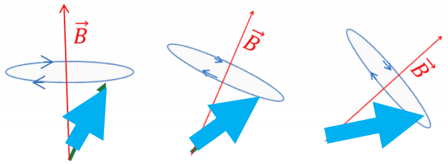
Guide fields and nutators

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

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

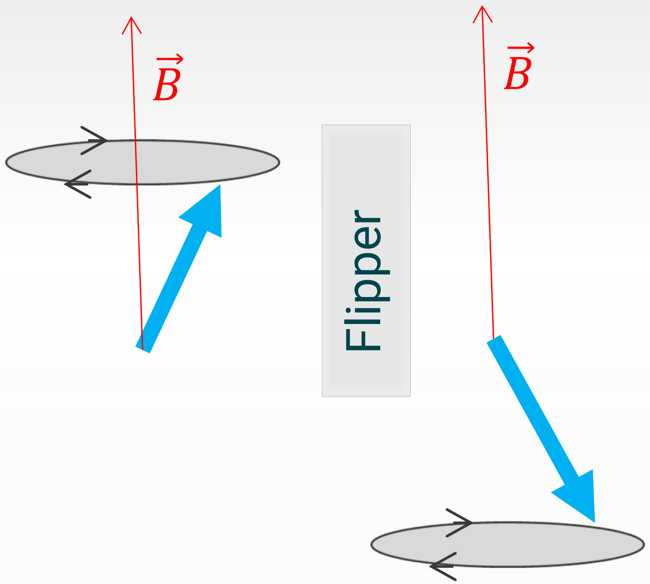
γ = -1.833E4 rad/Gauss-sec

- 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

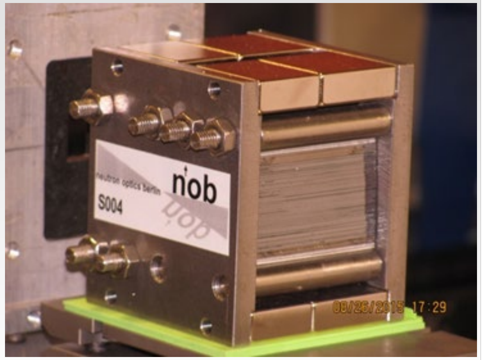


Polarization optics

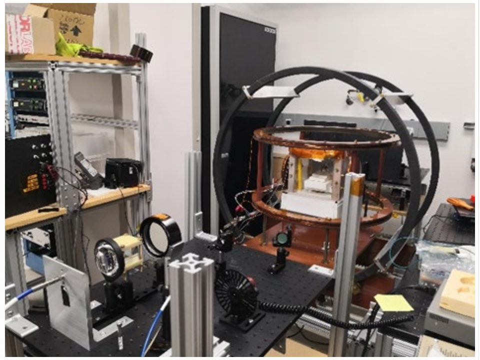
Filters

Heusler crystal

Polarizing Supermirror



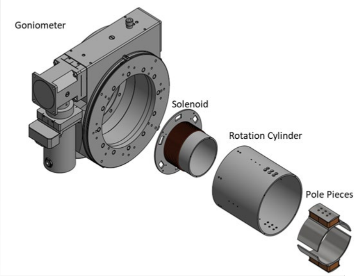
Nuclear-polarized ^{3}He



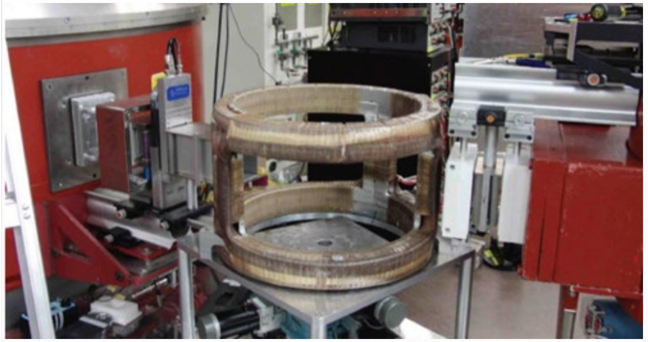
Guide fields and nutators

Permanent Magnet Yoked Assemblies

Rotatable nutator

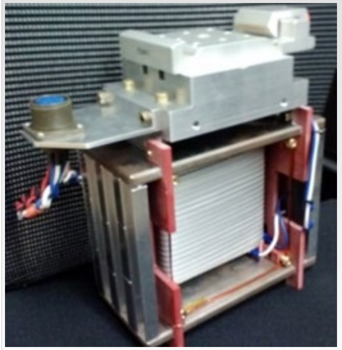


3D Coils



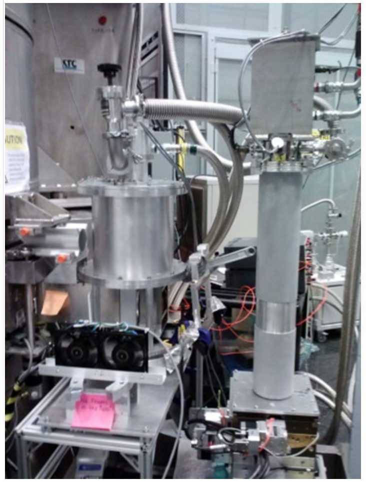
Flippers

Mezei



Radio-Frequency

Cryogenic (Meissner screen)



Adiabatic Fast Passage /w ^{3}He

Scattering changes accessed by different CONFIGURATIONS

Ways to measure changes in scattered intensity and/or changes in neutron polarization orientation

Add *changes to scattered intensity* to the Contrast / Character Matrix

Absorption

^{3}He filters absorb just 1 spin state*

Coherent & Strong

Dynamic Nuclear Polarization

- When 'polarize[4]' t
  ^{1}H nuclei
  - IMAGINE-X

Coherent cross-talk or interference

C herent &
netic

When 'polarizing[4]' your sample

- Ferromagnets
- Ferrimagnets
- Paramagnets
- Constructive / deconstructive interference for specific Bragg peaks: e.g. Heusler crystals

Magnetic chiral structures

Incoherent & Strong

Scatters only one spin state for ^{1}H

- Naphtaline as polarization filter for unscattered beam*

Incoherent & Magnetic

No change

Incoherent Character Coherent

Strong force Contrast Magnetism

*N. Niketic *et al*, *J. Appl. Cryst.* (2015). **48**, 1514-1521

OAK RIDGE National Laboratory | HIGH FLUX ISOTOPE REACTOR

Add *Vector Reorientation* to the Contrast / Character Matrix

Scatter from sample ***changes*** neutron polarization

Absorption

Character: Coherent ↕ Incoherent

Contrast: Strong force ↔ Magnetism

