

Techniques for neutron spin manipulations

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Content

- ✦ Beam polarisation vector
- ✦ Spin flippers and Spin filters
- ✦ Cross-section & scattered polarisation vector
- ✦ PND — Polarised neutron diffraction (powder, crystal)
- ✦ UPA — Uniaxial polarisation analysis
- ✦ SNP — Spherical neutron polarimetry
- ✦ PNSE — Polarimetric neutron spin-echo

Content

- ✦ **Beam polarisation vector**
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Beam polarisation vector

neutron spin & neutron magnetic moment

- The neutron carries a spin \vec{s} which is an internal angular momentum with a quantum number $s = 1/2$. The general spin wave of an itinerant neutron is:

$$|\chi\rangle = a|+\rangle + b|-\rangle \text{ where } |a|^2 + |b|^2 = 1$$

- The 3 components of this angular momentum are given by the Pauli matrices representing $\vec{\sigma} = 2\vec{s}/\hbar$:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Beam polarisation vector

neutron spin & neutron magnetic moment

- The neutron carries a magnetic moment:

$$\mu_n = \gamma_n \mu_B \vec{\sigma} \text{ where } \gamma_n = -1.913$$

- The gyromagnetic ratio of the neutron is the ratio between the magnetic moment and the spin moment:

$$\vec{\mu}_n = \gamma_L \vec{s}$$

$$\text{where } \gamma_L = \frac{2\gamma_n \mu_B}{\hbar} = -1.832 \cdot 10^8 \text{ rad.s}^{-1} \cdot \text{T}^{-1}$$

NB: the magnetic moment and spin are opposed.

Beam polarisation vector

polarisation of a neutron beam

- The neutron beam is a statistical ensemble of several quantum states and the beam polarisation $\vec{P} = \langle \vec{\sigma} \rangle$.
- We use the density matrix formalism to describe this statistical quantum system:

$$\hat{\rho} = \frac{1}{2} \left(\mathbb{1} + \vec{\sigma} \cdot \vec{P} \right) = \frac{1}{2} \begin{bmatrix} 1 + P_z & P_x - iP_y \\ P_x + iP_y & 1 - P_z \end{bmatrix}$$

Only 3 real numbers are required to describe this 2x2 matrix, i.e. the statistical quantum situation.

Beam polarisation vector

polarisation of a neutron beam

- The beam polarisation can therefore be seen as a vector in space:

$$\vec{P} = \langle \vec{\sigma} \rangle = \text{trace} (\hat{\rho} \vec{\sigma})$$

- We can measure each of the 3 orthogonal components in any arbitrary direction \vec{u} in space:

$$P_u = \text{trace} [\hat{\rho} (u_x \sigma_x + u_y \sigma_y + u_z \sigma_z)]$$

Beam polarisation vector

polarisation of a neutron beam

- Experimentally, we always measure the component parallel to the field direction (quantisation axis):

$$P = \frac{(r_{p,+} - r_{b,+}) - (r_{p,-} - r_{b,-})}{(r_{p,+} - r_{b,+}) + (r_{p,-} - r_{b,-})}$$

$$\sigma_P^2 = 4 \frac{(r_{p,+} - r_{b,+})^2 (\sigma_{r_{p,-}}^2 + \sigma_{r_{b,-}}^2) + (r_{p,-} - r_{b,-})^2 (\sigma_{r_{p,+}}^2 + \sigma_{r_{b,+}}^2)}{(r_{p,+} - r_{b,+} + r_{p,-} - r_{b,-})^4}$$

where r is a neutron count rate, p/b stand for peak/background, +/- for the spin states.

Beam polarisation vector

polarisation of a neutron beam

- For historical reasons, some people prefer to measure the *flipping ratio*:

$$R = \frac{r_{p,+} - r_{b,+}}{r_{p,-} - r_{b,-}} \quad \left(\text{and } P = \frac{R - 1}{R + 1} \right)$$

$$\sigma_R^2 = \frac{(r_{p,+} - r_{b,+})^2 (\sigma_{r_{p,-}}^2 + \sigma_{r_{b,-}}^2) + (r_{p,-} - r_{b,-})^2 (\sigma_{r_{p,+}}^2 + \sigma_{r_{b,+}}^2)}{(r_{p,-} - r_{b,-})^4}$$

but it has no physical meaning and P is recommended.

Beam polarisation vector

polarisation of a neutron beam

- ✦ You can optimise the distribution of the times spent on the peak, the background and the [+] and [-] spin states to reduce the error bar.

Hopelessly, only [+] / [-] counting times can be optimised with a 2D detector.

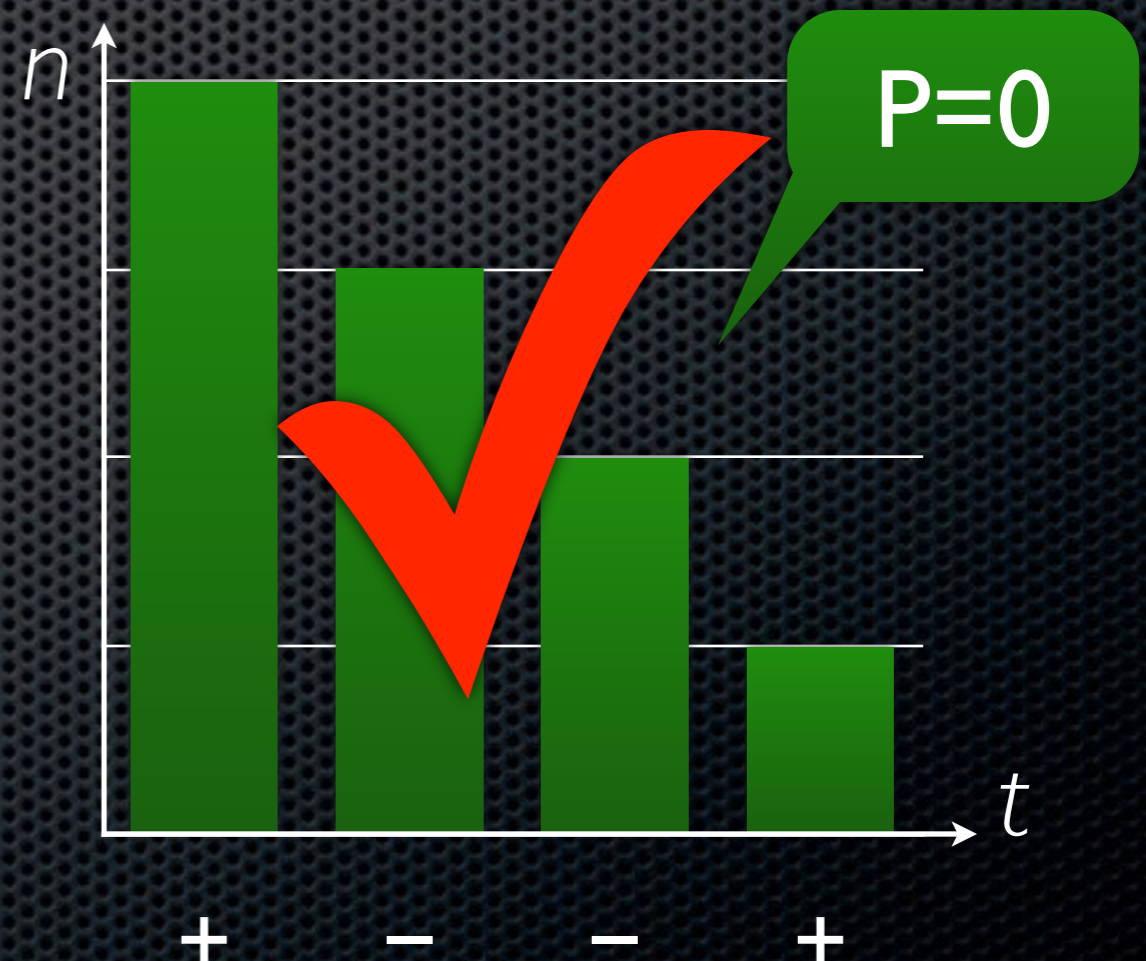
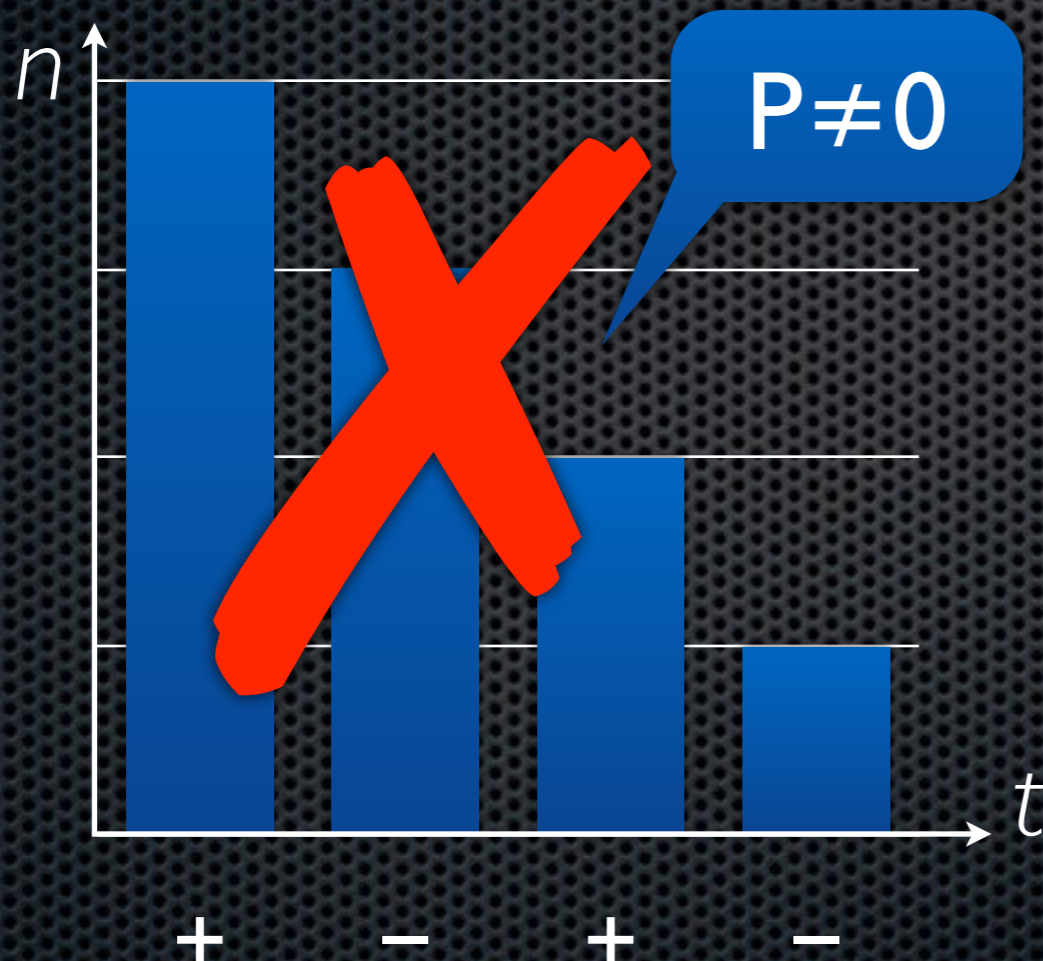
See <http://www.ill.eu/sane/software/xop-plugins-for-igor-pro/neutron-scattering-xop/> for an Igor Pro XOP providing all routines.



Beam polarisation vector

polarisation of a neutron beam

- You must compensate for the variations of the incident flux: choose the right sequence and a stable detector.



Beam polarisation vector

polarisation of a neutron beam

- Using a *flipping control unit*, you can also minimise the error bar by taking advantage of the high-precision clock of your counter:

$$P_{opt} = \frac{M_b t_p t_{b,+} t_{b,-} (N_{p,+} t_{p,-} - N_{p,-} t_{p,+}) - M_p t_b t_{p,+} t_{p,-} (N_{b,+} t_{b,-} - N_{b,-} t_{b,+})}{M_b t_p t_{b,+} t_{b,-} (N_{p,+} t_{p,-} + N_{p,-} t_{p,+}) - M_p t_b t_{p,+} t_{p,-} (N_{b,+} t_{b,-} + N_{b,-} t_{b,+})}$$

$$\sigma_{P_{opt}}^2 = \frac{M_b t_p^2 t_{b,+}^2 t_{b,-}^2}{P_d^2} \left[\begin{array}{l} ((1 + P_{opt}) t_{p,+} N_{p,-} - (1 - P_{opt}) t_{p,-} N_{p,+})^2 + \\ M_b \left((1 + P_{opt})^2 t_{p,+}^2 N_{p,-}^2 + (1 - P_{opt})^2 t_{p,-}^2 N_{p,+}^2 \right) \end{array} \right] + \frac{M_p t_b^2 t_{p,+}^2 t_{p,-}^2}{P_d^2} \left[\begin{array}{l} ((1 + P_{opt}) t_{b,+} N_{b,-} - (1 - P_{opt}) t_{b,-} N_{b,+})^2 + \\ M_p \left((1 + P_{opt})^2 t_{b,+}^2 N_{b,-}^2 + (1 - P_{opt})^2 t_{b,-}^2 N_{b,+}^2 \right) \end{array} \right]$$

with $P_d =$ denominator of P_{opt}

Beam polarisation vector

polarisation of a neutron beam

- ✦ Heusler Cu_2MnAl crystals: monochromatised beam, large $\lambda/2$ contamination, ≈ 15 cm height max. (mag. saturation), 95% polarisation with some variation on the beam section.
- ✦ Polarising supermirrors: efficient above $\approx 2\text{\AA}$, 85-95% polarisation but angular dependent unless in crossed geometry (reduced transmission).
- ✦ ^3He spin filters: polarisation decoupled from optical functions, compromise polarisation/transmission.

