Polarization-analysed SANS at the ESS

13/07/2026

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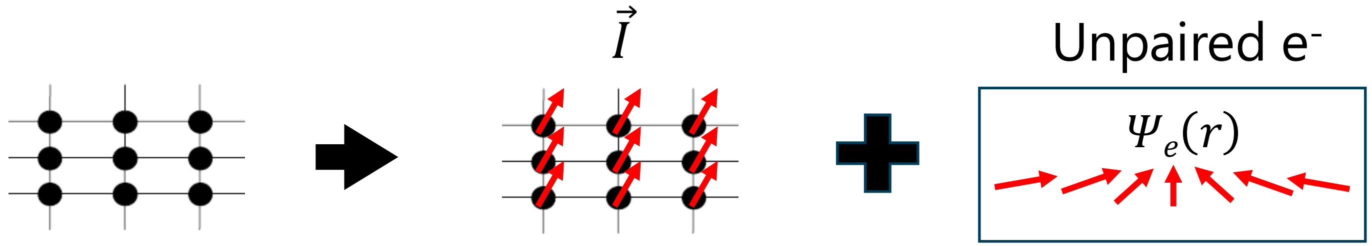
EUROPEAN
SPALLATION
SOURCE

Agenda

1.1 Introduction to Polarization Analysis: Use Cases



$$\hat{V} = V_{nuc}^{coh} + V_{nuc}^{inc} + V_{nuc}^{spin} + V_{el}^{spin}$$

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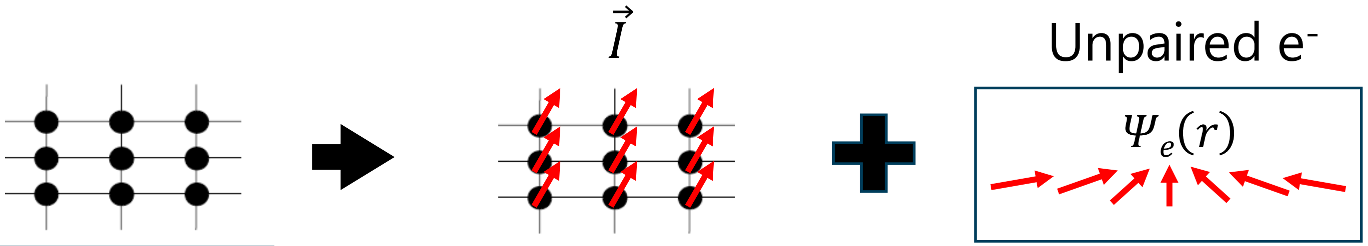

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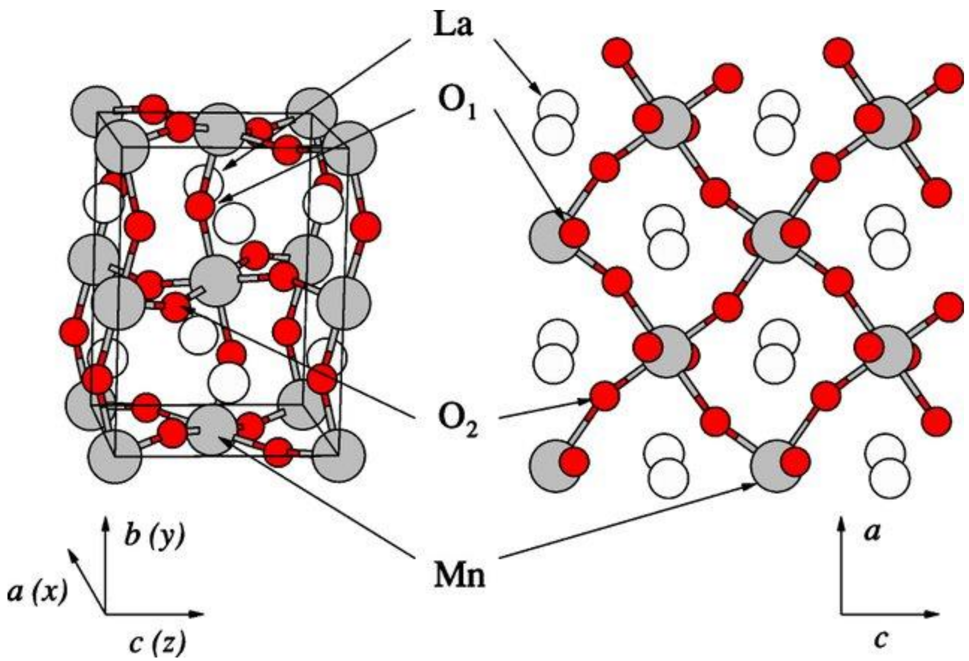

G. Trimarchi et al., PHYSICAL REVIEW B **71**, 035101 (2005)
Example: $LaMnO_3$

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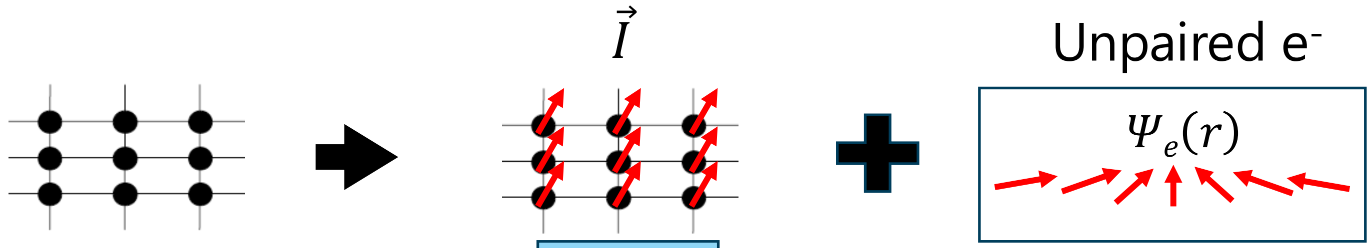