Coherent & Strong

No spin flip for
- Nuclear coherent scattering

Coherent cross-talk or interference

Coherent & Magnetic

Sometimes spin flip
- Known dependence on momentum transfer $\vec{Q}$

Incoherent & Strong

$\frac{2}{3}$ spin flip for
- Spin-incoherent scattering (^{1}H & V)

No spin flip for
- Isotope incoherent scattering
- Suppressed coherent (TiZr)

Incoherent & Magnetic

Random spin flip

Formulas on next page leverage lattice periodicity & coherent scattering

Coherence mechanism #1:
Leverage ***lattice periodicity*** for single crystals or powders
(think Bragg's law, Block equations, etc.)

Useful for ***diffraction*** and ***coherent inelastic scatting*** in comparable Q ranges

Leads to 'Maleev-Blume' equations with '***simple***' formulas relating various contributions to scattering ***into*** changes in neutron scattering intensity and/or polarization state

Will utilize Maleev-Blume vector equations as instructional aid for this introduction

Coherence mechanism #2:
Leverage ***# density variations*** leading into optical density variations

Useful for **small angle neutron scattering (SANS)** and **reflectometry**

For e.g. 1D multilayer systems, NOT periodic so must ***directly solve Schrodinger's equation***

Similar approach to coherent interference effects
(here often called 'contrast matching')

Add *changes to* ***scattered intensity*** to the Contrast / Character Matrix

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

Coherent & Strong	$N^\dagger N$	Coherent & Magnetic	$\vec{\boldsymbol{M}}_\perp^\dagger \vec{\boldsymbol{M}}_\perp + i\vec{\boldsymbol{P}}\cdot\left(\vec{\boldsymbol{M}}_\perp^\dagger \times \vec{\boldsymbol{M}}_\perp\right)$
Incoherent & Strong	$I_n + I_{si}$	Incoherent & Magnetic	

Coherent Strong ⇄ Coherent Magnetic (cross terms):

$$\vec{\boldsymbol{P}}\cdot\vec{\boldsymbol{M}}_\perp^\dagger N + \vec{\boldsymbol{P}}\cdot\vec{\boldsymbol{M}}_\perp N^\dagger$$

[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).