Beam polarisation vector

the action of a magnetic field

- In a magnetic field, the polarisation rotates around the field in a Larmor precession with the frequency:

$$\omega_L(\text{rad/s}) = 18\,325\, B(\text{G})$$

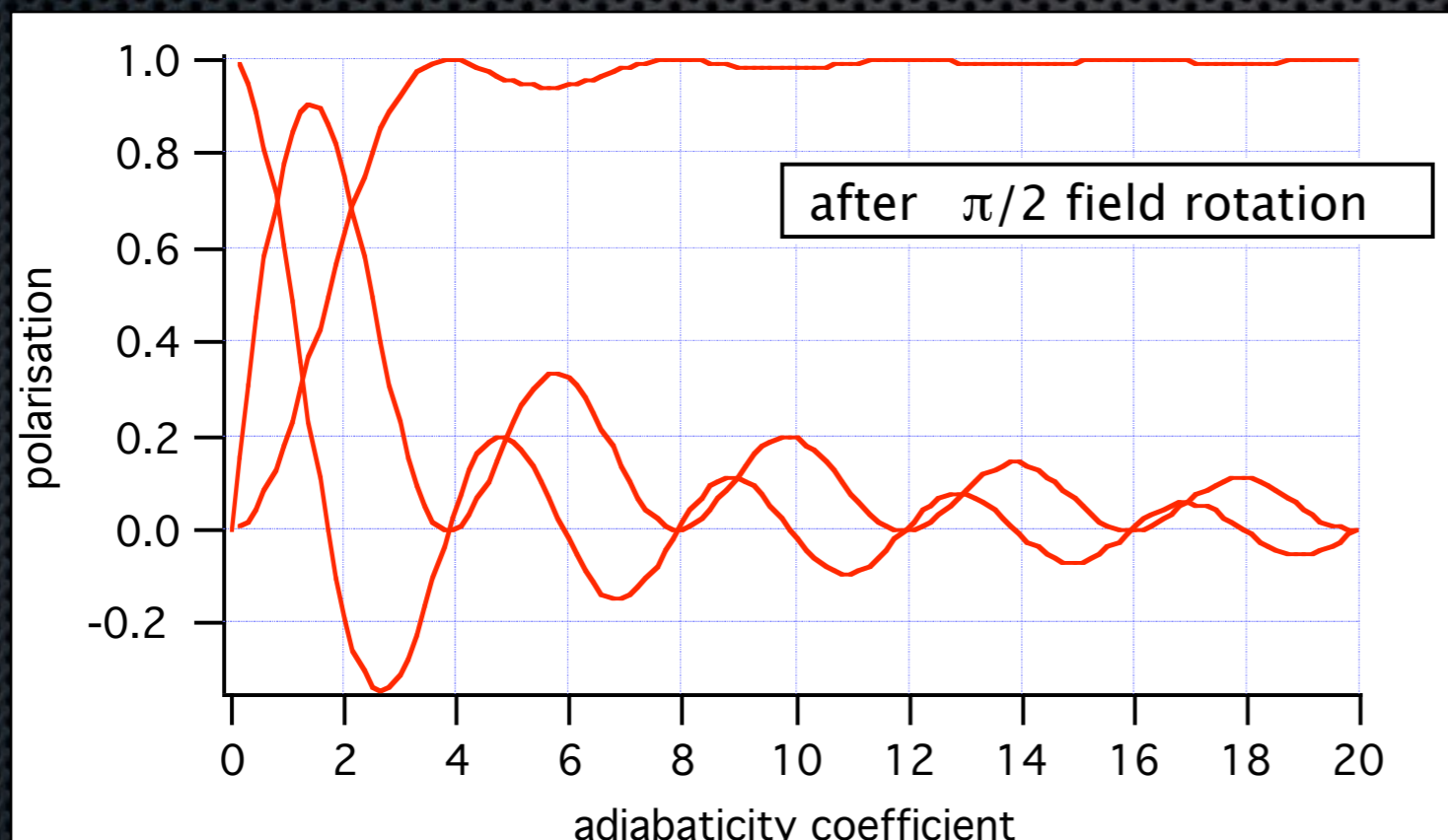
- With B aligned along the z -axis, we find:

$$\begin{cases} P_x(t) = \cos(\omega_L \cdot t) P_x(0) - \sin(\omega_L \cdot t) P_y(0) \\ P_y(t) = \sin(\omega_L \cdot t) P_x(0) + \cos(\omega_L \cdot t) P_y(0) \\ P_z(t) = P_z(0) \end{cases}$$

Beam polarisation vector

the action of a magnetic field

- If the guiding field rotates slowly compared to the Larmor precession frequency, the polarisation is transported adiabatically.



$$E = \frac{\omega_L}{\omega_B} \gg 30$$

Zeeman
energy
conserved

Beam polarisation vector

the action of a magnetic field

- If the guiding field rotates slowly compared to the Larmor precession frequency, the polarisation is transported adiabatically.

Typically, for a 90° rotation over 10 cm

λ [Å]	0.4	1	4	10
B [G]	255	102	25	10

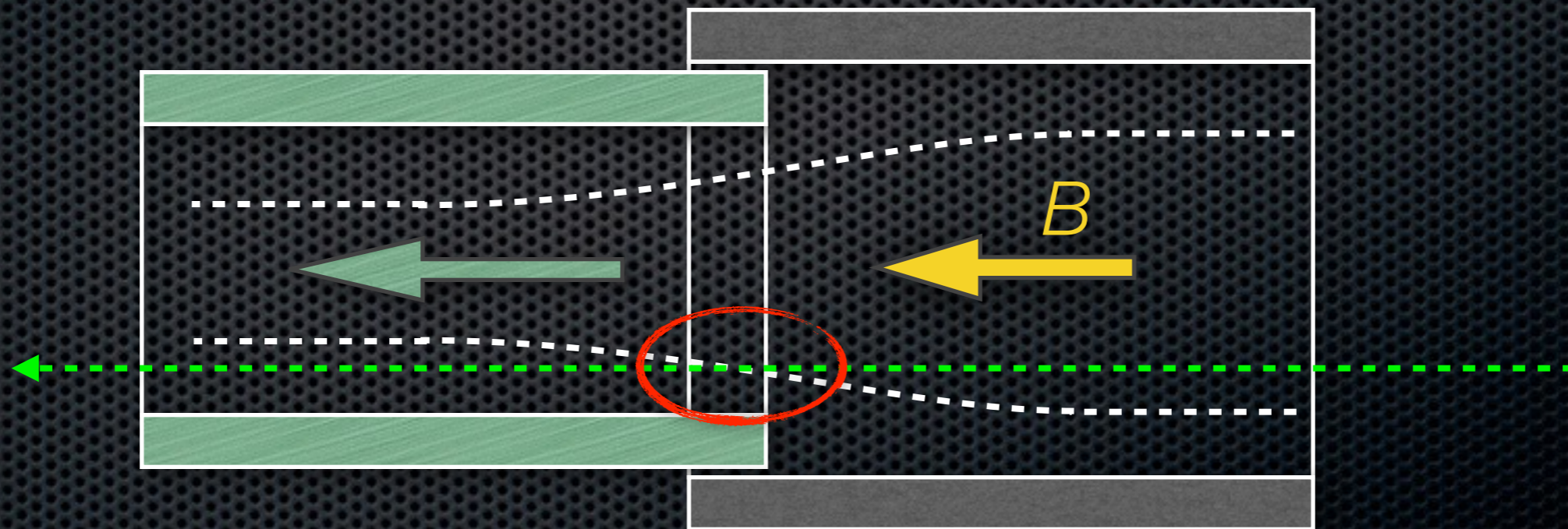
$$E = \frac{\omega_L}{\omega_B} \gg 30$$

Zeeman
energy
conserved

Beam polarisation vector

the action of a magnetic field

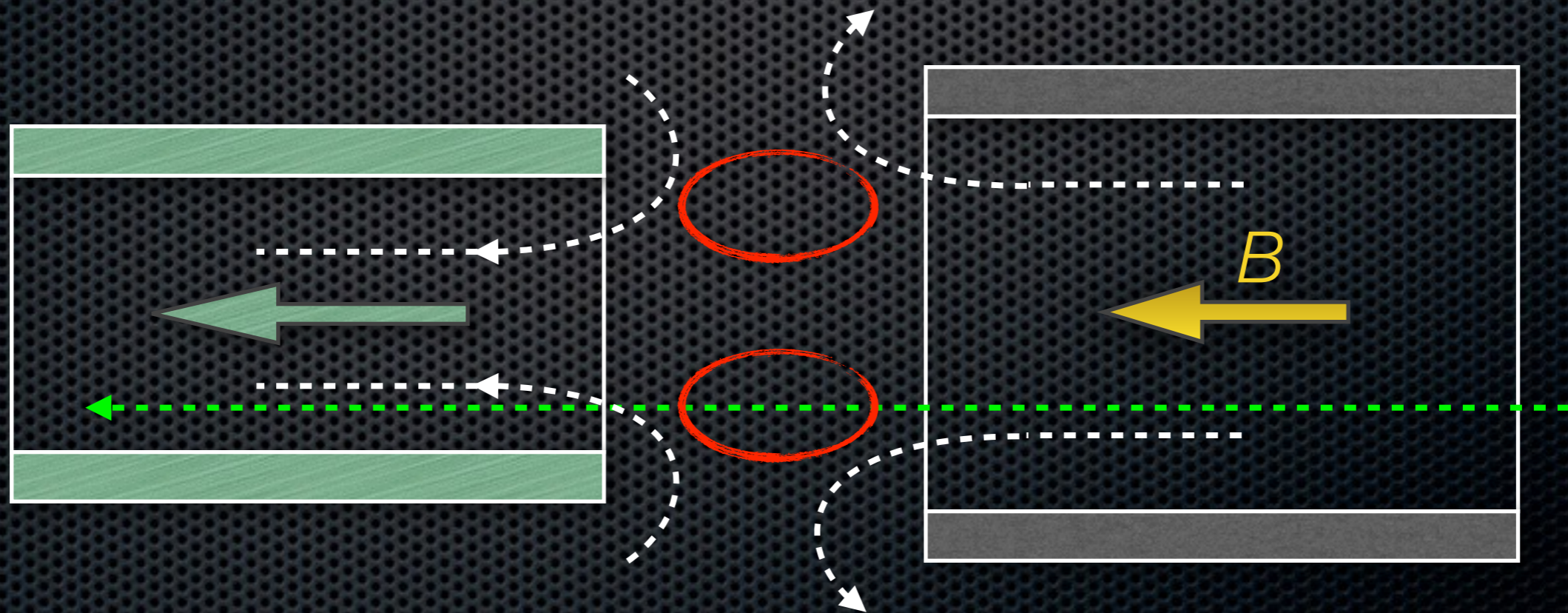
- When setting up guiding fields, always be careful with the reduction of the field amplitude at the location where neutrons see a field rotation.