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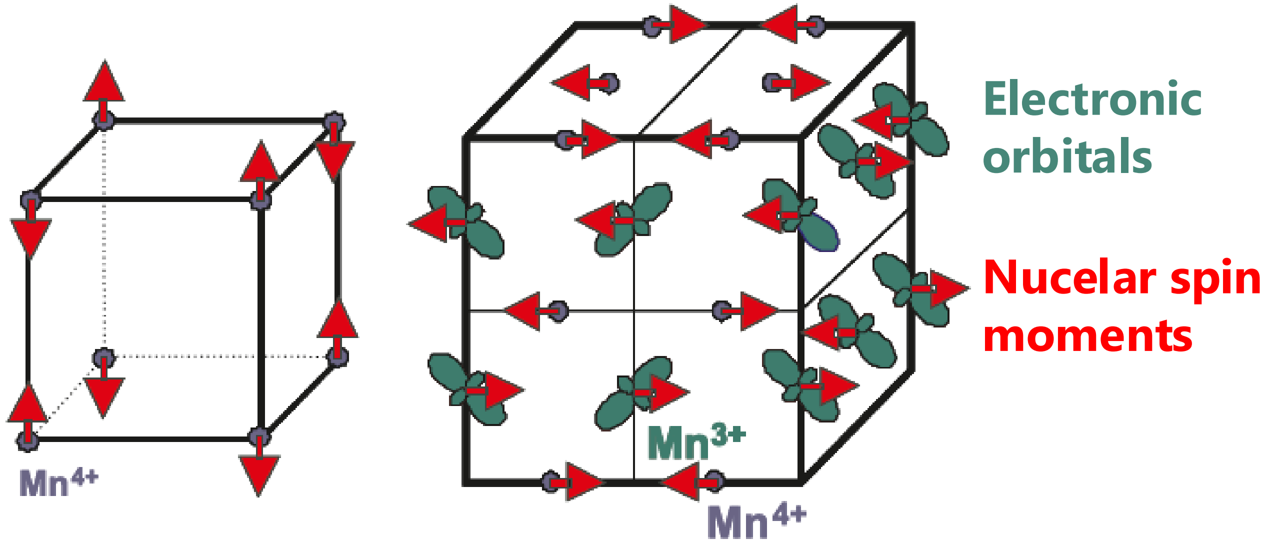

M. Angst, Laboratory course "Neutron Scattering", Ch. 12 (2015). Example: $LaMnO_3$

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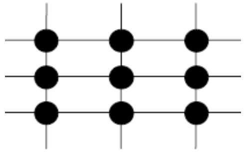
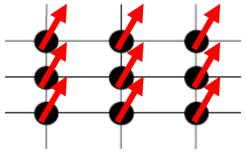
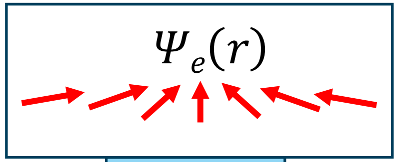


$\vec{I}$



Unpaired e^-



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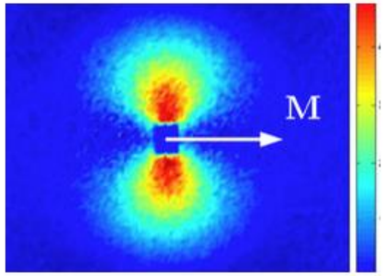
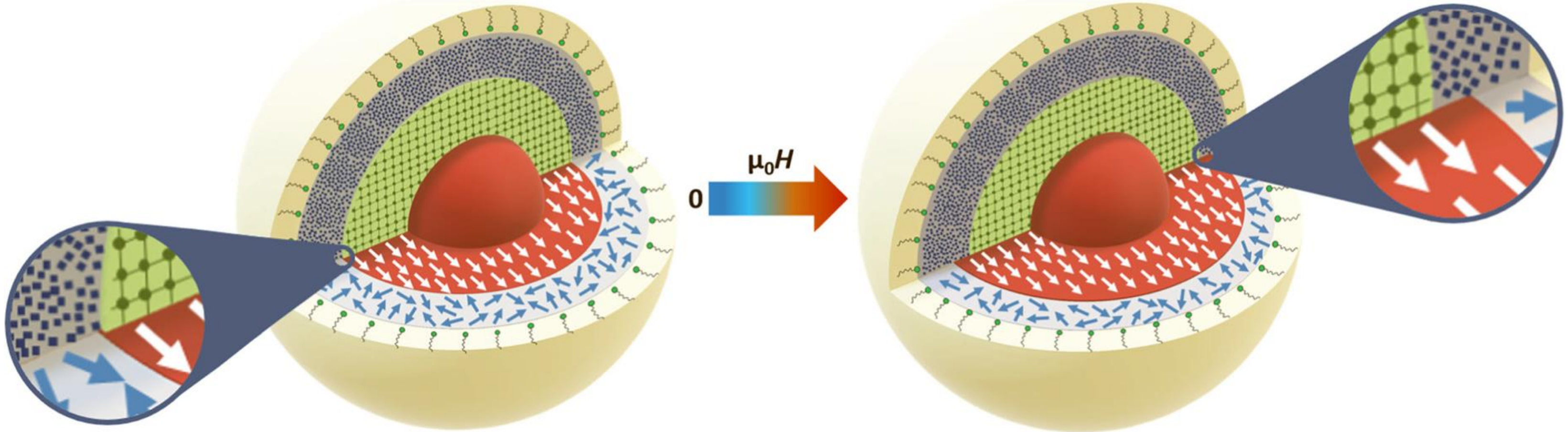
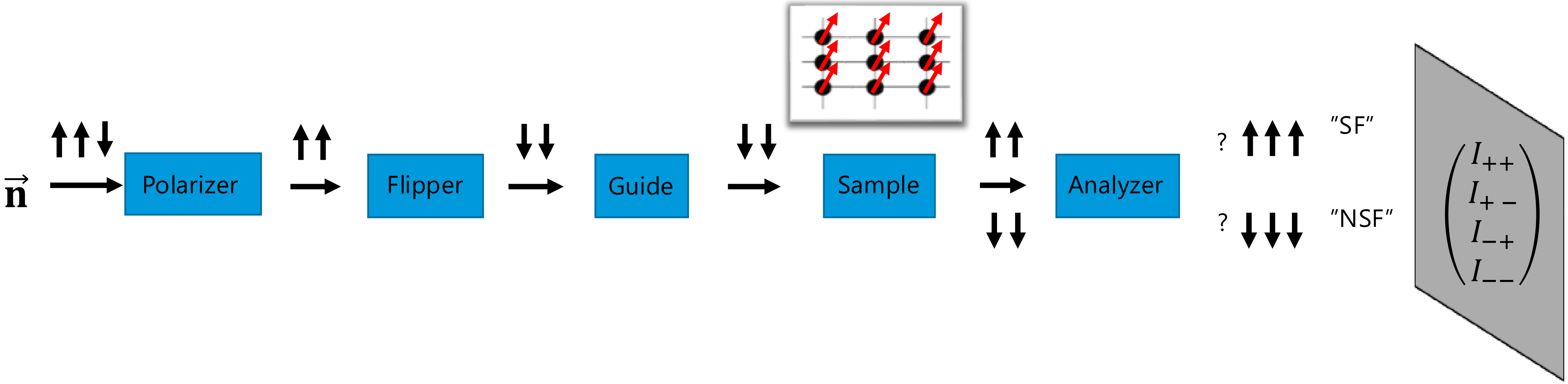