Maleev-Blume vector equations for single crystals & powders

Add ***Vector Reorientation*** to the Contrast / Character Matrix

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

Coherent & Strong

$$\vec{\boldsymbol{P}}(N^{\dagger}N)$$

$$iN(\vec{\boldsymbol{P}}\times\vec{\boldsymbol{M}}_{\perp}^{\dagger}) - iN^{\dagger}(\vec{\boldsymbol{P}}\times\vec{\boldsymbol{M}}_{\perp}) + N\vec{\boldsymbol{M}}_{\perp}^{\dagger} + N^{\dagger}\vec{\boldsymbol{M}}_{\perp}$$

herent & gnetic

$$(\vec{\boldsymbol{P}}\cdot\vec{\boldsymbol{M}}_{\perp}^{\dagger})\vec{\boldsymbol{M}}_{\perp} + (\vec{\boldsymbol{P}}\cdot\vec{\boldsymbol{M}}_{\perp})\vec{\boldsymbol{M}}_{\perp}^{\dagger} - \vec{\boldsymbol{P}}(\vec{\boldsymbol{M}}_{\perp}^{\dagger}\vec{\boldsymbol{M}}_{\perp}) - i(\vec{\boldsymbol{M}}_{\perp}^{\dagger}\times\vec{\boldsymbol{M}}_{\perp})$$

Incoherent & Strong

$$\vec{\boldsymbol{P}}\left(I_n - \frac{1}{3}I_{si}\right)$$

Incoherent & Magnetic

[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).

Meet the "Vector" family

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

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
$\boldsymbol{P}, \boldsymbol{P}^1$	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

Changes in scattered intensity

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

Changes in neutron orientation

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

[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).

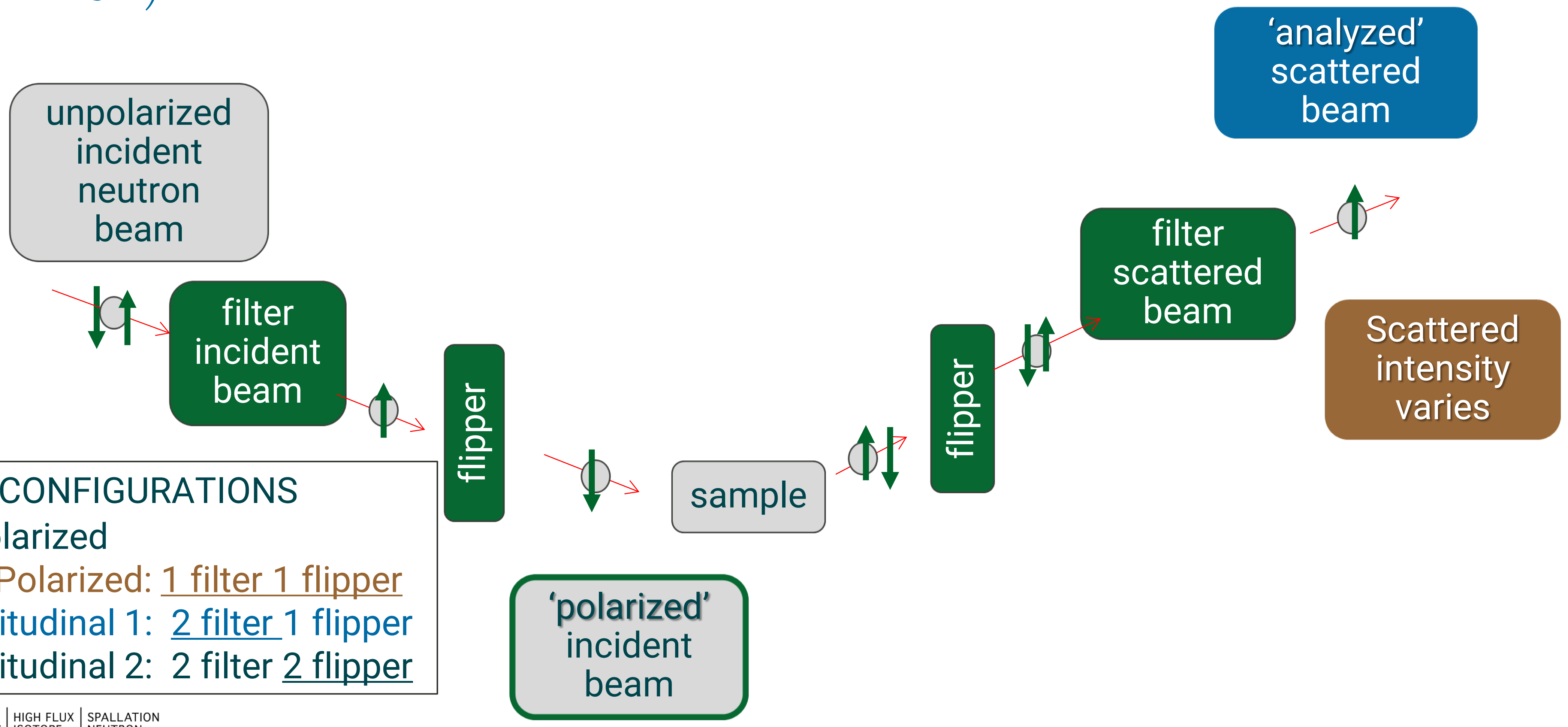
CONFIGURATIONS, what they access, and their optics