Beam polarisation vector

the action of a magnetic field

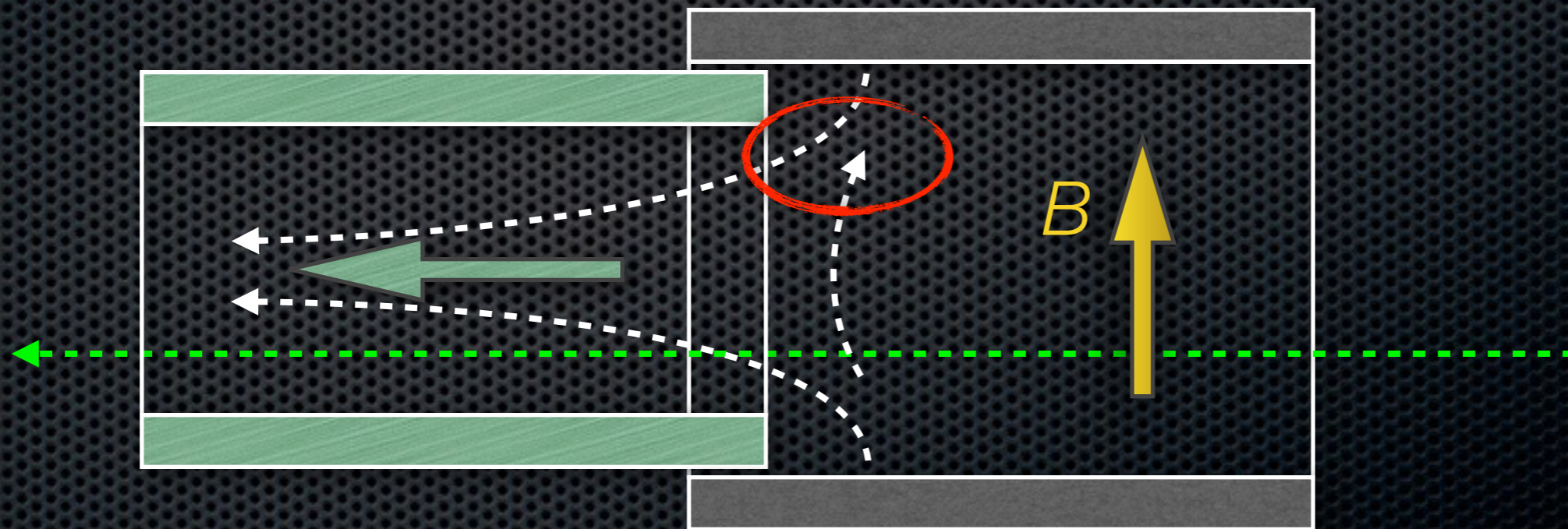
- The gaps between guiding field coils can lead to depolarisation, even when the fields are parallel. Also true for permanent magnets.



Beam polarisation vector

the action of a magnetic field

- ✦ In spin rotators, the loss of polarisation generally comes from the region where the fields cancel, which is also where the field (polarisation) rotates.



Beam polarisation vector

the action of a magnetic field

- The Magnaprobe is a very useful tool. It illustrates very well the true shape of the magnetic field...

but NOT its magnitude !

λ [Å]	0.4	1	4	10
B [G]	255	102	25	10



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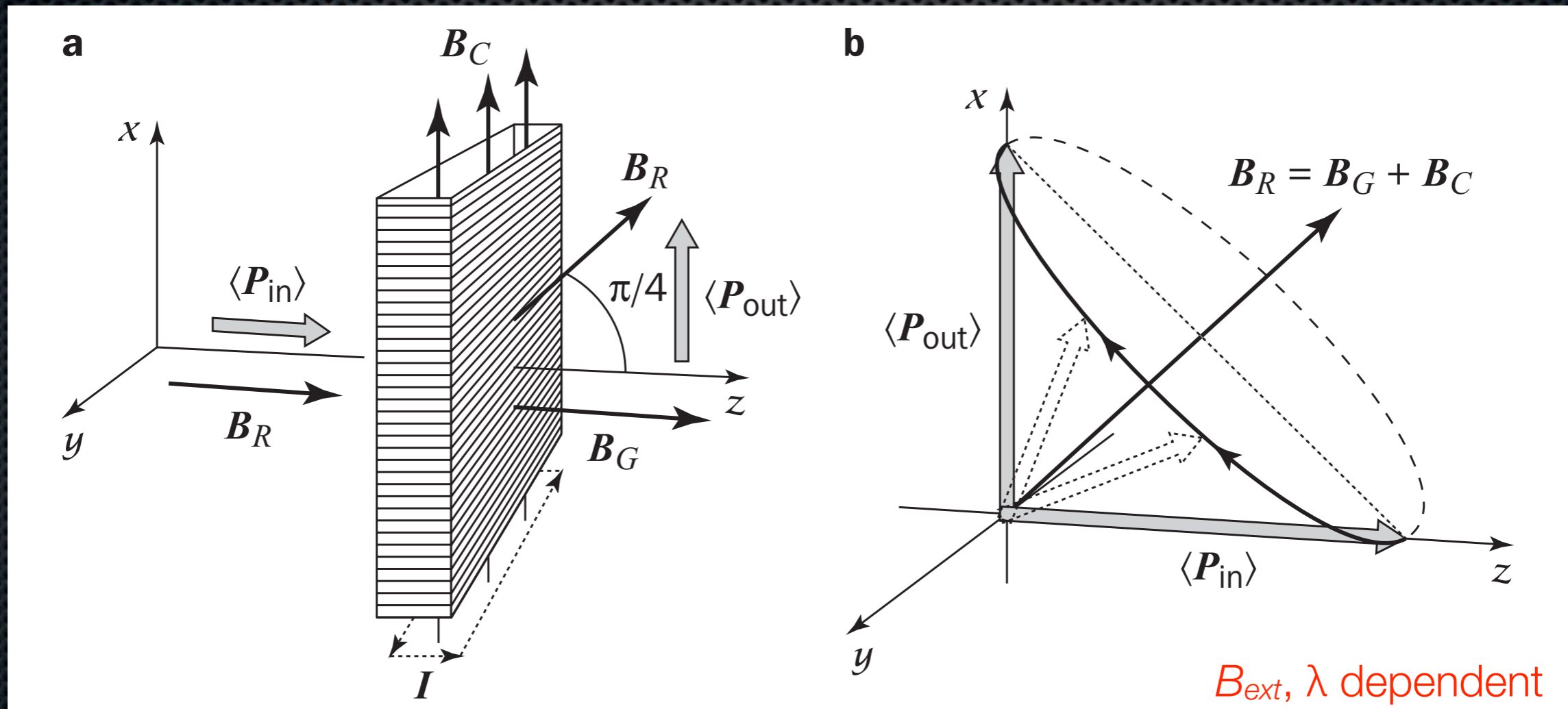
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Spin Flippers & Spin Filters

Mezei's flipper

- Example of a $\pi/2$ flipper: the neutrons enter and exit the coil non-adiabatically.

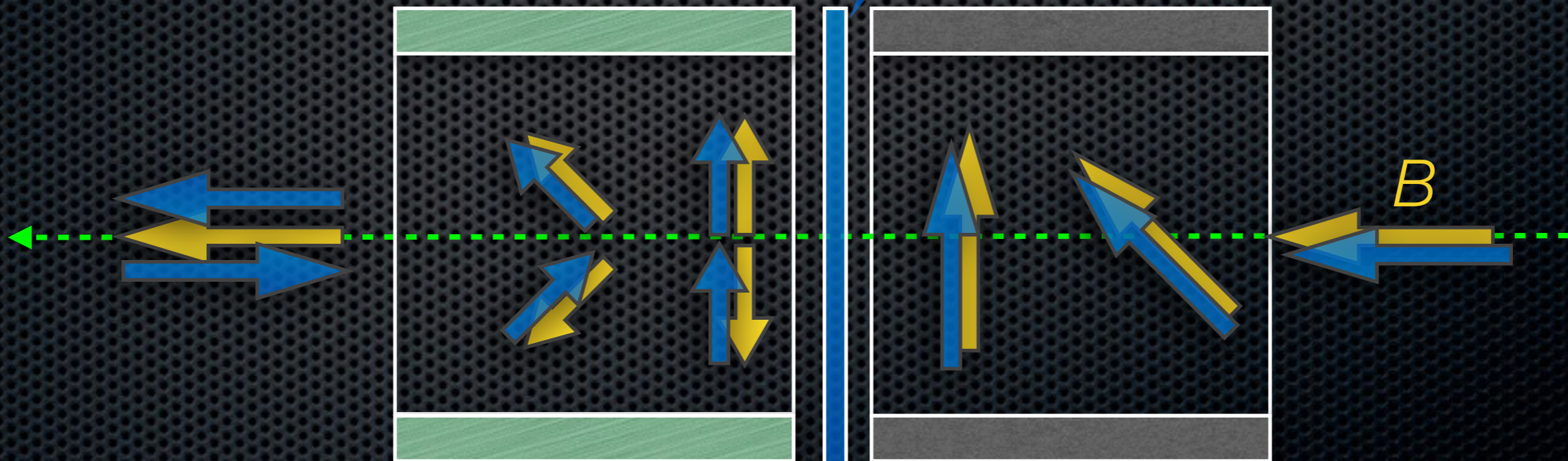


Spin Flippers & Spin Filters

Tasset's cryoflipper

- The neutrons enter the second coil non-adiabatically. Perfect flipper even in 400 Gauss stray field.

B_{ext} and λ independent
but Al and Nb in the beam



Spin Flippers ...

Tasset's cryoflipper

- ✦ 99.9% efficient
- ✦ $\lambda > 0.4 \text{ \AA}$
- ✦ 10L liquid He
- ✦ 3 weeks autonomy
- ✦ Al & Nb in beam
- ✦ To be cooled down in zero field !

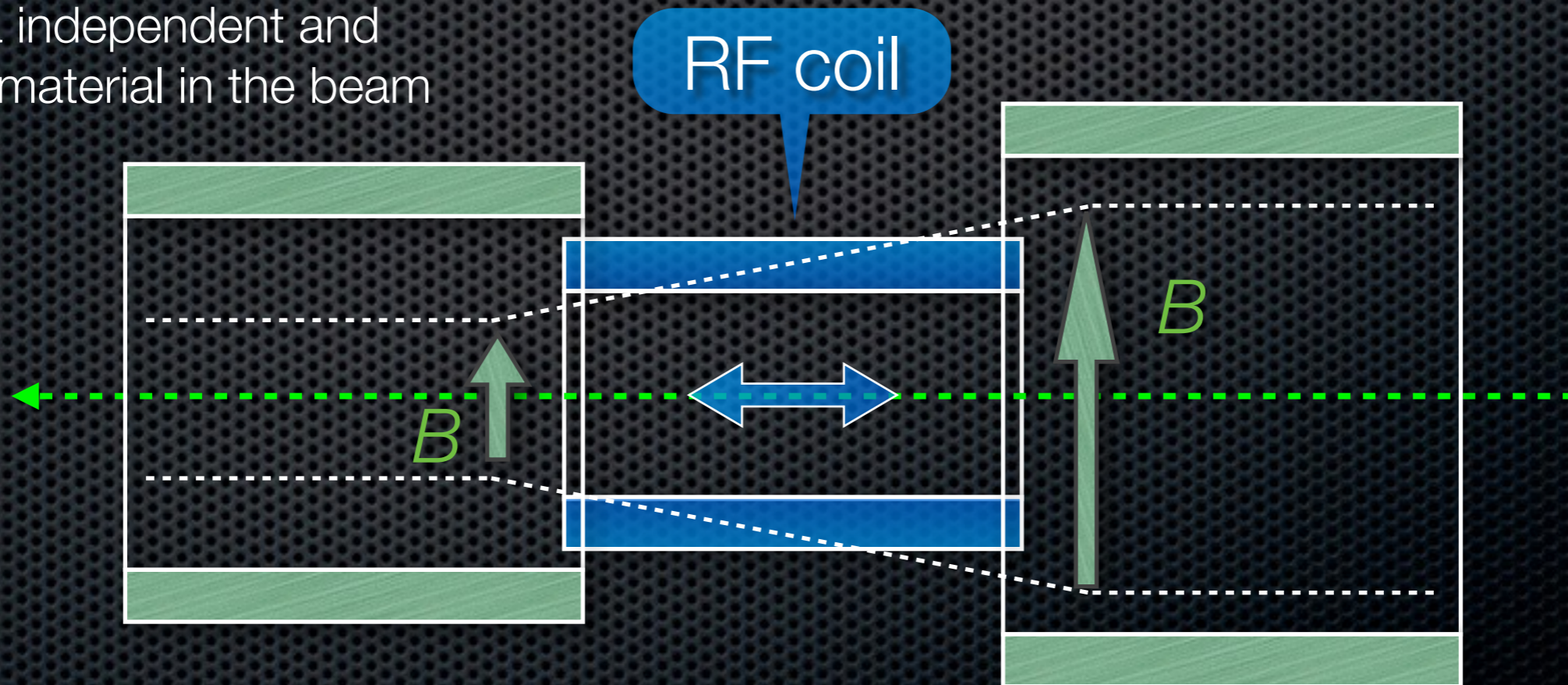


Spin Flippers & Spin Filters

RF adiabatic flipper

- In the rotating frame of the neutron, the polarisation follows the effective field and rotates adiabatically.

