SANS-STAP

Report on the polarization analysis data reduction workflow

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PRESENTED BY: ANNIKA STELLHORN, HAL LEE

2024-10-23

Agenda

2. Overview – Polarised data reduction

The method to reduce polarised data is based on transmission matrices.

$$\begin{pmatrix} I_{++} \\ I_{+-} \\ I_{-+} \\ I_{--} \end{pmatrix} = \begin{pmatrix} T_{A+} & T_{A-} & \cdot & \cdot \\ T_{A-} & T_{A+} & \cdot & \cdot \\ \cdot & \cdot & T_{A+} & T_{A-} \\ \cdot & \cdot & T_{A-} & T_{A+} \end{pmatrix} \begin{pmatrix} 1 & 0 & \cdot & \cdot \\ 1-T_{F2} & T_{F2} & \cdot & \cdot \\ \cdot & \cdot & 1 & 0 \\ \cdot & \cdot & 1-T_{F2} & T_{F2} \end{pmatrix} \begin{pmatrix} 1 & 0 & \cdot & \cdot \\ 0 & 1 & \cdot & \cdot \\ 1-T_{F1} & 0 & T_{F1} & 0 \\ 0 & 1-T_{F1} & 0 & T_{F1} \end{pmatrix} \begin{pmatrix} T_{P+} & \cdot & T_{P-} & \cdot \\ \cdot & T_{P+} & \cdot & T_{P-} \\ T_{P-} & \cdot & T_{P+} & \cdot \\ \cdot & T_{P-} & \cdot & T_{P+} \end{pmatrix} \begin{pmatrix} S_{++} \\ S_{+-} \\ S_{-+} \\ S_{--} \end{pmatrix}$$

Before reduction | Analyser | Flipper after sample (Off transmits spin+) | Flipper before sample (Off transmits spin+) | Polariser | After reduction

Polariser, analyser matrix elements

Supermirror: $T_{p,A} \pm = \frac{1 \pm e_{p,A}}{2}$,

[3]He spin filter: $T_{p,A} \pm = \exp(-O)\exp(-O P_{He}(t))$.

$e_{p,A}$ = efficiency, 1=perfect, 0=not (note: *not* polarisation).

$O(\lambda)$ = wavelength dependent "Opacity" of ^{3}He cell

$=$ (Pressure) (Absorption x-section) (^{3}He path length)

$P_{He}(t)$ = time-dependent ^{3}He polarisation

Process of polarised data reduction

Get the transmission matrix elements from calibration measurements

Multiply matrices $\hat{T} = \widehat{T_A}\ \widehat{T_{F2}}\ \widehat{T_{F1}}\ \widehat{T_P}$, invert matrix & calculate $\vec{S} = \hat{T}^{-1}\vec{I}$.

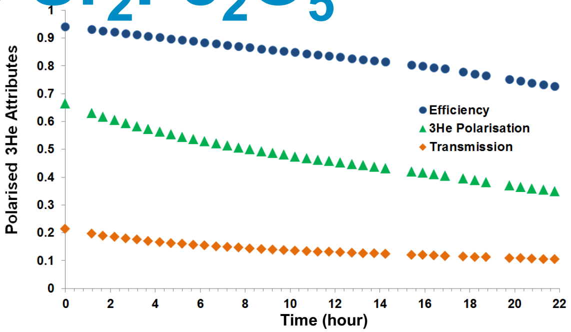
Same method applies across different scattering methods and choice of polarisation equipment.
Reduce data during experiment, not waiting after experiment!

Reference: Andrew Wildes, Review of Scientific Instruments 70(11):4241 - 4245 · December 1999.

2. Test case: Magnetic order in Brownmillerite $Sr_2Fe_2O_5$

Step1: Unpolarised direct beam transmission.
Get time-dependent transmission matrix elements of polariser & analyser. (note: spin +/- selection efficiency 99.995%)
Step 2: Correct sample measurements.

^{3}He polarisation decay example

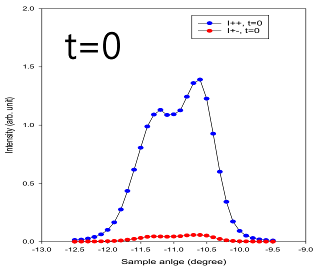


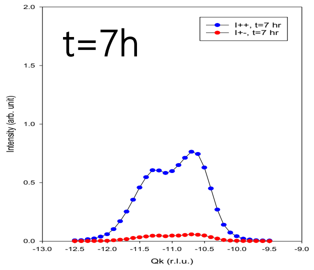
Known chemical peak

(0 8 0)

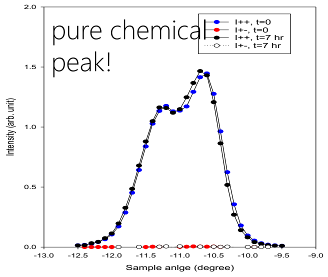
I++: Blue
I+-: Red

Measurements done at different times





corrected

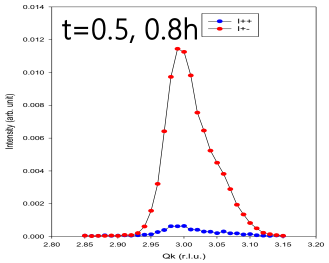


Sanity check: Must have

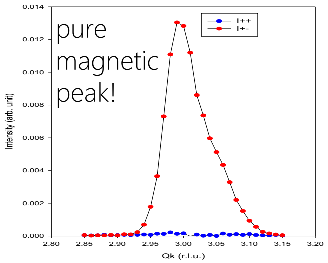
1. Virtually no spin-flip.
2. Non-spin-flip at different times are virtually identical.

Magnetic peak?
Mixed?