D. Zakutna et al., PHYSICAL REVIEW X 10, 031019 (2020).

1.2 Introduction to Polarization Analysis: Data Reduction



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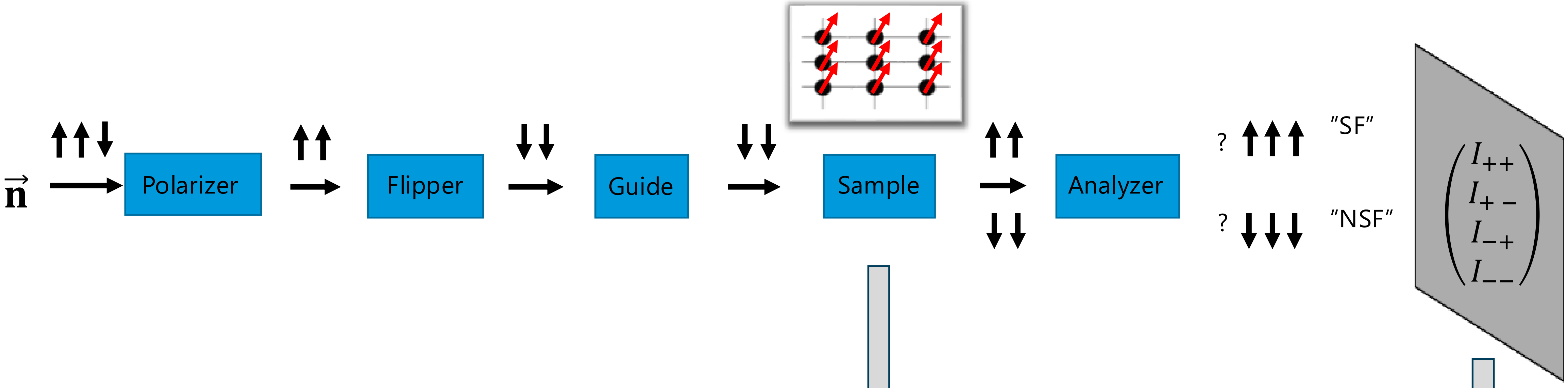

Effect on measured intensities?

$$\frac{d\boldsymbol{\sigma}}{d\Omega} = \begin{pmatrix} S_{++} \\ S_{+-} \\ S_{-+} \\ S_{--} \end{pmatrix} \xleftarrow{\ ?\ } \begin{pmatrix} I_{++} \\ I_{+-} \\ I_{-+} \\ I_{--} \end{pmatrix}$$