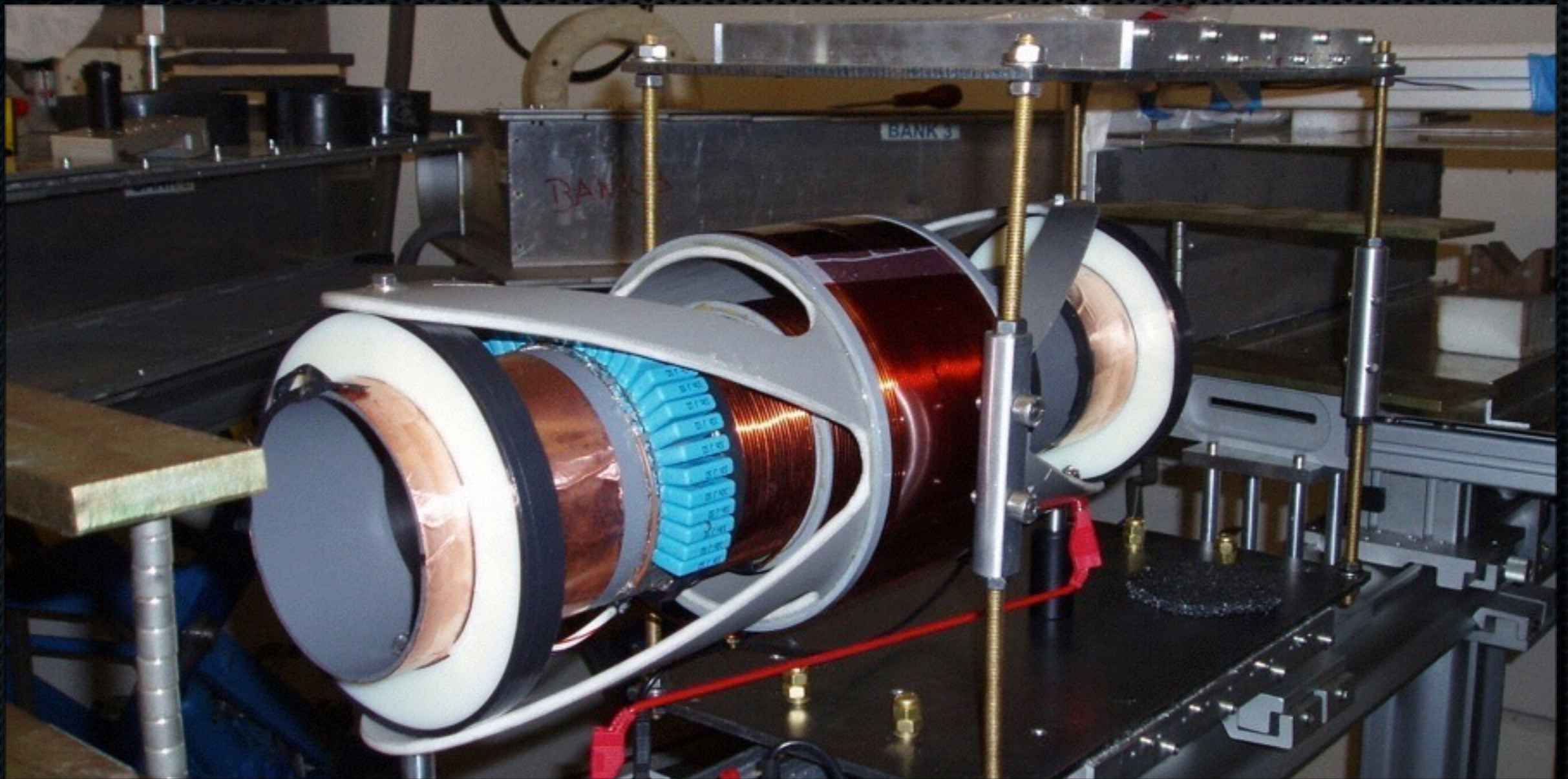
λ independent and
no material in the beam



Spin Flippers & Spin Filters

RF adiabatic flipper

153 kHz/10 A adiabatic flipper for $\lambda > 0.4 \text{ \AA}$



Spin Flippers & Spin Filters

^3He spin filters: optimised opacity

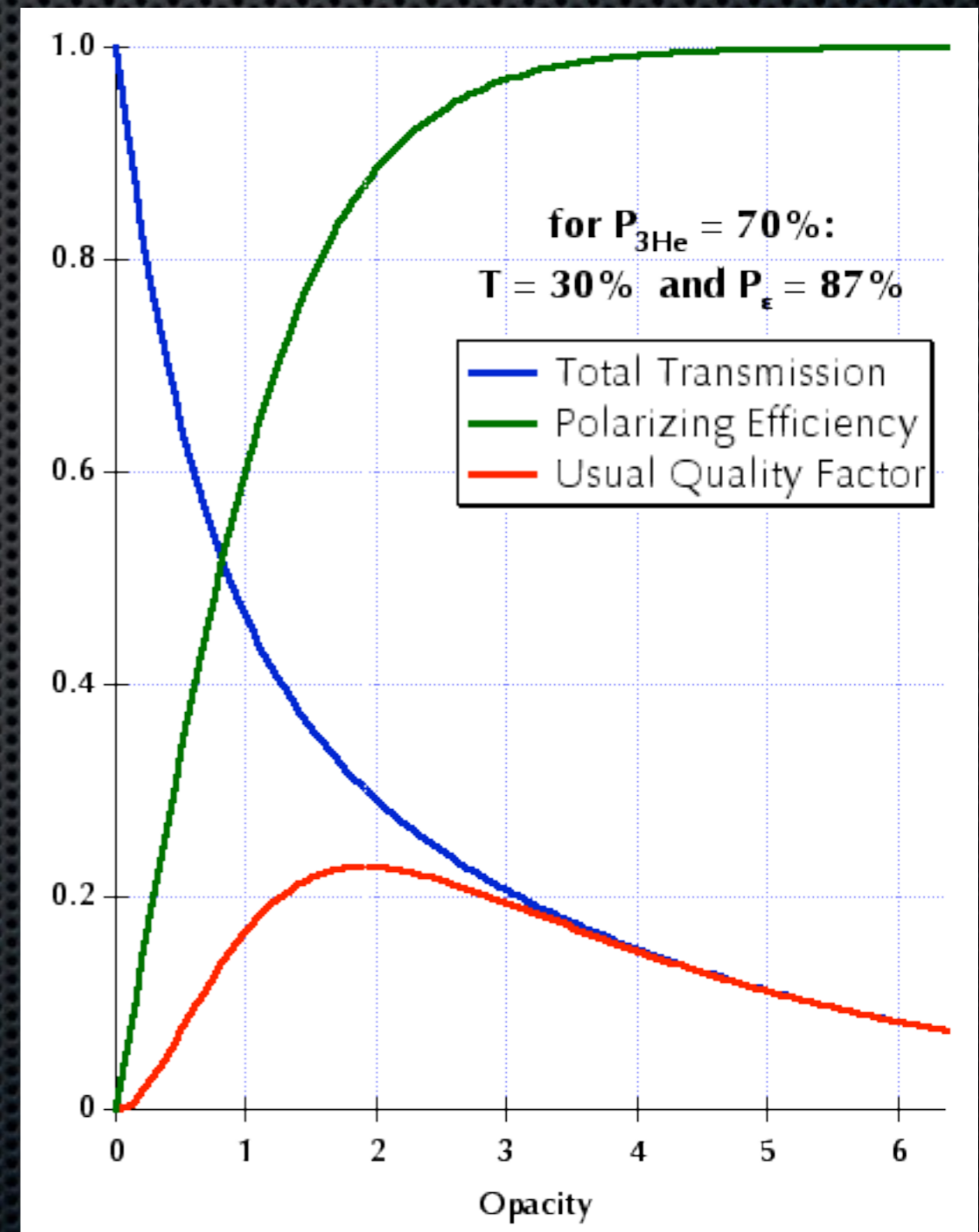
- Spin filters are characterised by their opacity:

$$\mathcal{O} = N \ell \sigma_{\parallel}$$
$$\simeq 0.0797 p[\text{bar}] \ell[\text{cm}] \lambda[\text{\AA}]$$

- The total transmission and polarising efficiency are:

$$T_n \propto \cosh(\mathcal{O} P_{3\text{He}})$$

$$P_{\epsilon} = \tanh(\mathcal{O} P_{3\text{He}})$$



Spin Flippers & Spin Filters

^3He polarising techniques: MEOP & SEOP

MEOP

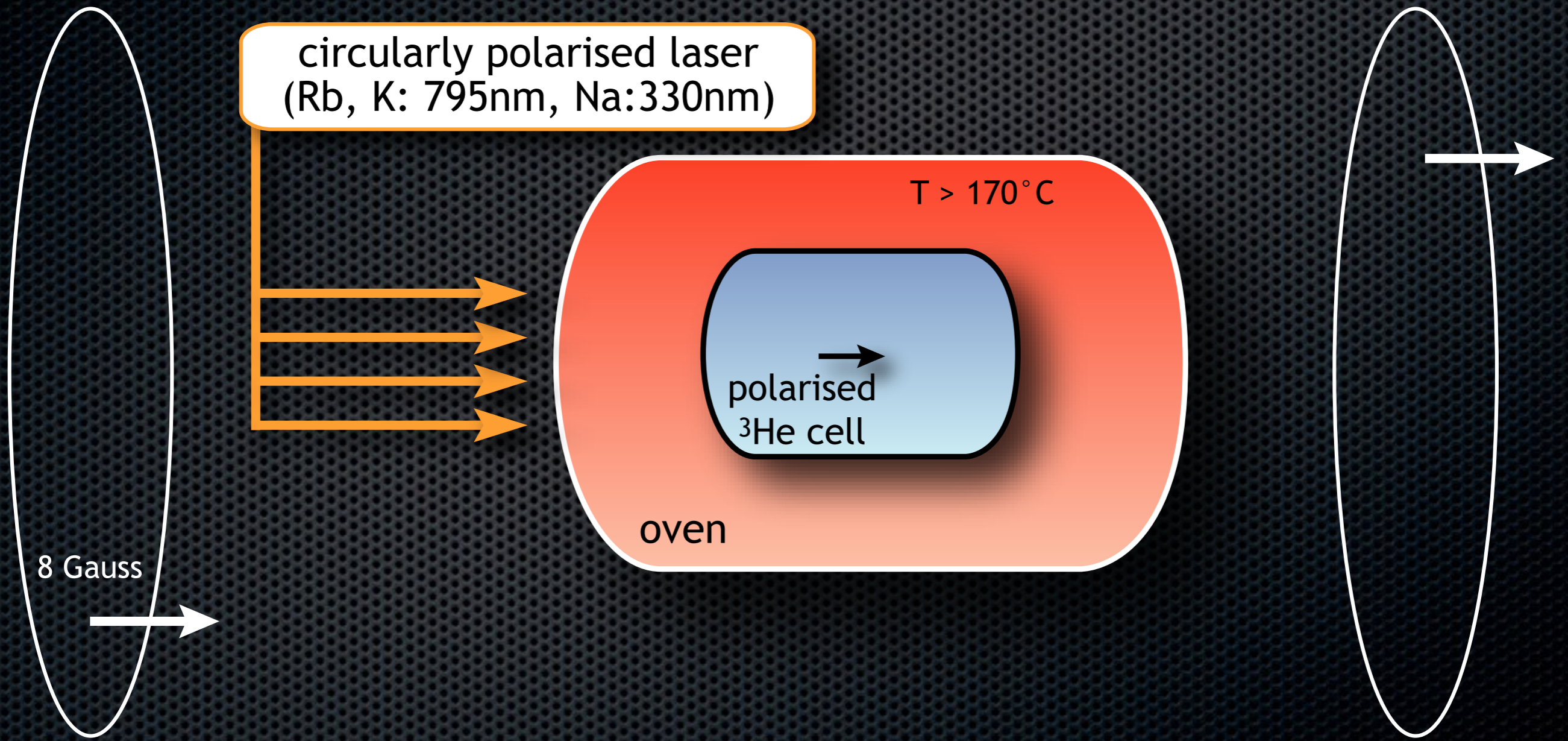
- low pressure (≈ 0.7 mbar) followed by compression
- cell ready in 1-2 hours
- 70 - 80% ^3He polarisation on instrument
- large system delivering gas remotely

SEOP

- directly at nominal pressure (1-4 bar)
- cell ready after 1-2 days
- 70 - 80% ^3He polarisation on instrument
- system that can generally be installed on beam