(1 3 2)
H // Q

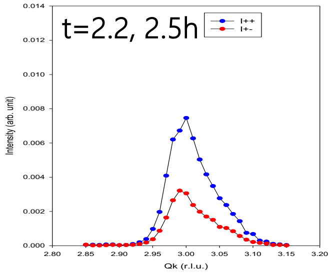


corrected



(1 3 2)
H ⊥ Q

I++: Blue
I+-: Red



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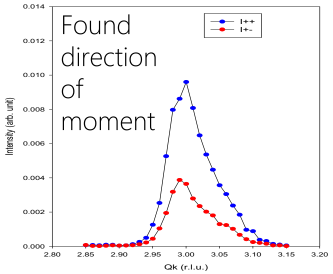
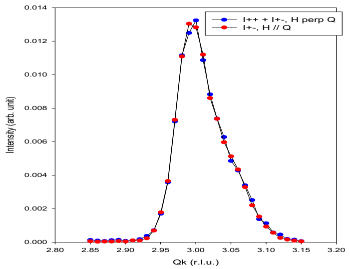


Sanity check: Must have

$$I_{++}(H \perp Q) + I_{+-}(H \perp Q) = I_{+-}(H//Q)$$



Confirmed

Reference: Josie E. Auckett, Wai Tung Lee, Kirrily C. Rule, Alexey Bosak, and Chris D. Ling, *Inorganic Chemistry* **2019** *58* (18), 12317-12324

2. Implemented workflow

EUROPEAN SPALLATION SOURCE

Which beamline components?
- Supermirrors
- ^{3}He-cells
- Flippers

Which polarization option?
- Half-polarized
- Full-polarized

Which DB characterization?
- Incoming **unpolarized** beam
- Incoming **polarized** beam

Transmission functions of elements:

$\hat{T}^{\pm,He}(t,\lambda)$
- Opacity from:
  a) pressure ("in-situ")
  b) Depolarization ("ex-situ")
- Choose to insert as P/A

$\hat{T}^{\pm,SM}(\lambda)$
- Parameters from commissioning
- Choose to insert as P/A

$\hat{T}^{Flipper}$
- Insert?
  a) Yes: f < 1
  b) No: f = 1

→ $\widehat{PA}$

Data-reduction at ESS-DMSC

scipp

Annika Stellhorn
Simon Heybrock
Johannes Kasimir
Hal Lee

PA-reduction:

$$\begin{pmatrix} I^{++} \\ I^{+-} \\ I^{-+} \\ I^{--} \end{pmatrix}(t,\lambda) \Rightarrow \frac{1}{N}\sum_N PA\left(\frac{I(t,\lambda)}{Beaml.-corrections}\right) \Rightarrow \begin{pmatrix} S^{++} \\ S^{+-} \\ S^{-+} \\ S^{--} \end{pmatrix}(t,\lambda)$$

In-situ & single channel correction possible!

[1] Scipp esspolarization, https://github.com/scipp/esspolarization/, accessed: 2024-10-07

2. Implemented workflow – Example ^{3}He-cell

EUROPEAN SPALLATION SOURCE

1. Calculation of ^{3}He opacity

a) Via cell-parameters ("in-situ")
   - Fix cell length, pressure, temperature

$$O(\lambda) = \frac{\sigma_0}{k_B T} \mathrm{pl}\lambda = O_0\lambda$$

b) Via depolarization measurements ("ex-situ")
   - Fix empty-glass transmission

$$O(\lambda) = -ln[\frac{I^{DB,depol,cell}}{I^{DB,no\ cell}} \frac{1}{T^g(\lambda))}] = O_0\lambda$$

2. Calculation of time-dependent ^{3}He-polarization

$$A/P(t,\lambda) = \frac{I^{DB,\,cell}}{I^{DB,\,no\ cell}}$$

a) With an unpolarized incoming beam:

$$A/P^{unpol}(t,\lambda) = \mathrm{T^g}(\lambda) \cdot \exp(-O(\lambda)) \cdot \cosh(O(\lambda) \cdot P^{He}(t))$$

b) With a polarized incoming beam:

$$A/P^{\pm}(t,\lambda) = \mathrm{T^g}(\lambda) \cdot \exp(-O(\lambda) \mp O(\lambda) \cdot P^{He}(t))$$

- Gives the ^{3}He-polarization:

$$P^{He}(t) = \mathrm{C} \cdot \exp(-t/T^1)$$

3. Sample correction matrices

- Insert $M^{+/-}$ components of ^{3}He
- Choose further beamline components

$$\begin{pmatrix} S^{++} \\ S^{+-} \\ S^{-+} \\ S^{--} \end{pmatrix}(t,\lambda) = inv(\hat{T}^{+/-}(t,\lambda)) \cdot \begin{pmatrix} I^{++} \\ I^{+-} \\ I^{-+} \\ I^{--} \end{pmatrix}(t,\lambda)$$

[1] Sans polarization analysis https://github.com/scipp/esspolarization/blob/main/docs/user-guide/sans-polarization-analysis-methodology.ipynb

2. Implemented workflow – Example full-PA workflow

Definition of components and workflow (given by user):