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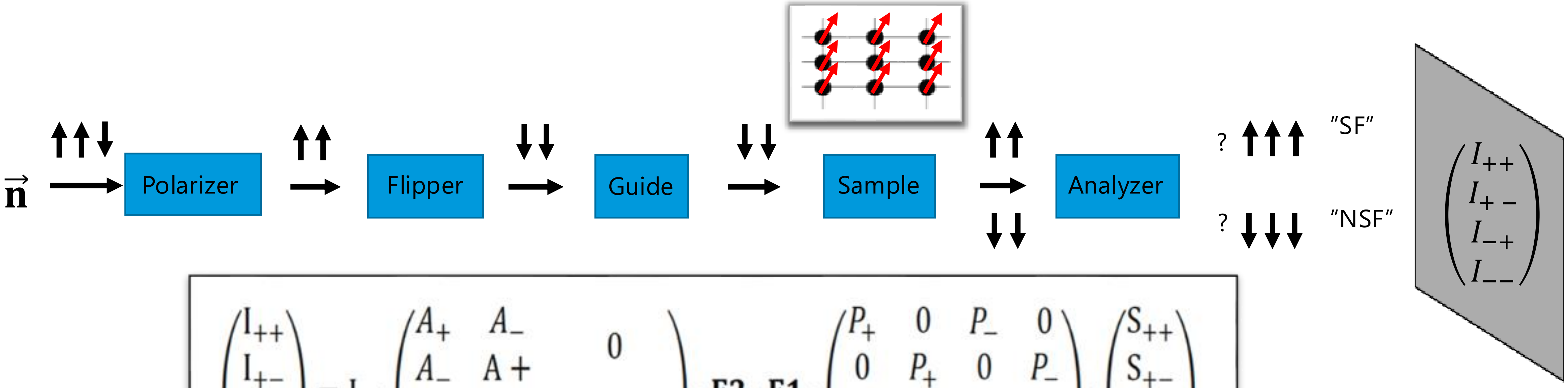


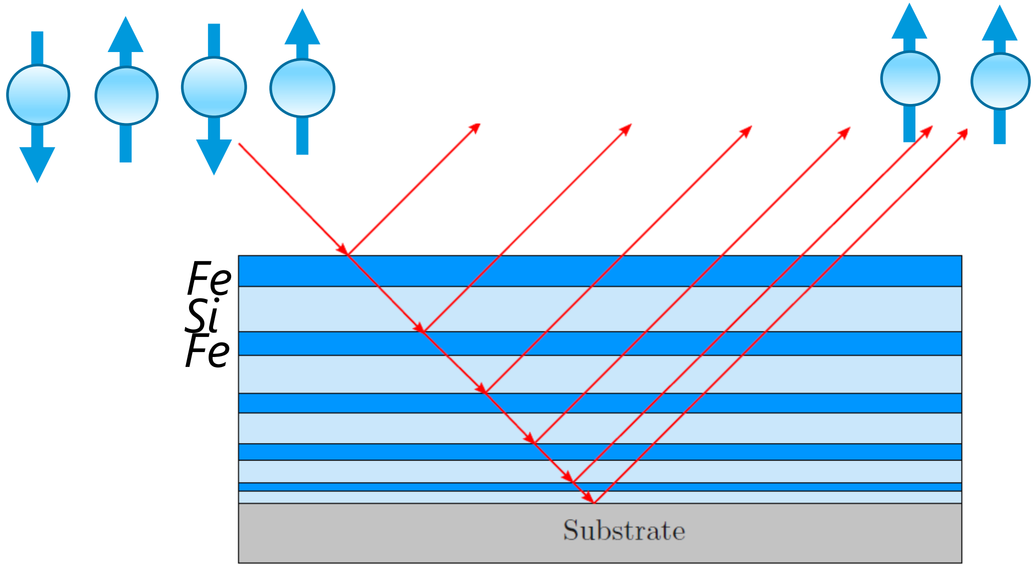
$$\begin{pmatrix} I_{++} \\ I_{+-} \\ I_{-+} \\ I_{--} \end{pmatrix} = I_0 \cdot \begin{pmatrix} A_+ & A_- & 0 & 0 \\ A_- & A+ & 0 & 0 \\ 0 & 0 & A_+ & A_- \\ 0 & 0 & A_- & A_+ \end{pmatrix} \cdot \mathbf{F2} \cdot \mathbf{F1} \cdot \begin{pmatrix} P_+ & 0 & P_- & 0 \\ 0 & P_+ & 0 & P_- \\ P_- & 0 & P_+ & 0 \\ 0 & P_- & 0 & P_+ \end{pmatrix} \cdot \begin{pmatrix} S_{++} \\ S_{+-} \\ S_{-+} \\ S_{--} \end{pmatrix}$$

P = Polariser spin-dependent transmission matrix
A = Analyser spin-dependent transmission matrix
F1, F2 = spin-flipper matrices, if present → If they work with 100% efficiency: ***F1, F2 = 1 (identity matrix)***

Supermirror: $P_\pm = T_P(1 \pm P)/2$, with T being the unpolarised neutron transmission.
^{3}He spin filter: $P_\pm = \exp(-O)\exp(\pm O P_{He})$ with O="Opacity" of ^{3}He cell and P_{He}=^{3}He polarisation
[P, A] = 0 → P & A commute, order does not matter
[P, F] ≠ 0 → the matrices must be in order!

1.3 Introduction to Polarization Analysis: Polarization Components

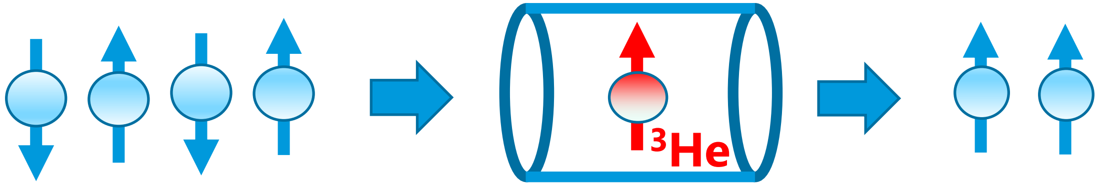
Supermirror



- Total reflection for one spin state, Transmission for other
- Time-independent
- Wavelength-dependent

$$P^{\pm}(t,\lambda) = \mathrm{T}(\lambda)(1 \pm P)/2$$

^{3}He-cell



- Filled with polarized ^{3}He atoms
- Transmission of neutrons with $s_n \parallel s_{He}$
- Wavelength-dependent

(a) Ex-situ pumped: Time-dependent

(b) In-situ pumped: Time-independent

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

2.1 Current Workflow for PA: Scipp implementations

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

$\rightarrow \widehat{PA}$

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
Calculation performed on single events

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

2.2 Current Workflow for PA: Integration with unpolarized SANS

1. **Data reduction to "non-polarization-related" corrections**
   - Masking
   - Normalization
   - Sample thickness correction
   - D(λ) determination

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

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!