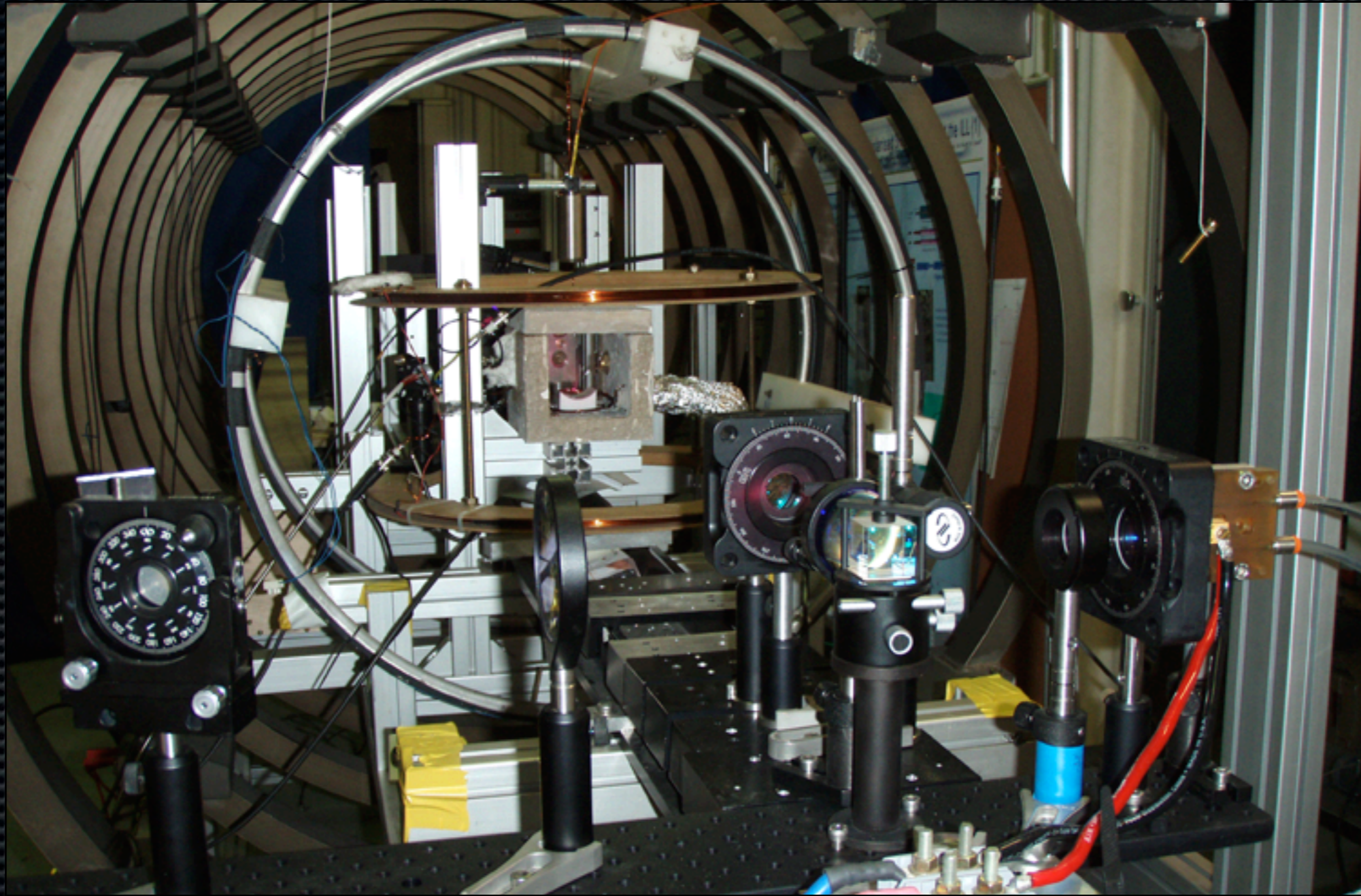
Spin Flippers & Spin Filters

^3He polarising techniques: SEOP station



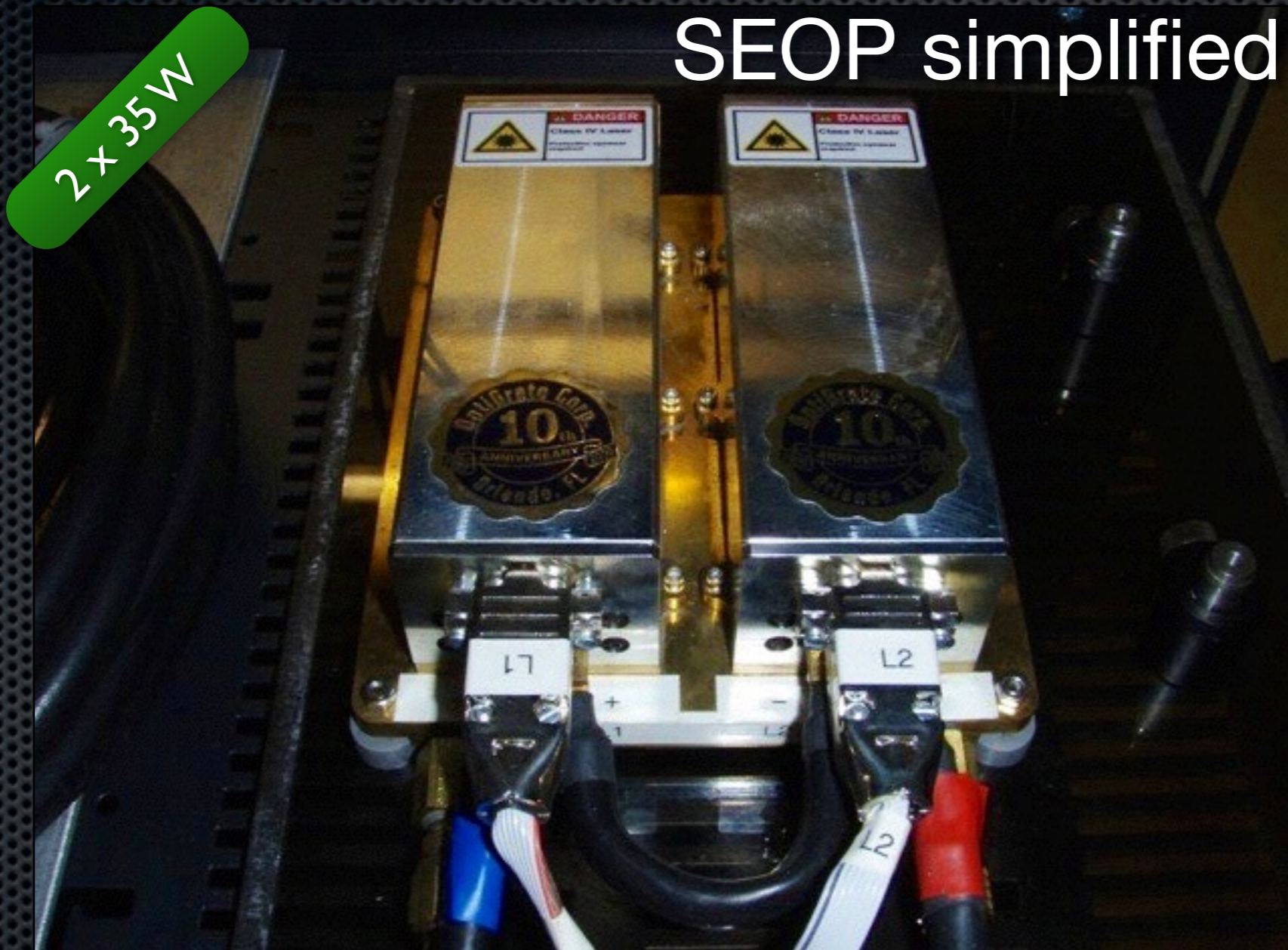
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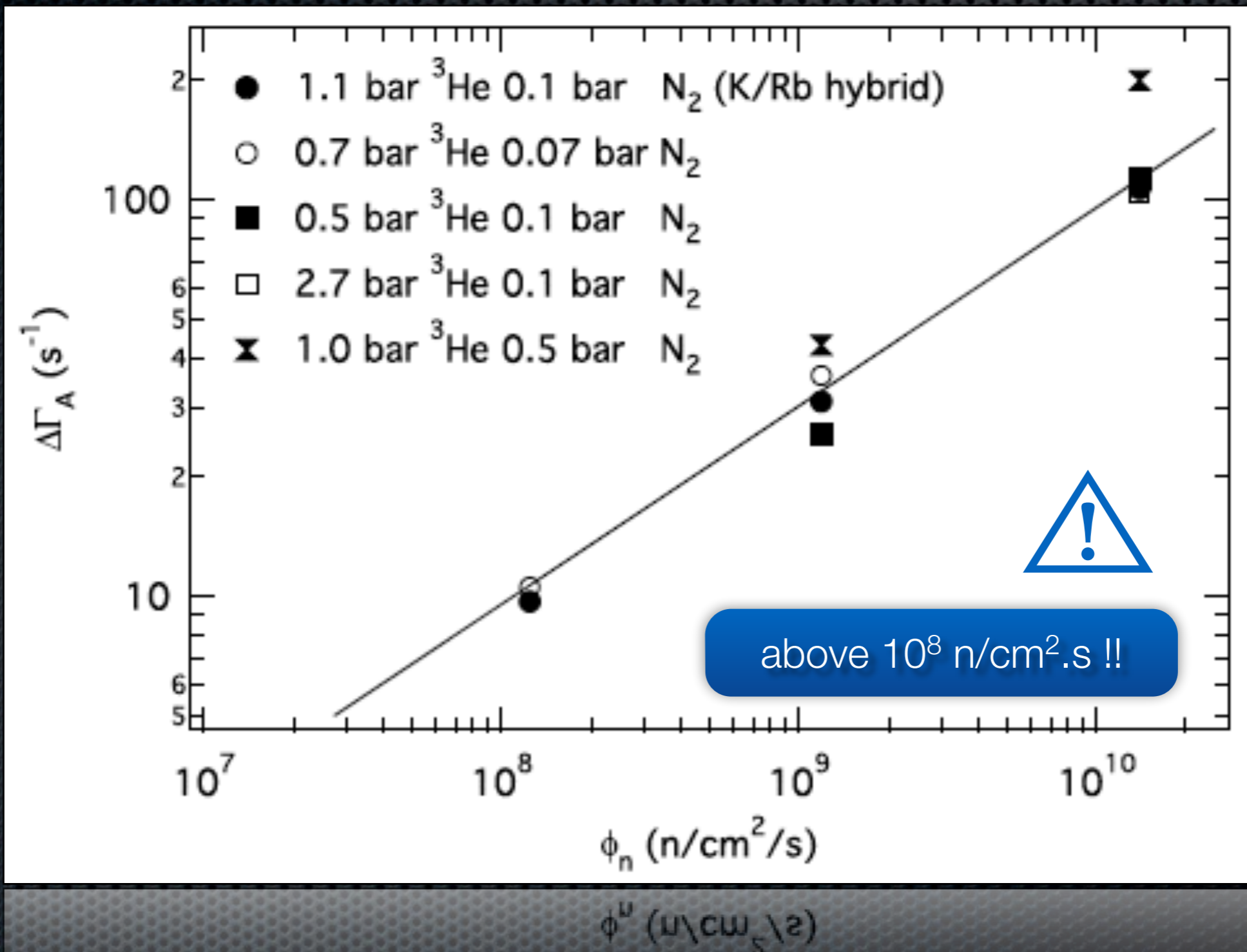
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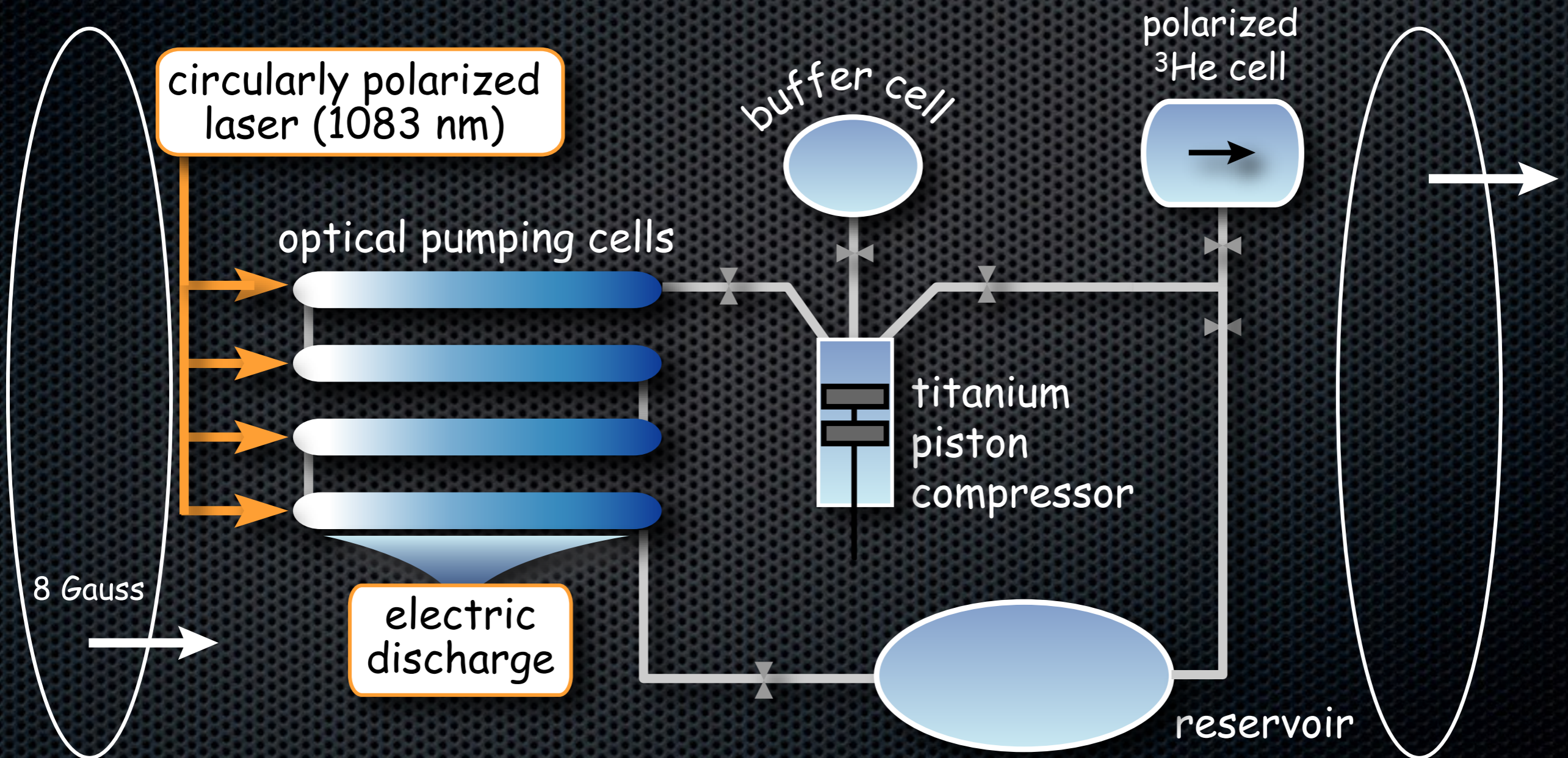
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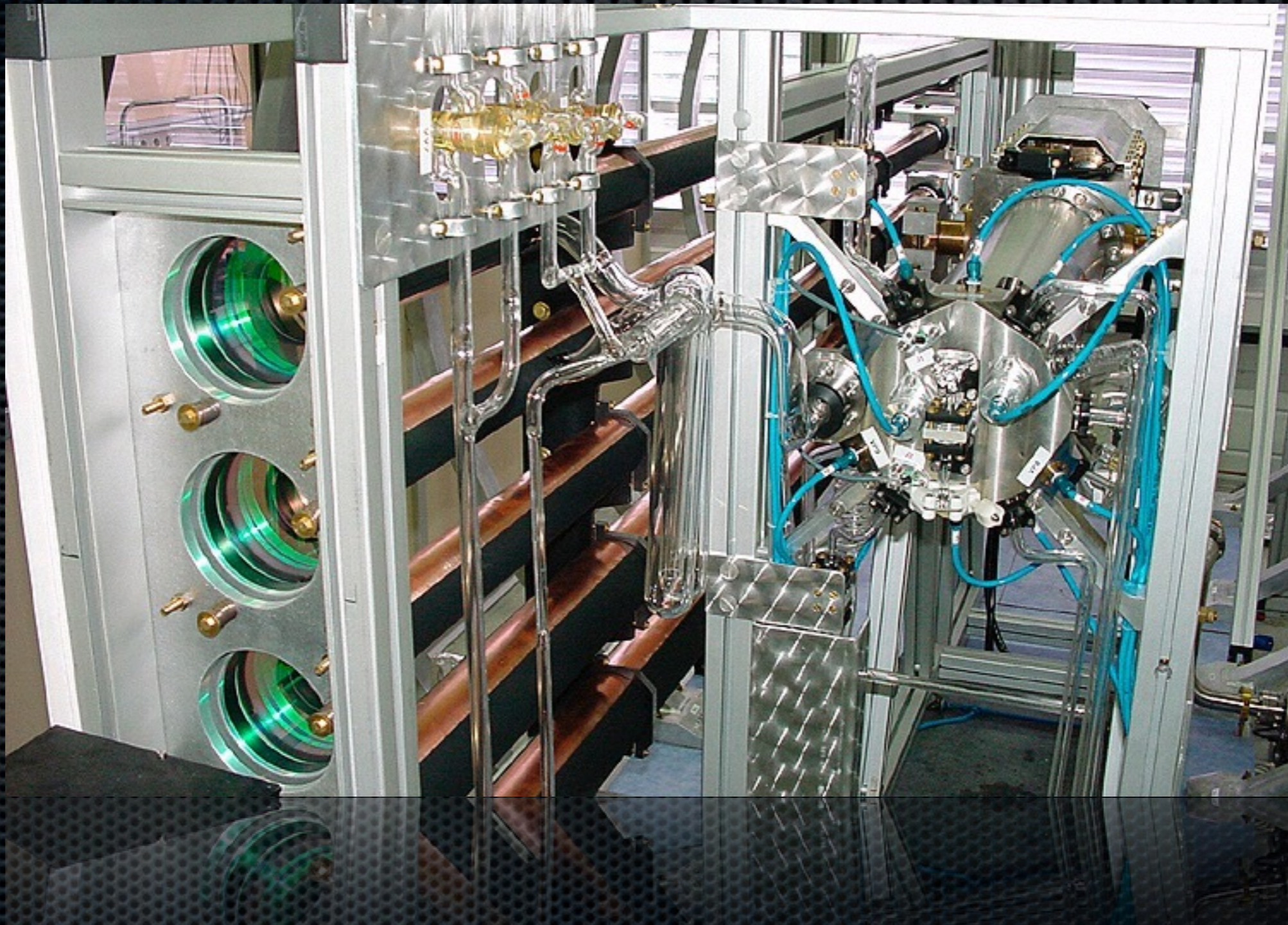
Spin Flippers & Spin Filters