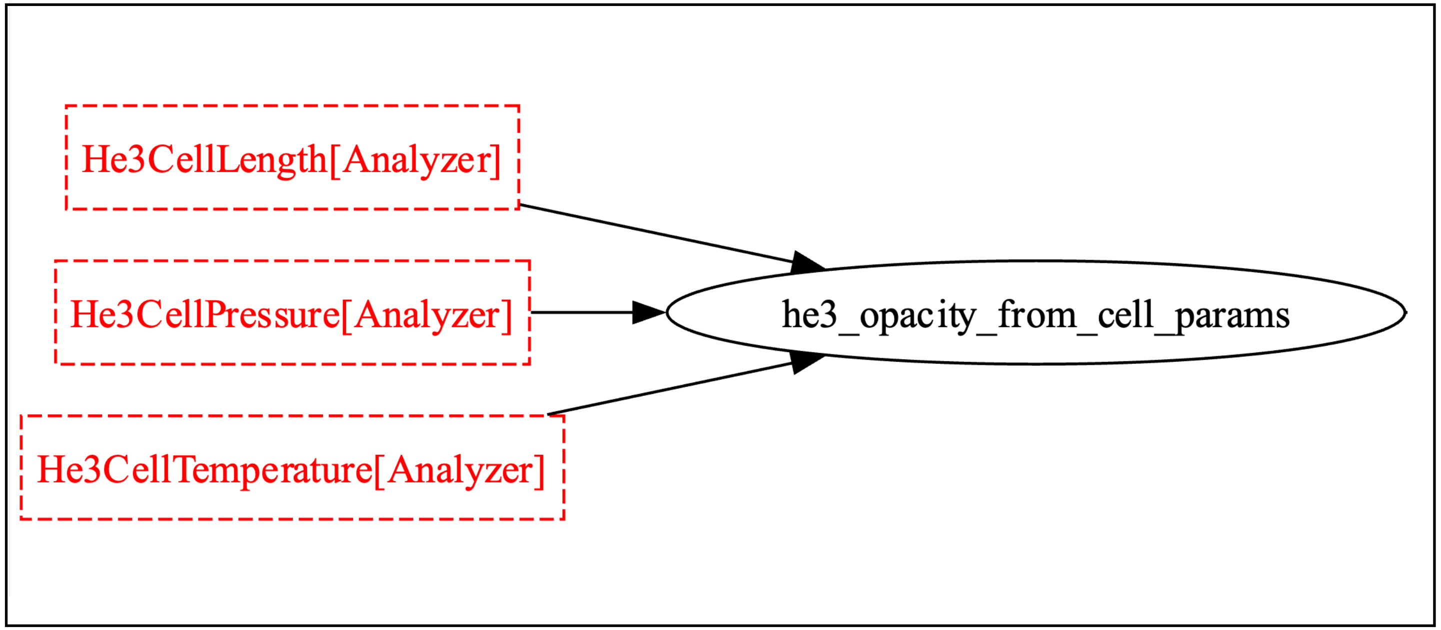
full_workflow = pol.PolarizationAnalysisWorkflow(
analyzer_workflow=he3_workflow – in-situ, polarized
polarizer_workflow=sm_workflow)

Calculation (not seen / varied by user):

$$A(t,\lambda) = \frac{I^{DB,\,cell}}{I^{DB,\,no\ cell}} \Rightarrow A^{\pm}(t,\lambda) = \mathrm{T^g}(\lambda) \cdot \exp(-O(\lambda) \mp O(\lambda) \cdot P^{He}(t)) \Rightarrow P^{He}(t) = \mathrm{C} \cdot \exp(-t/T^1)$$

DB-measurements:

- Insert cell-parameters → O_0



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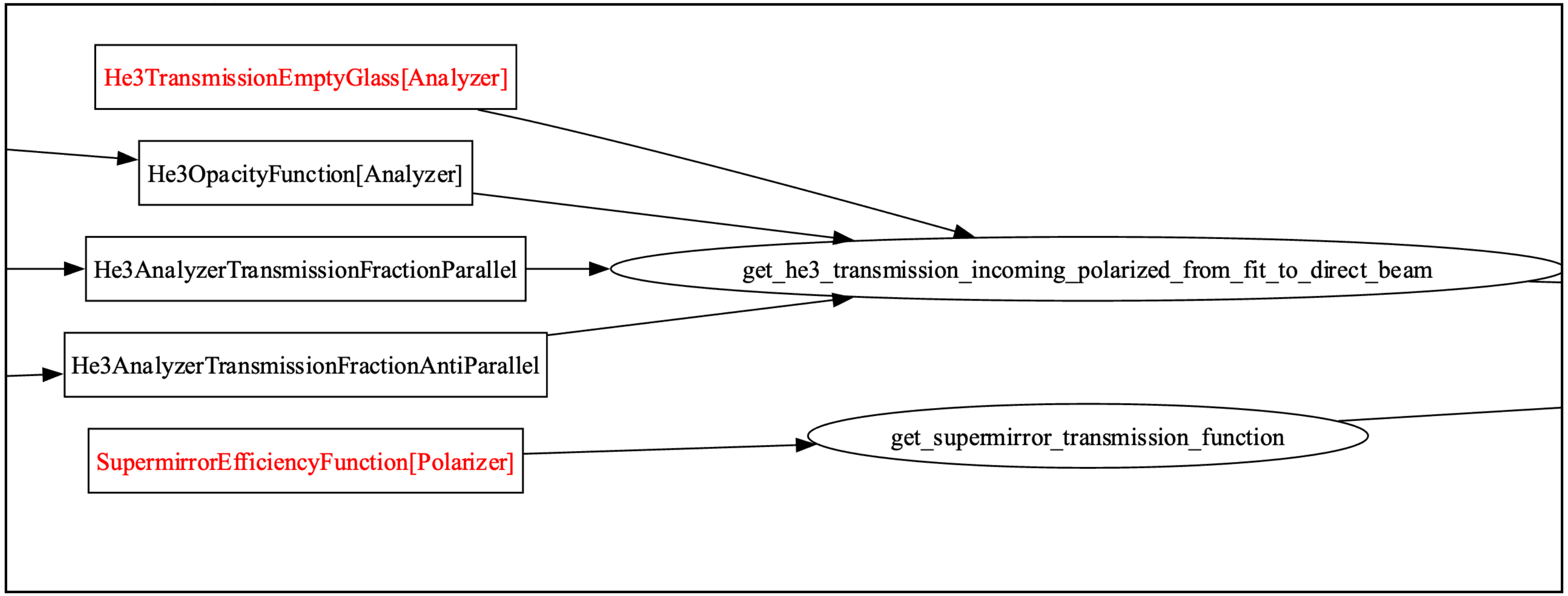
DB-measurements:

- Insert cell-parameters → O_0
- Insert $\mathrm{T^g}(\lambda)$
- Insert measurements of DB
- Insert SM $T^{\pm}$
- Get ^{3}He $T^{\pm}$