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

get

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

$P^{He}(t)$

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

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     - Get correction parameters
   - If SM correction:
     - Fix correction parameters!
   - If Sample correction:
     - Apply previously calculated correction parameters on “Beamline-corrected”-data

$$I(t,\lambda) = \frac{M_{cell}^{trans}}{M_{cell}^{inc}} \frac{M_{nocell}^{inc}}{M_{nocell}^{trans}} \quad \text{get} \Rightarrow \quad A/P^{\pm}(t,\lambda), \quad P^{He}(t)$$

$$I(t,\lambda) = PA\left(\frac{M_{sample}^{trans}}{M_{sample}^{inc}} \frac{M_{DB}^{inc}}{M_{DB}^{trans}}\right) \quad \text{get} \Rightarrow \quad \begin{pmatrix} S^{++} \\ S^{+-} \\ S^{-+} \\ S^{--} \end{pmatrix}(t,\lambda)$$

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2.2 Current Workflow for PA: Integration with unpolarized SANS

1. **"Unpolarized" data reduction**

$$\underbrace{I(spin, lambda, t)\left(\frac{1}{\Omega(x,y)}\left(\frac{\sum_{\Delta t_{shot}}\sum_{\Delta t_{bin}}\frac{C(channel,\lambda,t,x,y)dt}{T_{sample}(\lambda)D(\lambda,x,y)}}{\sum_{\Delta t_{shot}}\sum_{\Delta t_{bin}}M(channel,t,\lambda)}\right)(channel,\lambda,\overline{t_{pulse}})\right)}$$

2. **"Polarized" data reduction:**

$$\sum_{neutron\ pulses}\left(\begin{pmatrix} C^{++}_{PA.corr}(\lambda) \\ C^{+-}_{PA.corr}(\lambda) \\ C^{-+}_{PA.corr}(\lambda) \\ C^{--}_{PA.corr}(\lambda) \end{pmatrix}\right) = \sum_{neutron\ pulses}\left(inv\begin{pmatrix} T_{11}(\lambda) & \cdots & T_{14}(\lambda) \\ \vdots & \ddots & \vdots \\ T_{41}(\lambda) & \cdots & T_{44}(\lambda) \end{pmatrix}\begin{pmatrix} C^{++}_{mon.corr}(\lambda) \\ C^{+-}_{mon.corr}(\lambda) \\ C^{-+}_{mon.corr}(\lambda) \\ C^{--}_{mon.corr}(\lambda) \end{pmatrix}\right)$$