Changes in scattered intensity

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

Changes in neutron orientation

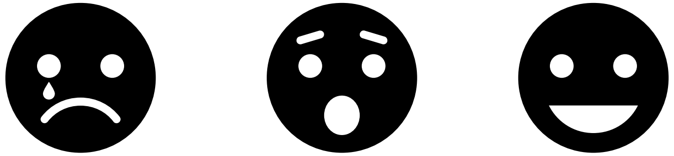
$$\boldsymbol{P}'I = \boldsymbol{P}\left(N^{\dagger}N - \frac{1}{3}I_{si}\right) + (\boldsymbol{P}\cdot\boldsymbol{M}_{\perp}^{\dagger})\boldsymbol{M}_{\perp} + (\boldsymbol{P}\cdot\boldsymbol{M}_{\perp})\boldsymbol{M}_{\perp}^{\dagger} - \boldsymbol{P}(\boldsymbol{M}_{\perp}^{\dagger}\boldsymbol{M}_{\perp})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



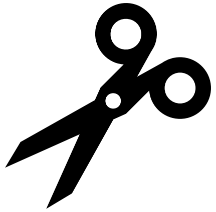
CONFIGURATIONS

- Unpolarized
- Half Polarized: 1 filter 1 flipper
- Longitudinal 1: 2 filter 1 flipper
- Longitudinal 2: 2 filter 2 flipper

<u>CAPABILITIES</u> truncate those equations
Yes, the Maleev-Blume equations are VERY busy

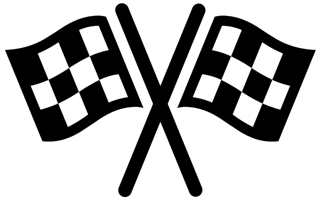


- Leverage *personality flaw* found in some scientists
  A. *Make assumptions* about the system you are studying
  B. Eliminate terms
  C. Simplify / Streamline the math



- Linear algebra
  - *N* equations & *N* unknowns → solvable problem

- Let's call the solutions to the streamlined equations "<u>Capabilities</u>"
  - Think word problems in reverse…



CONFIGURATIONS, CAPABILITIES and Capability Families

- "Configurations" are specific combinations of polarization optics enabling access to different Maleev-Blume equations
  - Will show examples of configurations in upcoming slides!
- "Capabilities" are specific solutions to streamlined Linear algebra problems
  - Can only be solved utilizing a subset of "Configurations"
  - Assume certain terms in Maleev-Blume equations aren't present
  - Polarization-state 'equation' is actually several equations
- "Capability families" are intuitive (?) groupings of those specific solutions