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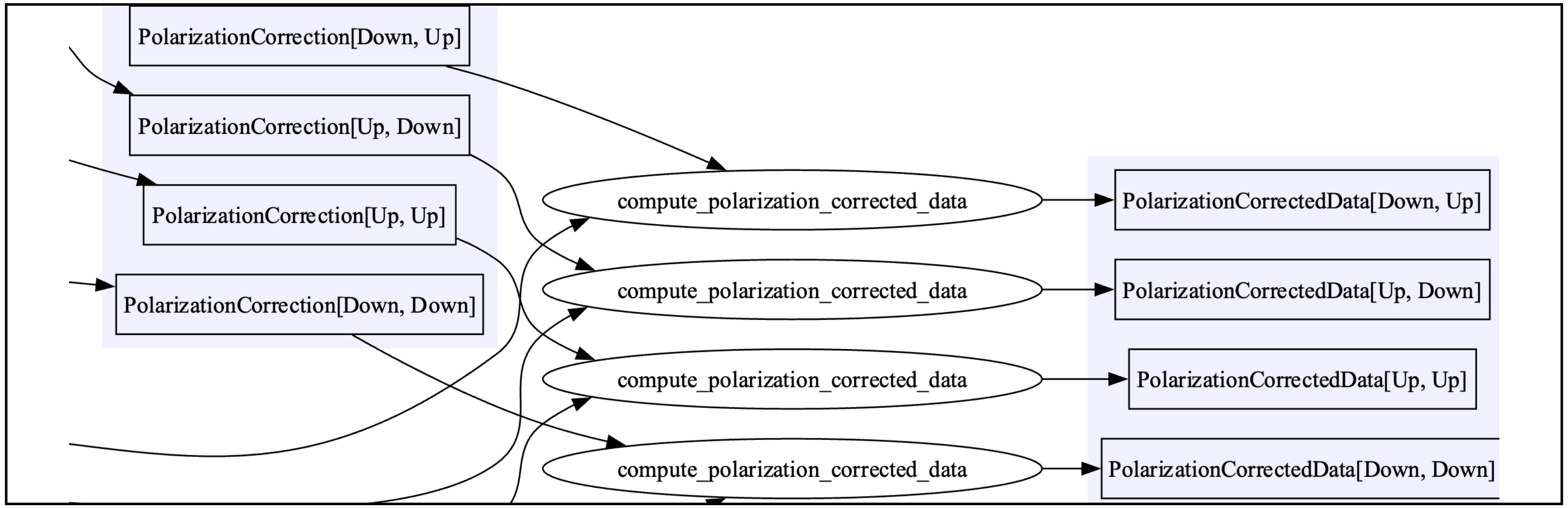
DB-measurements:

- Insert cell-parameters → O_0
- Insert $\mathrm{T^g}(\lambda)$
- Insert measurements of DB
- Insert SM $T^{\pm}$
- Get ^{3}He $T^{\pm}$

Sample measurements:

- Apply PA-correction
- Get cross-sections



3. Integration with unpolarized SANS workflow

EUROPEAN SPALLATION SOURCE

1. **Data reduction to "non-polarization-related" corrections**
   - Masking
   - Incident-beam correction
   - Sample thickness correction
   - Direct-beam-function

$$\begin{pmatrix} S^{++} \\ S^{+-} \\ S^{-+} \\ S^{--} \end{pmatrix}(t, \lambda) = \frac{1}{N}\sum_{N} PA \begin{pmatrix} I^{++} \\ I^{+-} \\ I^{-+} \\ I^{--} \end{pmatrix}(t, \lambda)^{\textbf{Beamline corrected}}$$

2. **Define transmission fractions (similar to LoKI workflow)**
   - If ^{3}He-cell correction:
     - "sample"=^{3}He-cell
     - Time-series of measurements for $P^{He}(t)$
     - Add depolarized ^{3}He-run
     - Get correction parameters
   - If SM correction:
     - Fix correction parameters!
   - If Sample correction:
     - Apply previously calculated correction parameters on "Beamline-corrected"-data

$$I(t, \lambda) = \frac{M_{cell}^{trans}}{M_{cell}^{inc}} \frac{M_{nocell}^{inc}}{M_{nocell}^{trans}}$$

get $\Rightarrow$ $A/P^{\pm}(t,\lambda)$, $P^{He}(t)$

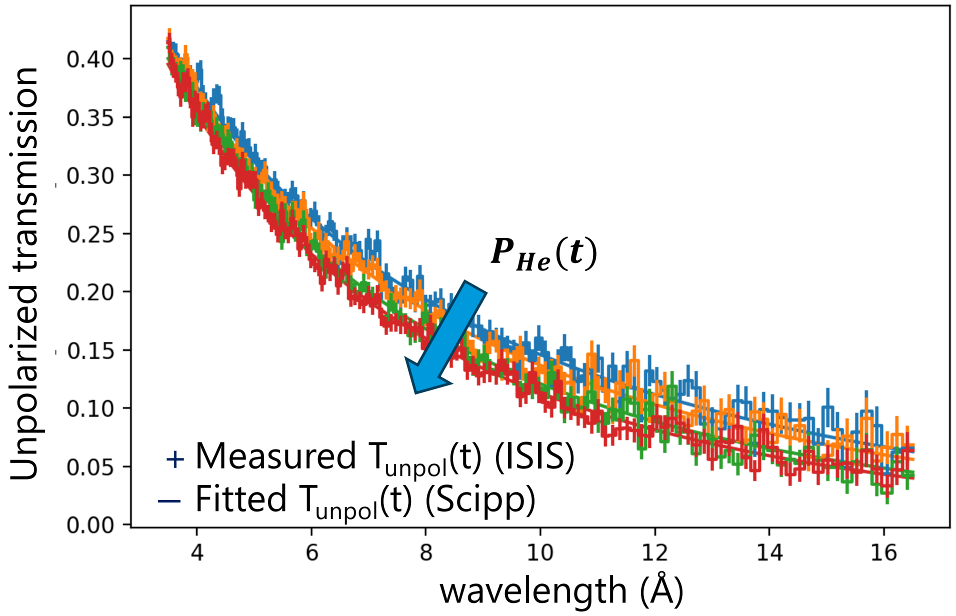
$$I(t, \lambda) = PA\left(\frac{M_{sample}^{trans}}{M_{sample}^{inc}} \frac{M_{DB}^{inc}}{M_{DB}^{trans}}\right)$$

get $\Rightarrow$ $\begin{pmatrix} S^{++} \\ S^{+-} \\ S^{-+} \\ S^{--} \end{pmatrix}(t, \lambda)$