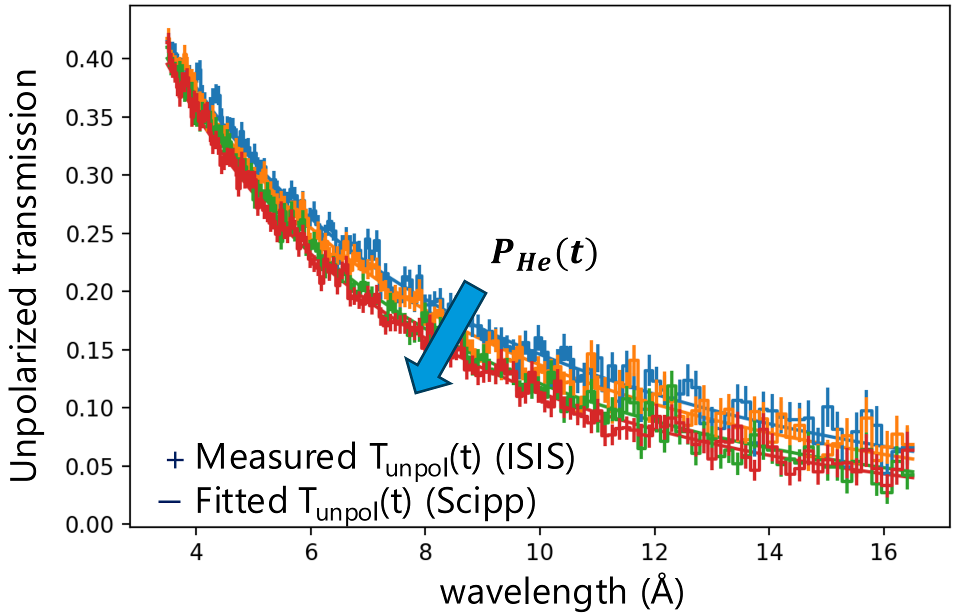
Sum up of neutron pulses

Polarization Efficiency Matrices

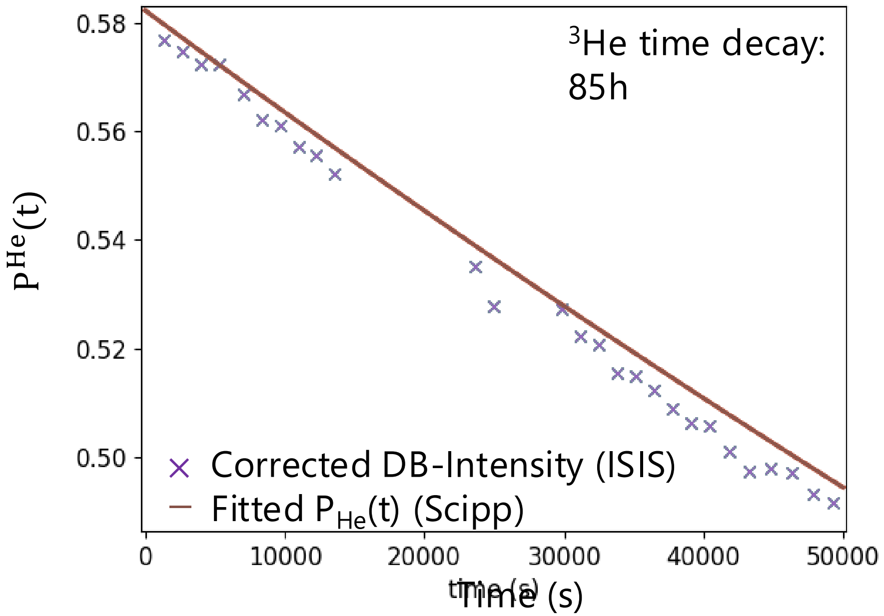
"Unpol." Beamline-corrected I

2.3 Current Workflow for PA: Tests

Direct-Beam Transmission measurements:



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

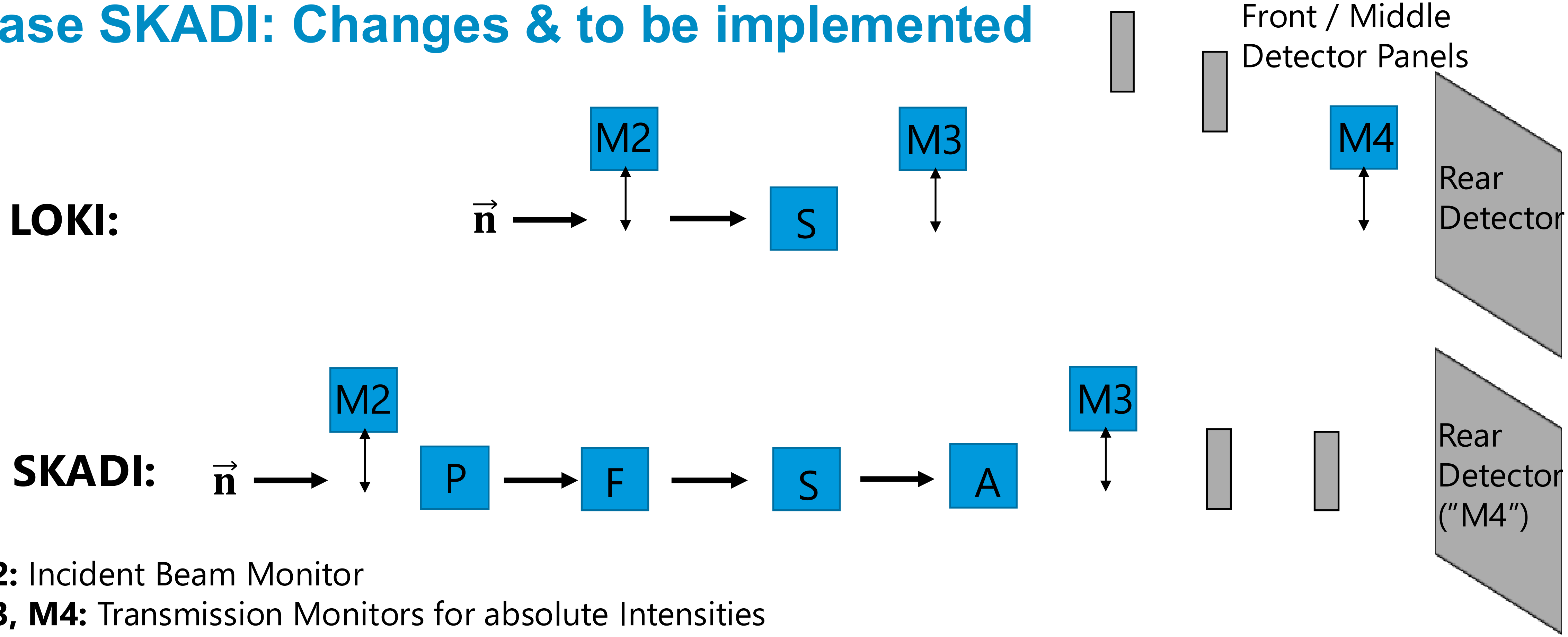


$$I(t,\lambda) = \frac{M_{cell}^{trans}}{M_{cell}^{inc}} \frac{M_{nocell}^{inc}}{M_{nocell}^{trans}}$$