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Spin Flippers & Spin Filters

^3He polarising techniques: MEOP station

Spin Flippers & Spin Filters

^3He spin filters: cells & magnetostatic cavities

- The main difficulty resides in the ability to build good cells and preserve the ^3He polarisation on the instrument:



Spin Flippers & Spin Filters

^3He spin filters: cells & magnetostatic cavities

- The main difficulty resides in the ability to build good cells and preserve the ^3He polarisation on the instrument:

$$\frac{1}{T_1} = \frac{1}{T_{wall}} + \frac{1}{T_{field}} + \frac{1}{T_{dipolar}}$$
$$= \gamma \frac{S}{V} + \frac{14\,400}{p [\text{bar}]} \left(\frac{1}{B_0} \frac{\partial B_{\perp}}{\partial r_{\perp} [\text{cm}]} \right)^2 + \frac{p [\text{bar}]}{830}$$

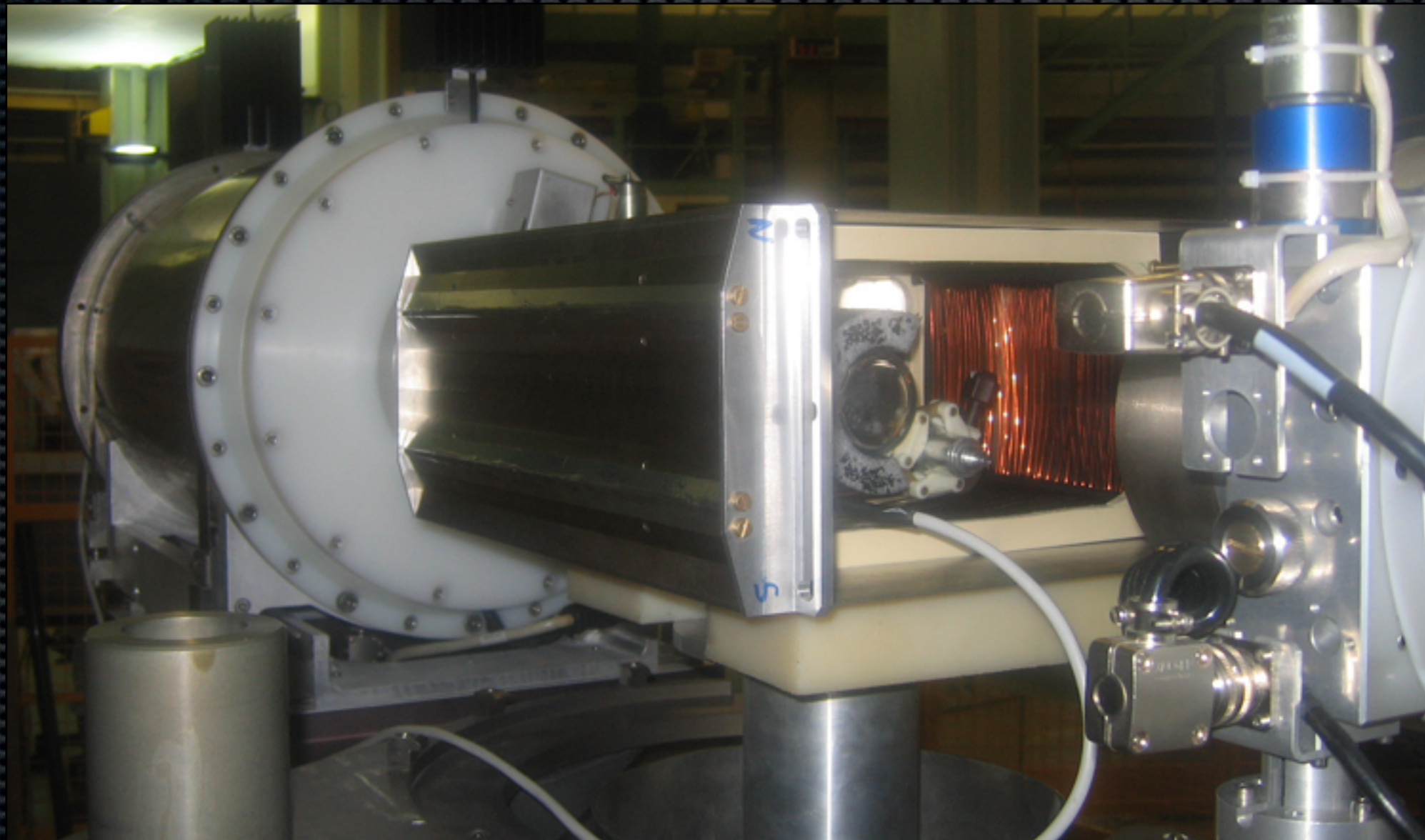
i.e. essentially $\frac{1}{B_0} \frac{\partial B_{\perp}}{\partial r_{\perp}} \ll 5 \cdot 10^{-4} \text{cm}^{-1}$



Spin Flippers & Spin Filters

^3He spin filters: cells & magnetostatic cavities

long T_1 + RF coil flipping ^3He polarisation



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Cross-section & scattered polarisation vector

theory: Maleyev, Blume, ... ($\vec{Q} = \vec{k}_i - \vec{k}_f$)

Contribution	Elastic scattering	Inelastic scattering
(n) Nuclear	$\sigma_n = NN^*$ $\{\vec{P}_f \sigma\}_n = \vec{P}_i \sigma_n$	$\sigma_n = \frac{k_f}{k_i} \mathcal{H} \left(N_{-\vec{Q}}, N_{\vec{Q}} \right)$ $\{\vec{P}_f \sigma\}_n = \vec{P}_i \sigma_n$
(m) Magnetic (I)	$\sigma_m = \vec{M}_\perp \cdot \vec{M}_\perp^*$ $\{\vec{P}_f \sigma\}_m = -\vec{P}_i \sigma_m + \dots$ $\dots 2\Re \left(\vec{M}_\perp \left(\vec{P}_i \cdot \vec{M}_\perp^* \right) \right)$	$\sigma_m = \frac{k_f}{k_i} S_{\alpha\beta} \delta_{\alpha\beta}$ $\{P_{f,\alpha} \sigma\}_m = \frac{k_f}{k_i} P_{i\beta} \dots$ $\dots [(S_{\alpha\beta} + S_{\beta\alpha}) - \delta_{\alpha\beta} \delta_{\beta\alpha}]$ $S_{\alpha\beta} = \mathcal{H} \left(M_{\perp,-\vec{Q}}^\alpha, M_{\perp,\vec{Q}}^\beta \right)$
(c) Magnetic (II)	$\sigma_c = \imath \vec{P}_i \cdot \left(\vec{M}_\perp^* \wedge \vec{M}_\perp \right)$ $\{\vec{P}_f \sigma\}_c = -\imath \left(\vec{M}_\perp^* \wedge \vec{M}_\perp \right)$	$\sigma_c = \frac{k_f}{k_i} \imath S_{\alpha\beta} \epsilon_{\alpha\beta\gamma} P_{i\gamma}$ $\{\vec{P}_f, \alpha \sigma\}_c = -\frac{k_f}{k_i} \imath \epsilon_{\alpha\beta\gamma} S_{\beta\gamma}$ $S_{\alpha\beta} = \mathcal{H} \left(M_{\perp,-\vec{Q}}^\alpha, M_{\perp,\vec{Q}}^\beta \right)$
(i) Nuclear- magnetic	$\sigma_i = 2\vec{P}_i \cdot \Re \left(N^* \vec{M}_\perp \right)$ $\{\vec{P}_f \sigma\}_i = 2\Re \left(N^* \vec{M}_\perp \right) +$ $2\vec{P}_i \wedge \Im \left(N^* \vec{M}_\perp \right)$	$\sigma_i = \frac{k_f}{k_i} \imath \vec{S}_+ \cdot \vec{P}_i$ $\{\vec{P}_f \sigma\}_i = \frac{k_f}{k_i} \left(\vec{S}_+ + \imath \vec{S}_- \wedge \vec{P}_i \right)$ $\vec{S}_\pm = \mathcal{H}_\pm \left(N_{-\vec{Q}}, \vec{M}_{\perp,\vec{Q}} \right)$