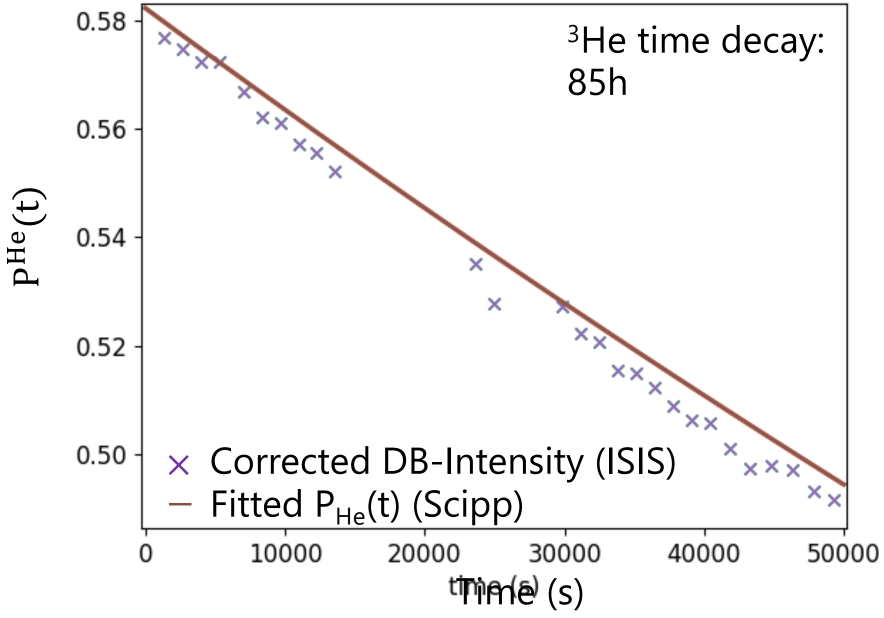
[1] Scipp esssans, https://github.com/scipp/esssans, accessed: 2024-10-07

4. Tests using polarization-analyzed data from ZOOM, ISIS

Direct-Beam Transmission measurements:



Fitting $P^{He}(t)$:



$$I(t,\lambda) = \frac{M_{cell}^{trans}\, M_{nocell}^{inc}}{M_{cell}^{inc}\, M_{nocell}^{trans}}$$

$$A^{unpol}(t,\lambda) = T^{g}(\lambda) \cdot \exp(-O(\lambda)) \cdot \cosh(O(\lambda) \cdot P^{He}(t))$$

$$P^{He}(t) = C \cdot \exp(-t/T^{1})$$

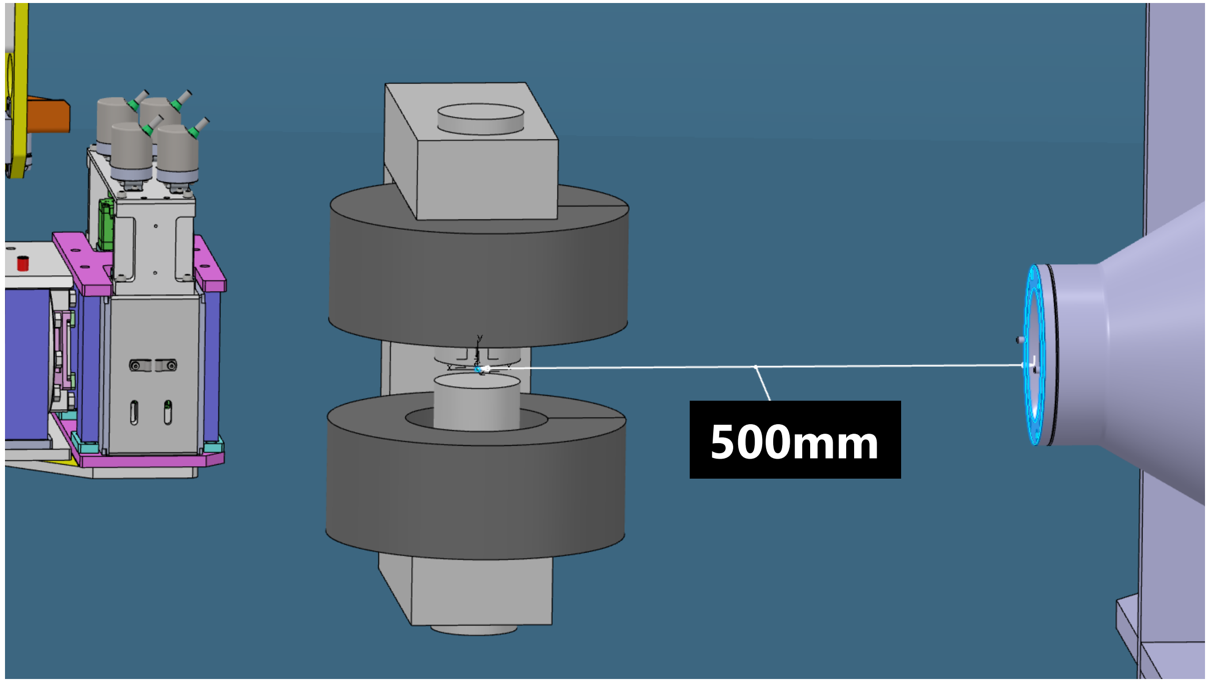
5. Outlook

SKADI with applied field (without PA):

- 2T water-cooled electromagnet (shared with ESTIA, DREAM)
  - **In purchase, ready for first science**