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

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

3. Case SKADI: Changes & to be implemented



M2: Incident Beam Monitor
M3, M4: Transmission Monitors for absolute Intensities

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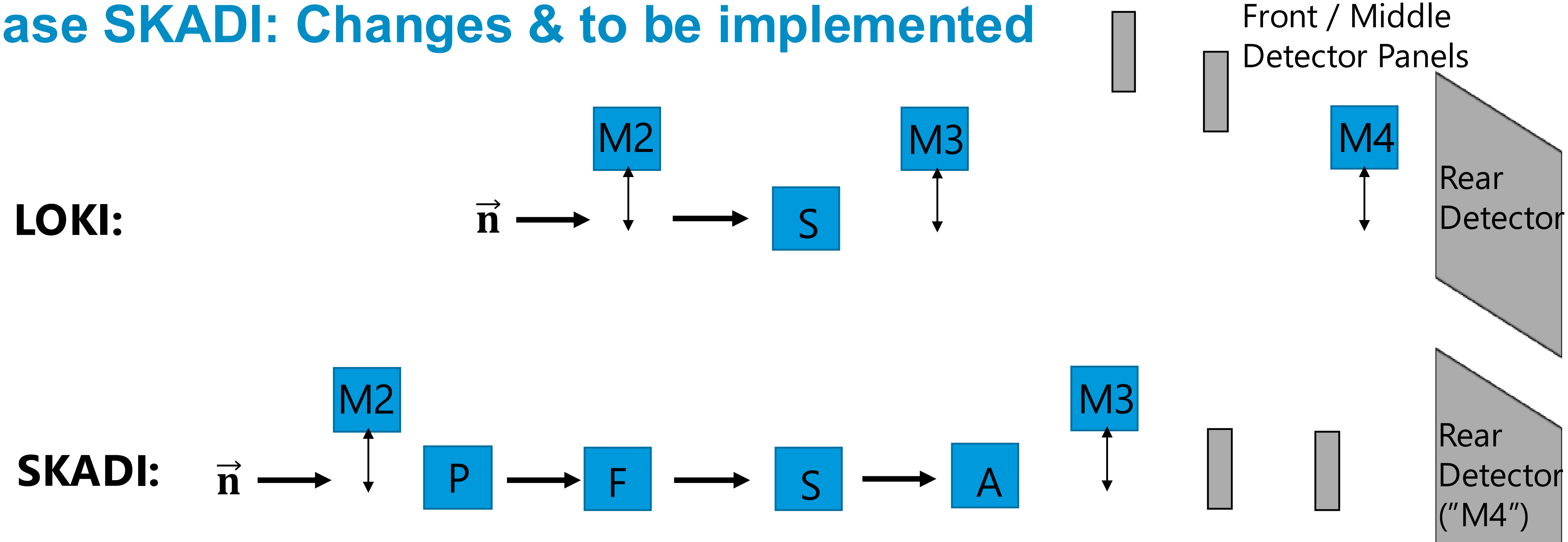

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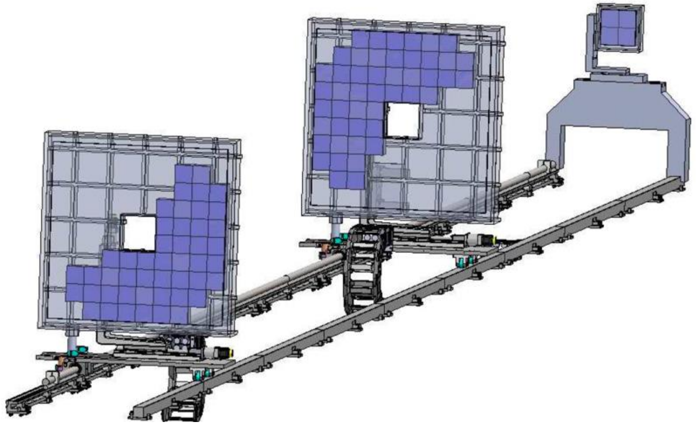
Changes in workflow from LoKI to SKADI & ToDo:

- Primary beam detector is not a seperate 1D monitor, but the SANS 2D rear detector
- Additional beam profile masking
- Different detector arrangements
- 1st phase: Ex-situ ^{3}He analyzer
- 2nd phase: In-situ ^{3}He analyzer



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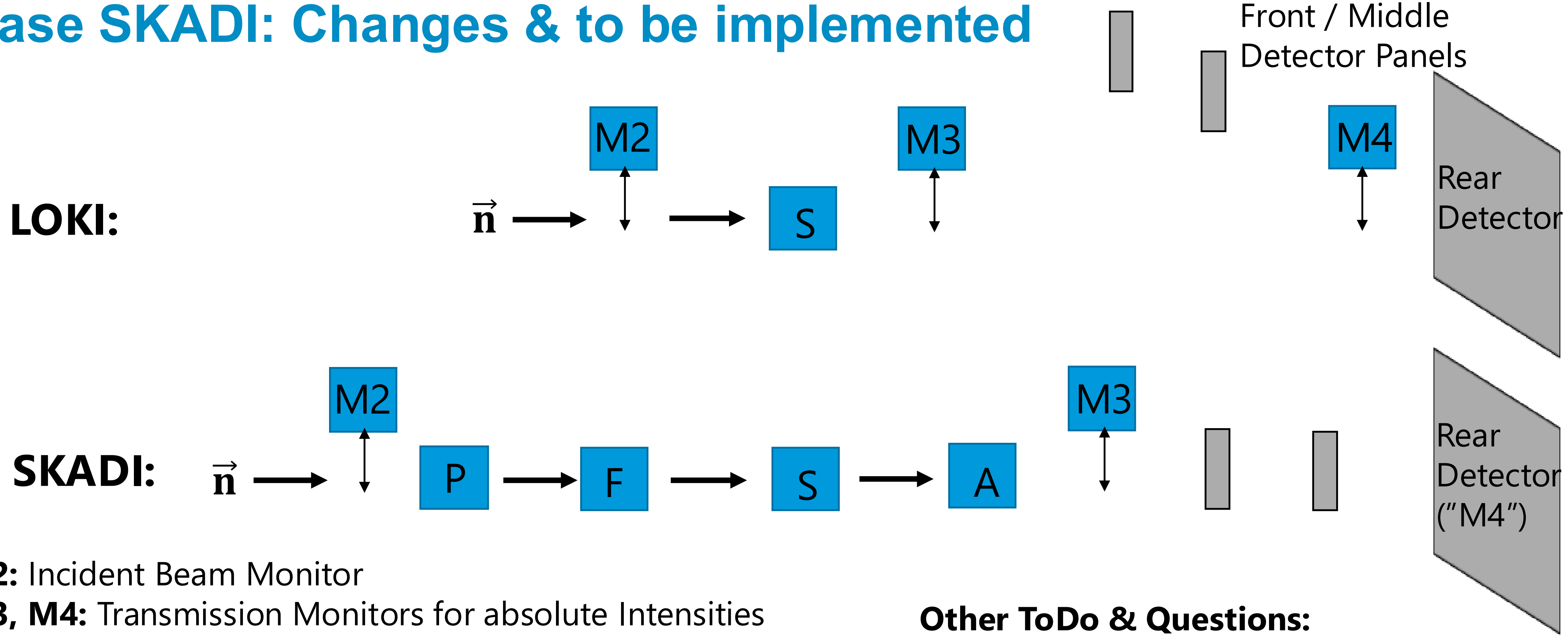