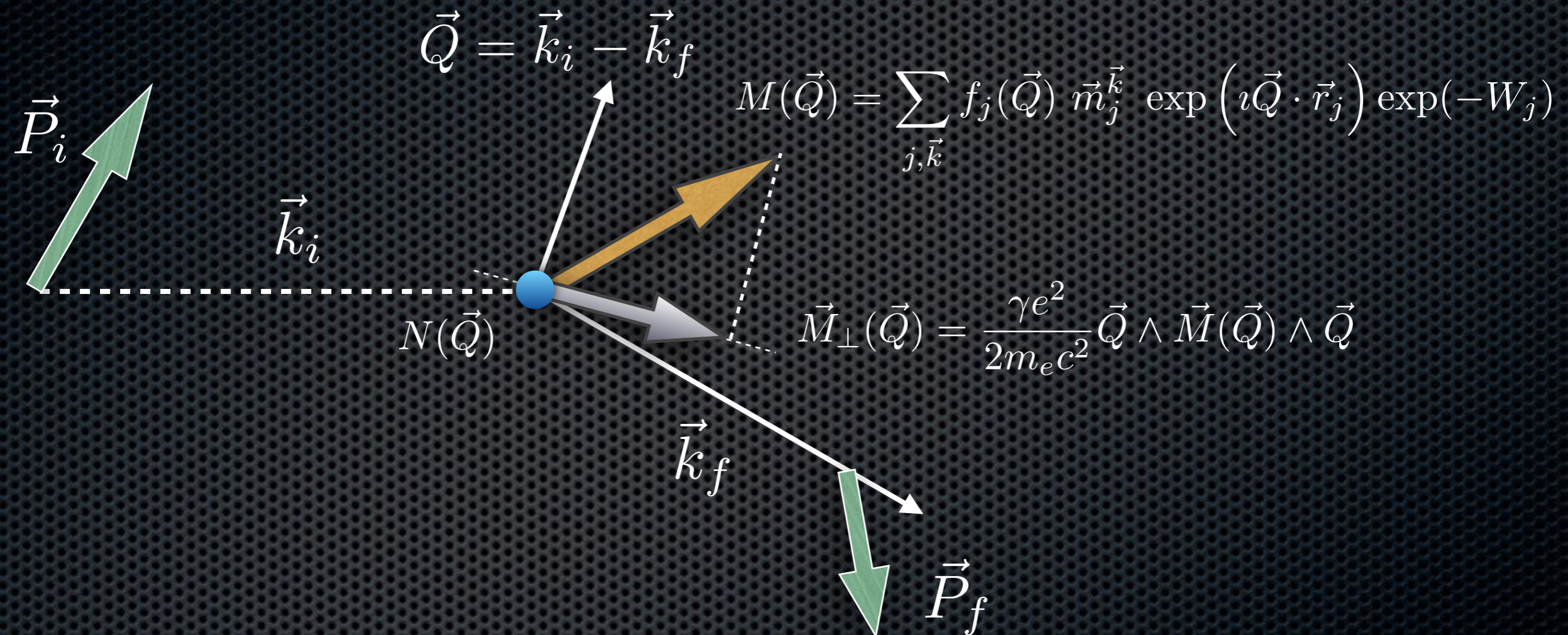
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(m) Magnetic (I)	$\sigma_m = \vec{M}_\perp \cdot \vec{M}_\perp^*$ $\{\vec{P}_f \sigma\}_m = -\vec{P}_i \sigma_m + \dots$ $\dots 2\Re \left(\vec{M}_\perp \left(\vec{P}_i \cdot \vec{M}_\perp^* \right) \right)$	$\sigma_m = \frac{k_f}{k_i} S_{\alpha\beta} \delta_{\alpha\beta}$ $\{P_{f,\alpha} \sigma\}_m = \frac{k_f}{k_i} P_{i\beta} \dots$ $\dots [(S_{\alpha\beta} + S_{\beta\alpha}) - \delta_{\alpha\beta} \delta_{\beta\alpha}]$ $S_{\alpha\beta} = \mathcal{H} \left(M_{\perp,-\vec{Q}}^\alpha, M_{\perp,\vec{Q}}^\beta \right)$
(c) Magnetic (II)	$\sigma_c = -i \vec{P}_i \cdot \left(\vec{M}_\perp^* \wedge \vec{M}_\perp \right)$ $\{\vec{P}_f \sigma\}_c = i \left(\vec{M}_\perp^* \wedge \vec{M}_\perp \right)$	$\sigma_c = -\frac{k_f}{k_i} i S_{\alpha\beta} \epsilon_{\alpha\beta\gamma} P_{i\gamma}$ $\{\vec{P}_f, \alpha \sigma\}_c = \frac{k_f}{k_i} i \epsilon_{\alpha\beta\gamma} S_{\beta\gamma}$ $S_{\alpha\beta} = \mathcal{H} \left(M_{\perp,-\vec{Q}}^\alpha, M_{\perp,\vec{Q}}^\beta \right)$
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Cross-section & scattered polarisation vector

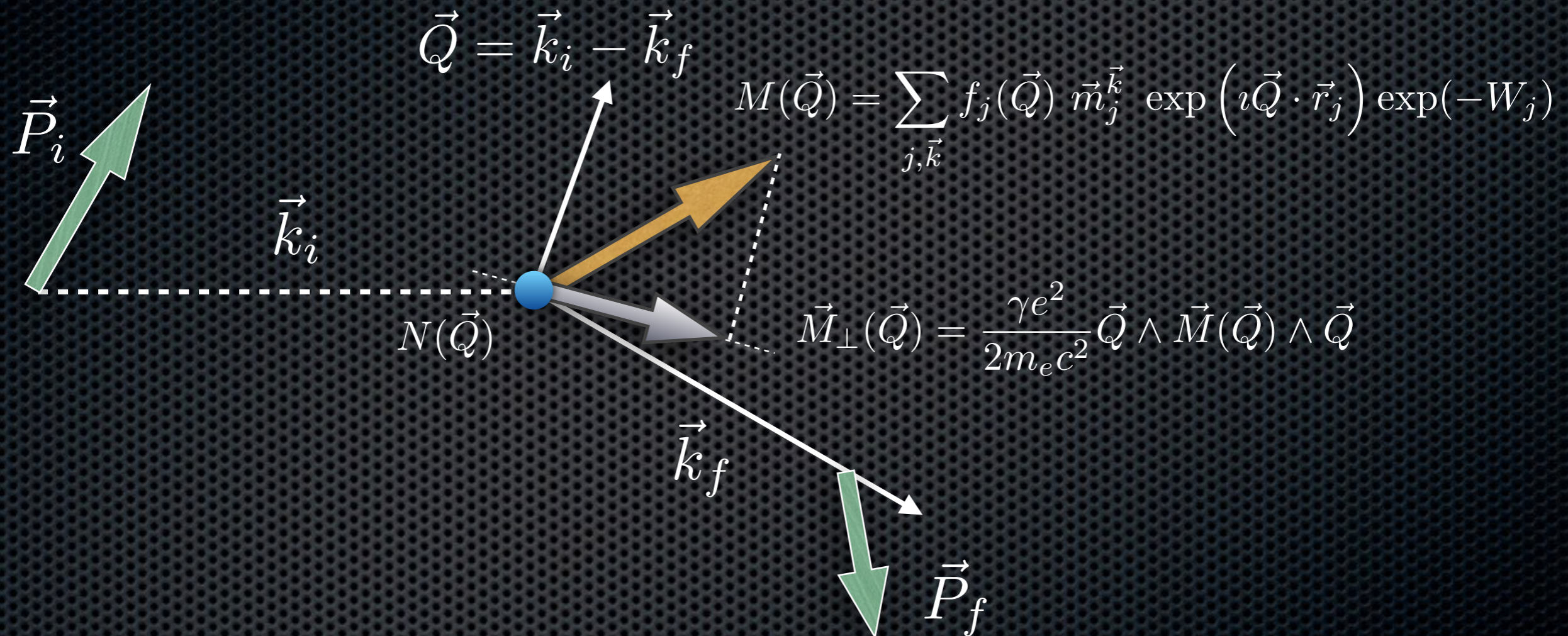
theory: Maleyev, Blume,...



In general, the polarisation of a neutron beam will change both in magnitude and direction upon scattering from a magnetic material.

Cross-section & scattered polarisation vector

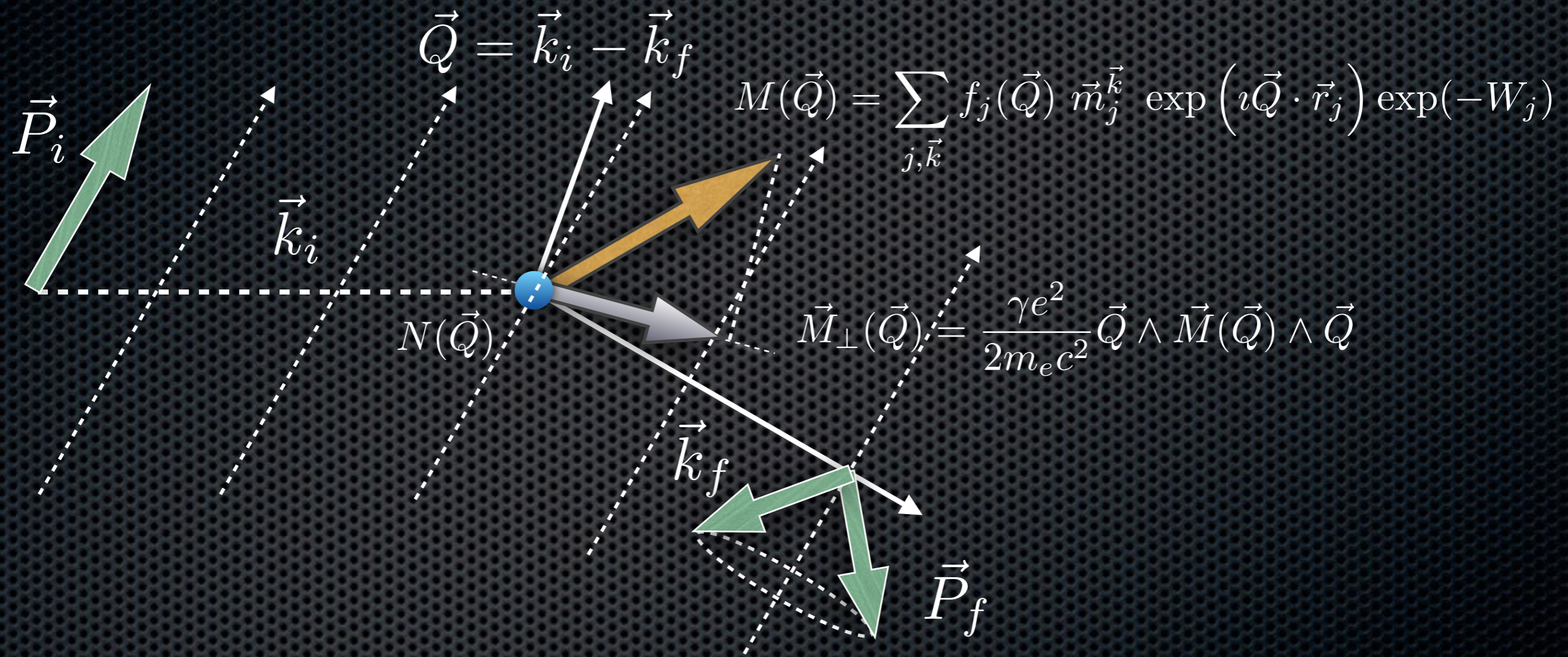
theory: Maleyev, Blume,...



The changes in direction that take place on scattering by a magnetic interaction vector are highly dependent on their relative orientations.

Cross-section & scattered polarisation vector

theory: Maleyev, Blume,...




 When a magnetic field is applied at the sample, the Larmor precessions lead to the loss of the components perpendicular to the field.
 

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Polarised neutron diffraction

applied to the measurement
of magnetisation distributions

- The nuclear-magnetic interference term is exploited to measure ferro- and para-magnetic distributions.

$$\frac{\partial \sigma}{\partial \Omega} = NN^* + \vec{M}_{\perp} \cdot \vec{M}_{\perp}^* + 2\vec{P}_i \cdot \Re(N^* \vec{M}_{\perp}) + i\vec{P}_i \cdot (\vec{M}_{\perp}^* \wedge \vec{M}_{\perp})$$

- The chiral term allows to measure the anti-ferromagnetic distributions of chiral systems.