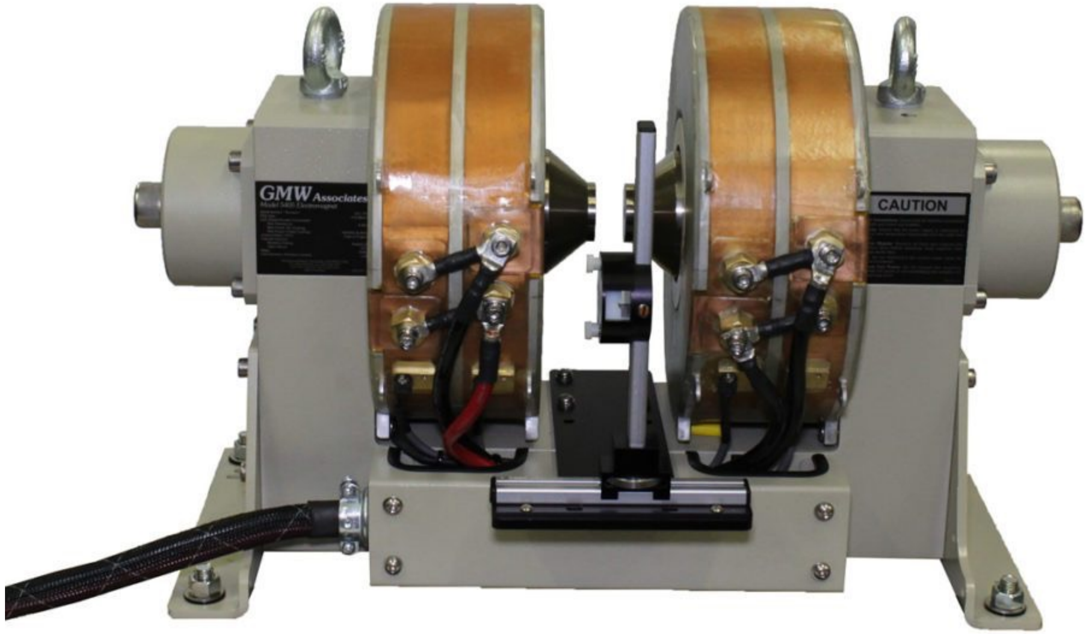
GMW 5405 Dipole EM

- inside SKADI



GMW 5405 Dipole EM

- ordered with additional overbar yoke



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  - **Next to be procured, after start of operation**

MA11 @ PSI

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SKADI with half-/full-PA:

- 5-7T full polarisation SANS/Refl asymmetric, self-shielded magnet (shared with ESTIA)
  - **Future-plan (many years after start of operation)**
  - **But: there is the need for full-PA on SKADI!**

AVM-1 @ ANSTO

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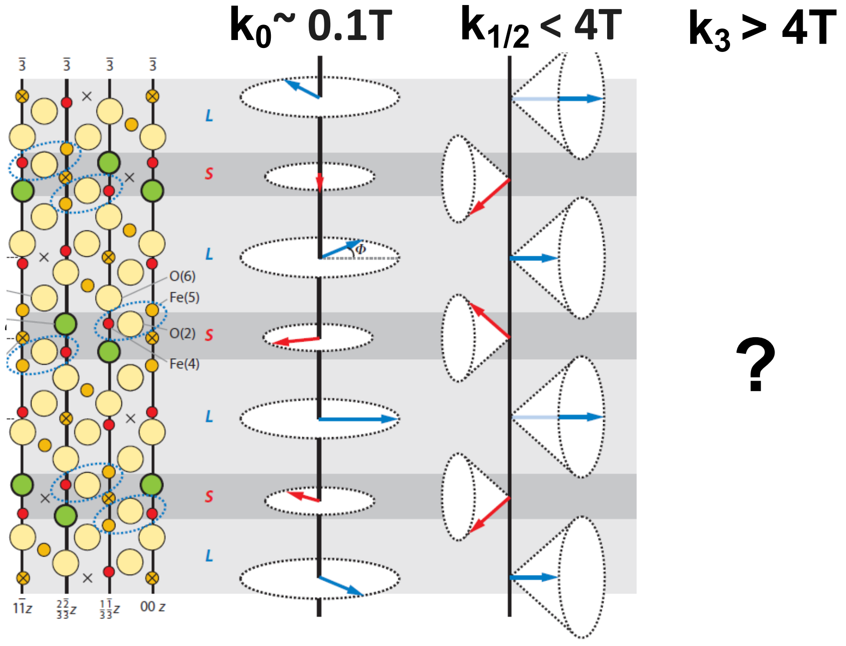
Ferroelectric materials

- Giant ME-effect [1]
- Magnetic phases (B, T, E)
- Example field range:
  - K_0 until 0.1T
  - $K_{1/2}$ > 0.2T, <4T
  - K_3 > 4T



[1] T. Kimura, *Annu. Rev. Condens. Matter Phys.* **3**, 93-110 (2012).