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Other ToDo & Questions:

- Reduction of full-PA test-measurements with incoming polarized beam missing
- Test supermirror matrix-component fitting
- Add option of sample depolarization
- Add interface for users?
- Proceed with previous scipp-workflow together with Oliver?
- Implementation of PA to Milans' script

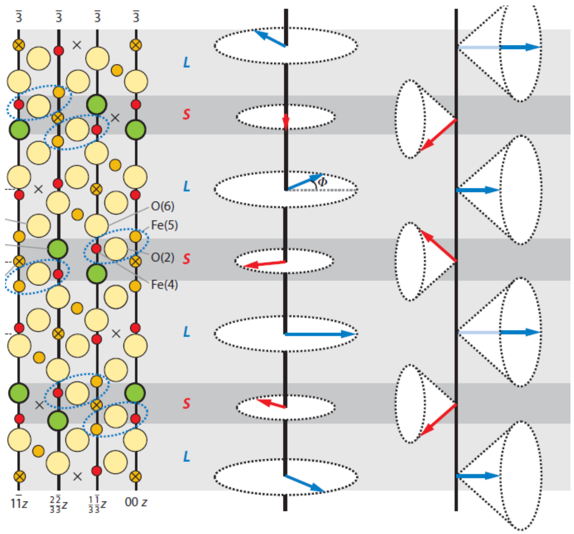
4. Future vision: instrument independent workflows?

Questions:

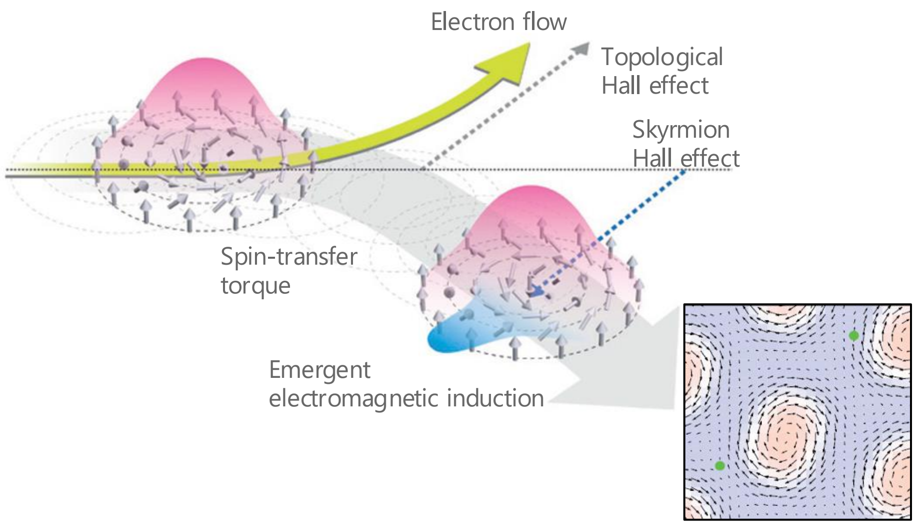
- Shall / can the SANS-workflow be transferred to other instruments?
  - E.g. Diffraction? Imaging?
- Plans for development of a GUI, including polarization components?
- Polarization-day for all polarization-equipped instruments?
  - Presenting status of data workflows
  - Presenting beamline-specific aspects
  - Discussing on "what can be taken over"?

ESS – the users' future choice for PA-measurements!!!

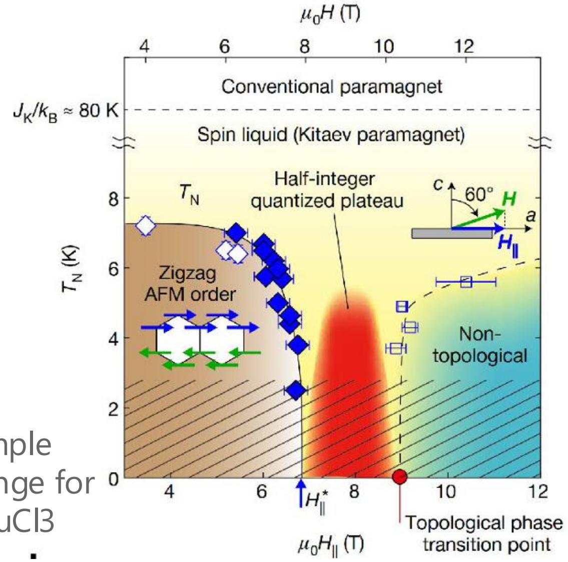
Ferroelectric materials



Skyrmions



Designer Quantum Matter



Example B-range for α−RuCl3

Attachments