Capability Families

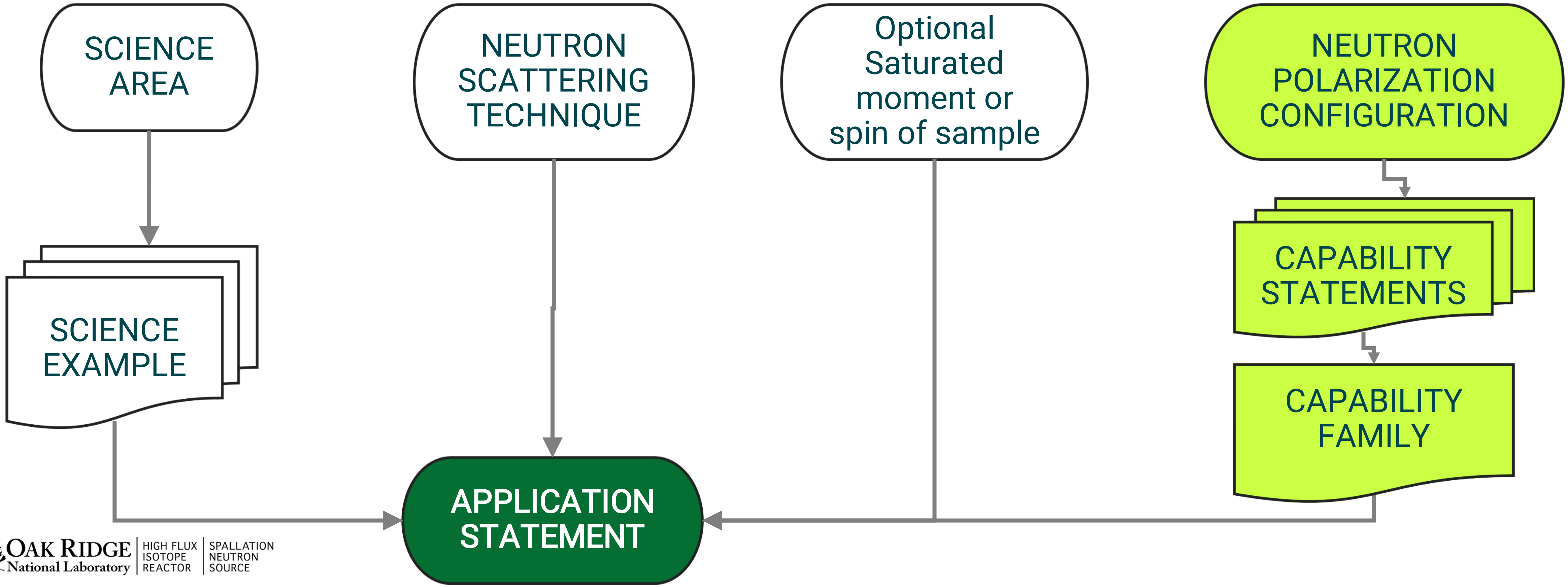
Isolate nuclear scattering	N & I_N
Isolate spin-incoherent scattering	I_{si}
Leverage dynamic nuclear polarization	$N \leftrightarrow I_{si}$
Solve Phase Problem	N & $\boldsymbol{M}_{\perp}$
Explore magnetic scattering	$\boldsymbol{M}_{\perp}$
Explore coinciding of nuclear and magnetic scattering	N with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

Color Key

Nuclear Scattering (coherent & isotope-incoherent)
Spin-Incoherent Scattering
Magnetic Scattering
Dynamic Nuclear Polarization
Other

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***]



Your invitation to take the red pill

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

For future reading

- Several dissertations
  - See instrument-specific publication lists
- Workshop slides, Polarization for Quantum Materials
  - Ovi, Masa, Yiqing & me, every other year
- Various online slide decks and tutorials
  - Kathryn Krycka, 'Neutron Polarization' slides & video at https://neutrons.ornl.gov/nxs/2021/lectures
  - 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