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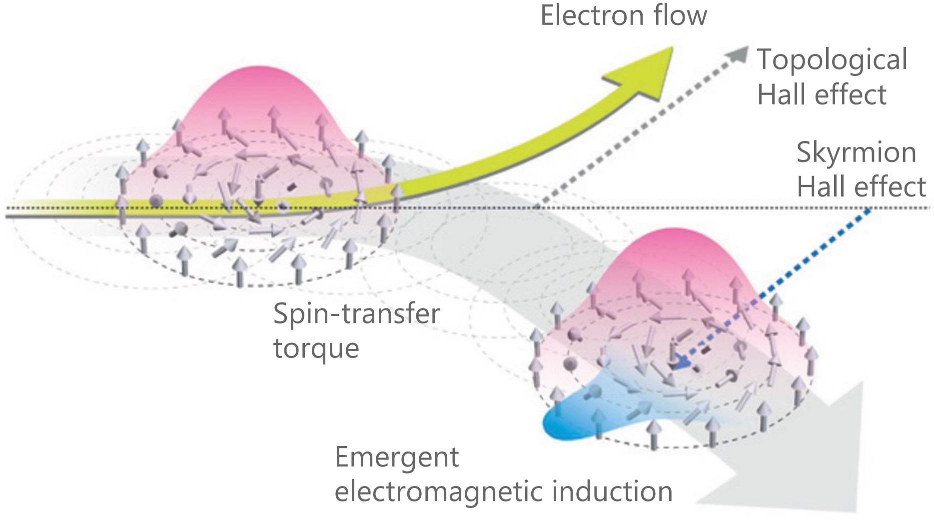
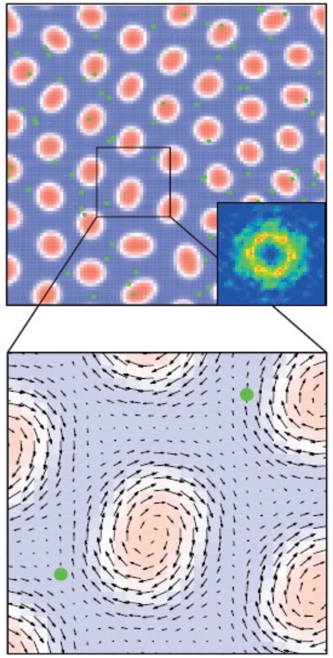
Skyrmions
- Under applied current[1]





[1] N. Nagaosa and Y. Tokura, *Nat. Nanotechnol.* **8**, 899-911 (2013)

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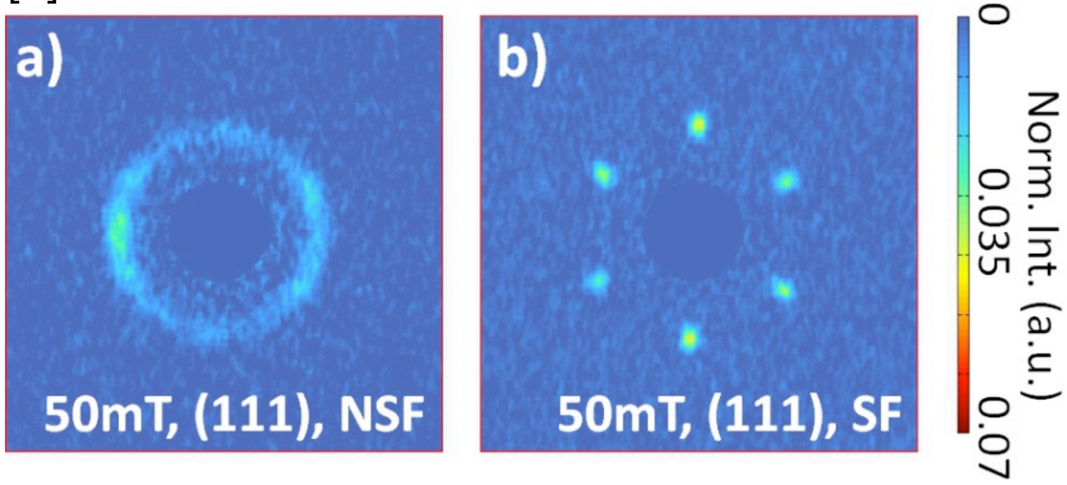
Skyrmions

- Under applied current[1]
- With cycloidal modulation[2]



[1] N. Nagaosa and Y. Tokura, *Nat. Nanotechnol.* **8**, 899-911 (2013)
[2] J. S. White et al., *Phys. Rev. B* **97**, 020401(R) (2018)

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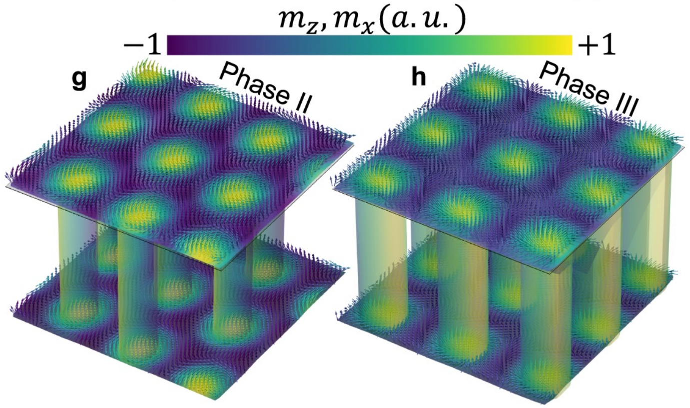
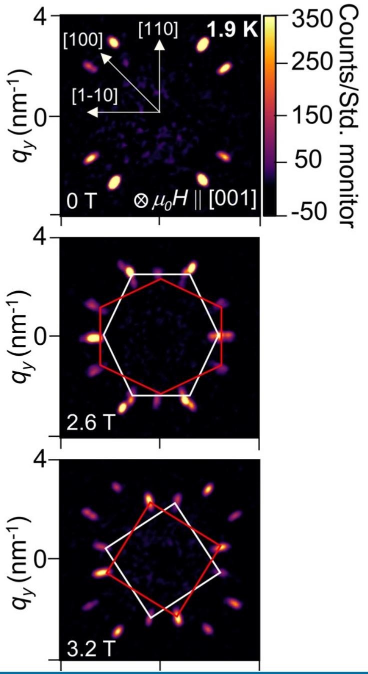
Skyrmions

- Under applied current[1]
- With cycloidal modulation[2]
- Square-hexagonal phase transition[3]





[1] N. Nagaosa and Y. Tokura, *Nat. Nanotechnol.* **8**, 899-911 (2013)
[2] J. S. White et al., *Phys. Rev. B* **97**, 020401(R) (2018)
[3] D. Singh et al., *Nat. Comm.* **14**, 8050 (2023)

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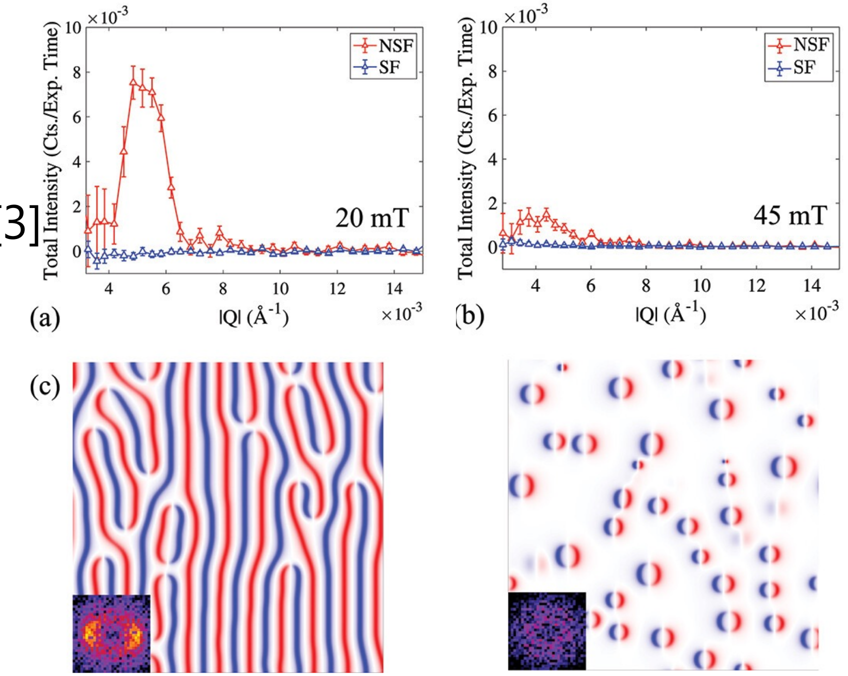
Skyrmions

- Under applied current[1]
- With cycloidal modulation[2]
- Square-hexagonal phase transition[3]
- Neel or Bloch pattern?[4]



[1] N. Nagaosa and Y. Tokura, *Nat. Nanotechnol.* **8**, 899-911 (2013)
[2] J. S. White et al., *Phys. Rev. B* **97**, 020401(R) (2018)
[3] D. Singh et al., *Nat. Comm.* **14**, 8050 (2023)
[4] V. Ukleev et al., *STAM* **25(1)** (2024)

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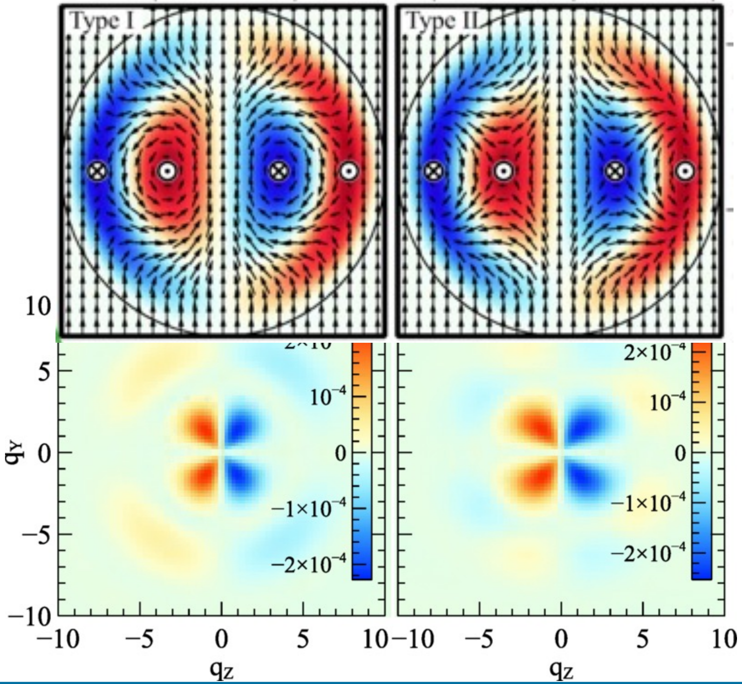
Hopfions

- In bulk magnetic materials
- Computed: chiral function of full-PA SANS scattering on type-I and type-II hopfions[1]



[1] K. L. Metlov and A. Michels, *Phys. Rev. B* **109**, L220408 (2024)

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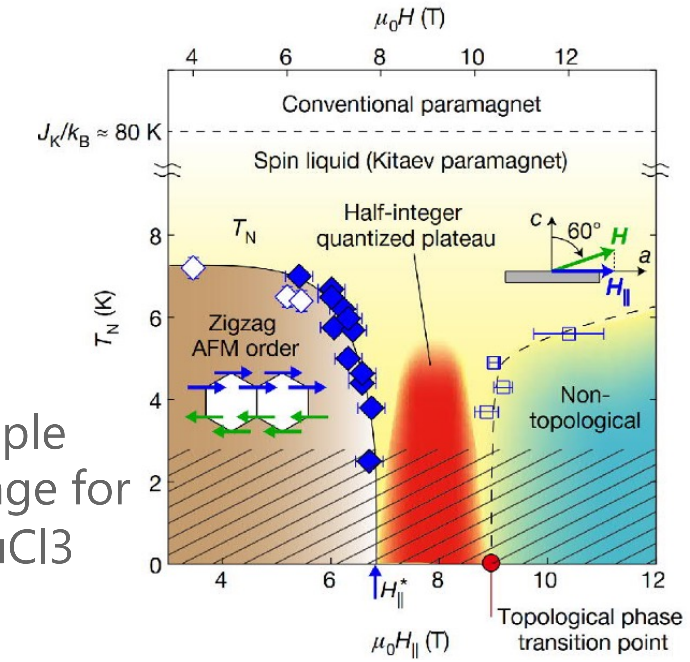
Designer Quantum Matter

- Artificially patterned domains
- Layered 2D vdW materials[1]
- E.g.:
  - topological superconductors,
  - quantum spin-liquids
  - flat band systems
- Polarized GISANS

Example B-range for α−RuCl3



[1] J. L. Lado and P. Liljeroth, arXiv:2102.11779v1 [cond-mat.mes-hall] 23 Feb 2021