Polarised neutron diffraction (powder)

magnetisation of systems
with no anisotropy and low magnetisation

- Method: flipping difference

$$\left(\frac{\partial\sigma}{\partial\Omega}\right)_+ = NN^* + M_{\perp}M_{\perp}^* + 2P_i N M_{\perp} + \cancel{iF_i \cdot 0}$$

$$\left(\frac{\partial\sigma}{\partial\Omega}\right)_- = NN^* + M_{\perp}M_{\perp}^* - 2P_i N M_{\perp} - \cancel{iF_i \cdot 0}$$

$$\Delta = 4P_i N M_{\perp}$$

➡ Background suppressed, higher sensitivity, easy to scale and to correct for polarisation

Polarised neutron diffraction (powder)

magnetisation of systems
with no anisotropy and low magnetisation

- ✦ The instrument is a powder diffractometer featuring:
 - ✦ a polariser and a flipper
 - ✦ a cryomagnet (typically 40 mK to 300 K, 1 to 10 T)
 - ✦ a radial oscillating collimator to get rid of the background when measuring without polarised neutrons
 - ✦ a method for determining the incident polarisation and the sample depolarisation

Polarised neutron diffraction (powder)

magnetisation
of systems with
no anisotropy and low
magnetisation

e.g.

molecular magnets
nano-scale samples
biological samples

...



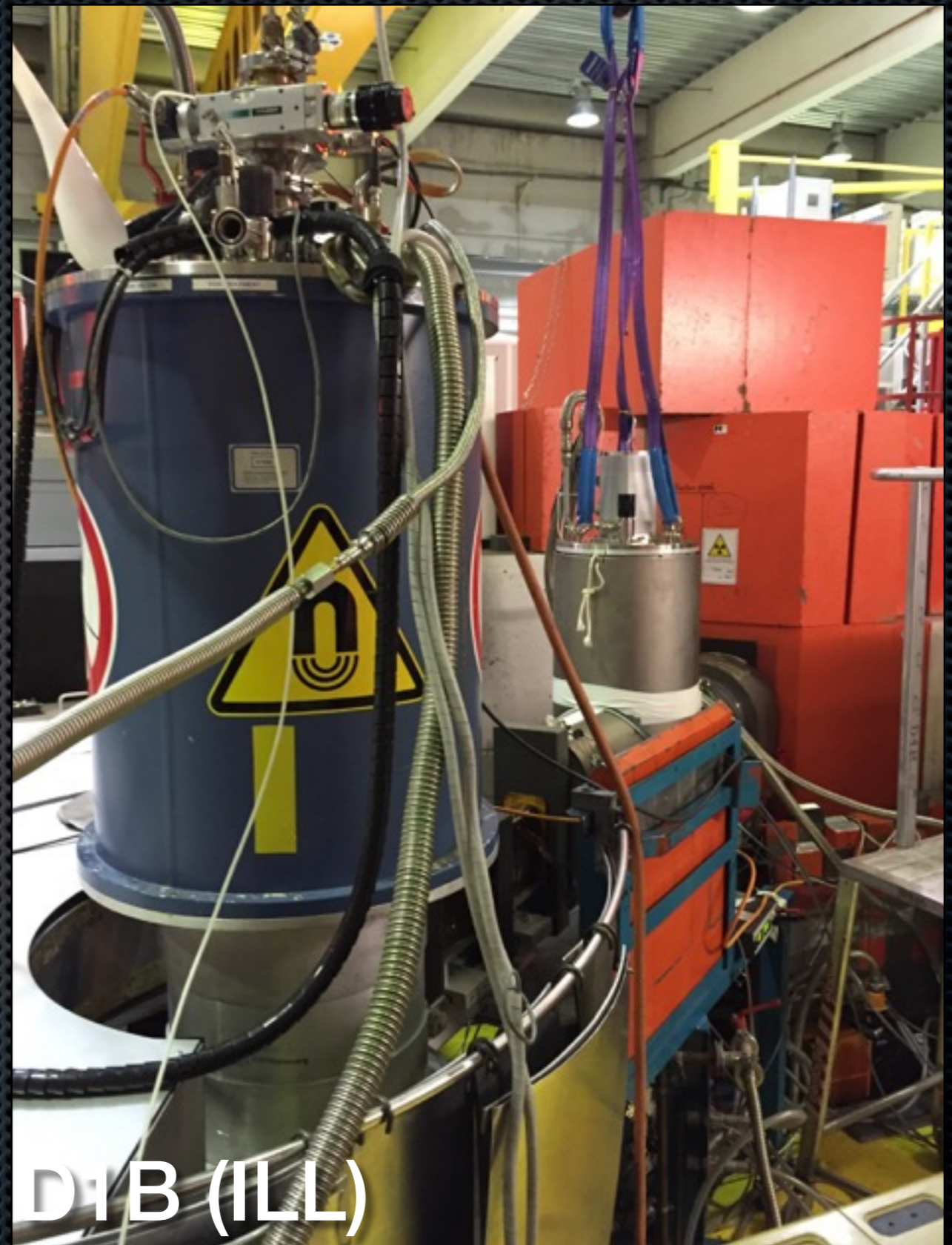
Polarised neutron diffraction (powder)

magnetisation
of systems with
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molecular magnets
nano-scale samples
biological samples

...



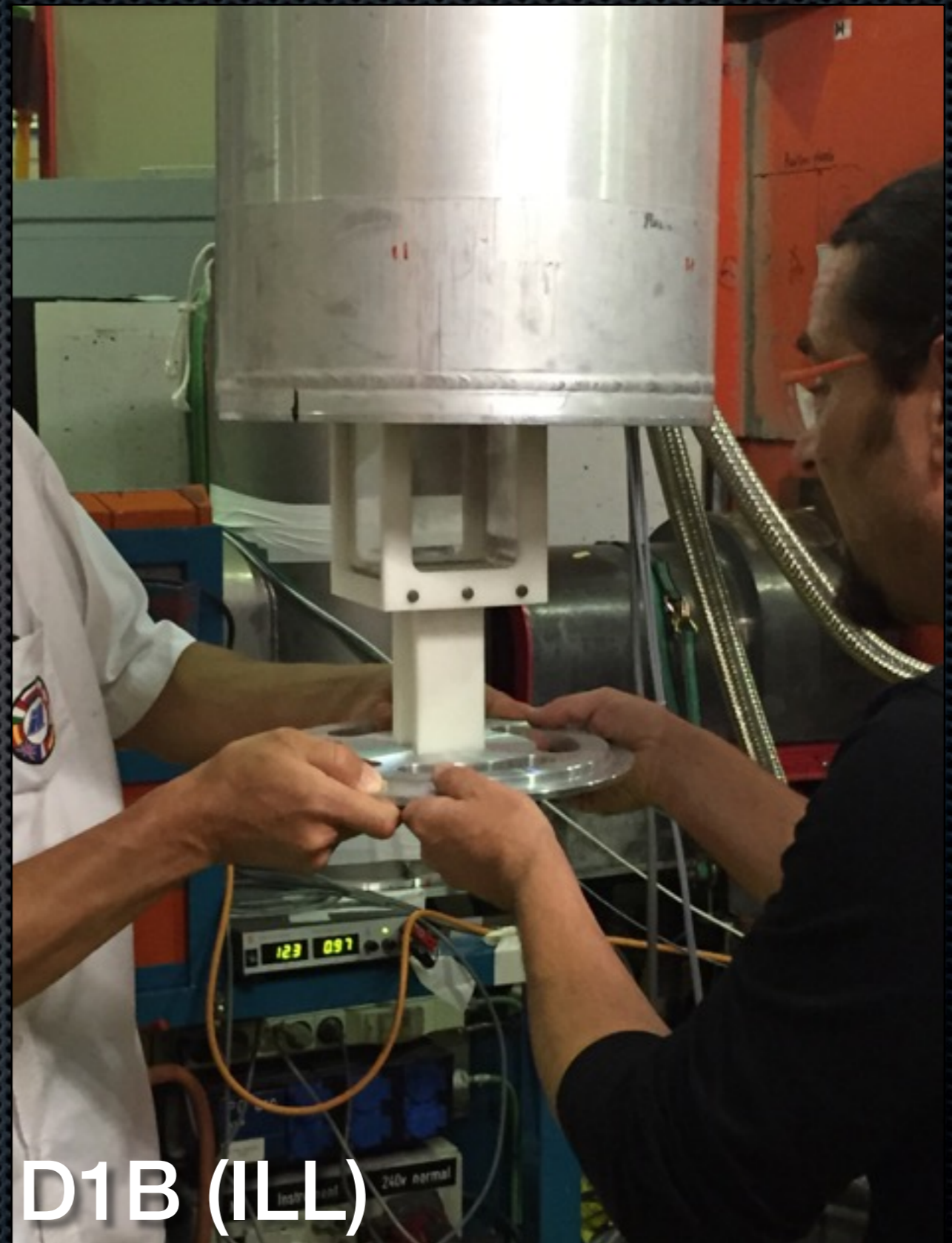
Polarised neutron diffraction (powder)

magnetisation
of systems with
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magnetisation

e.g.

molecular magnets
nano-scale samples
biological samples

...



Polarised neutron diffraction (powder)

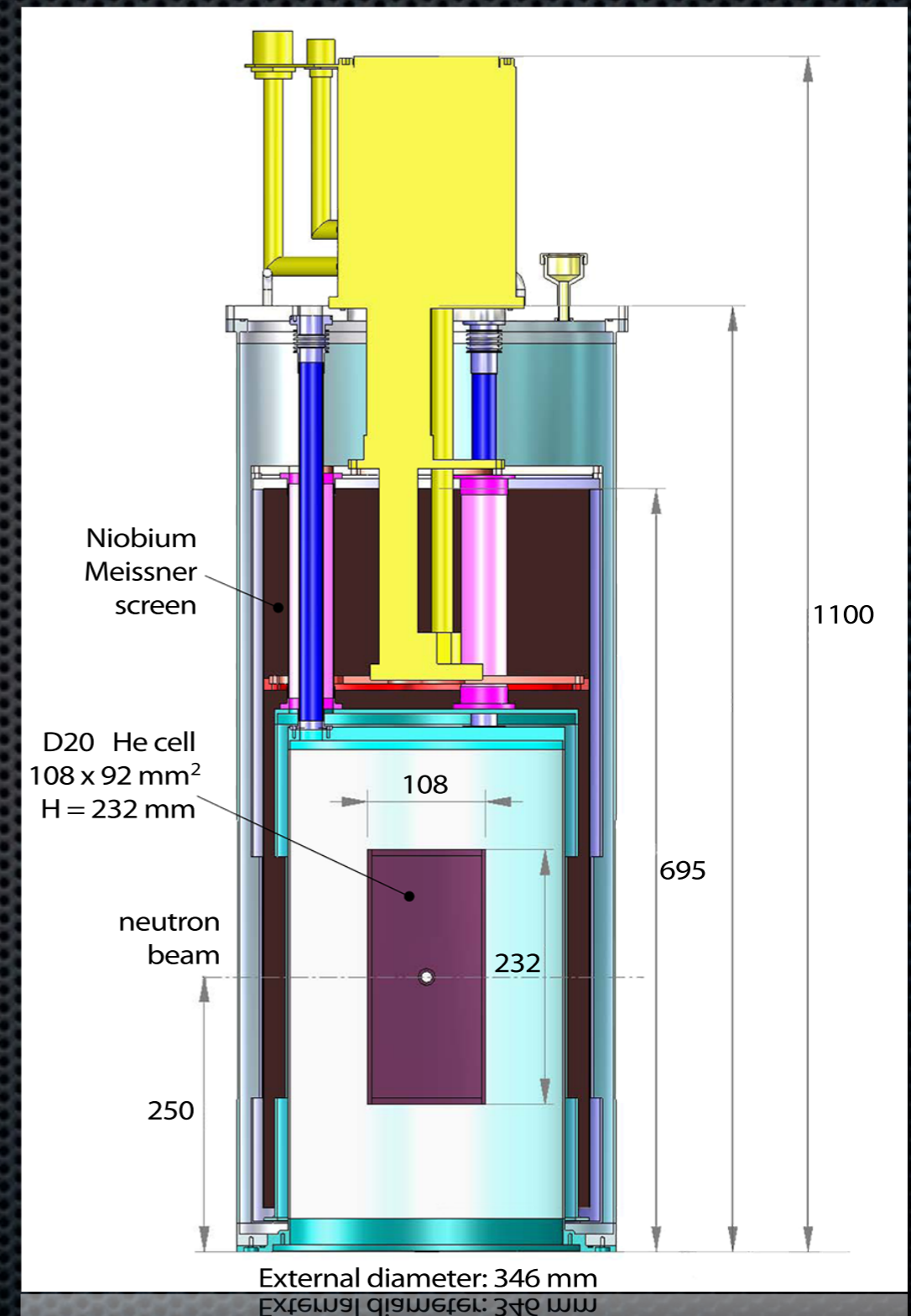
polariser/flipper used

Cryopol

neutron beam polarised
with a ^3He spin filter

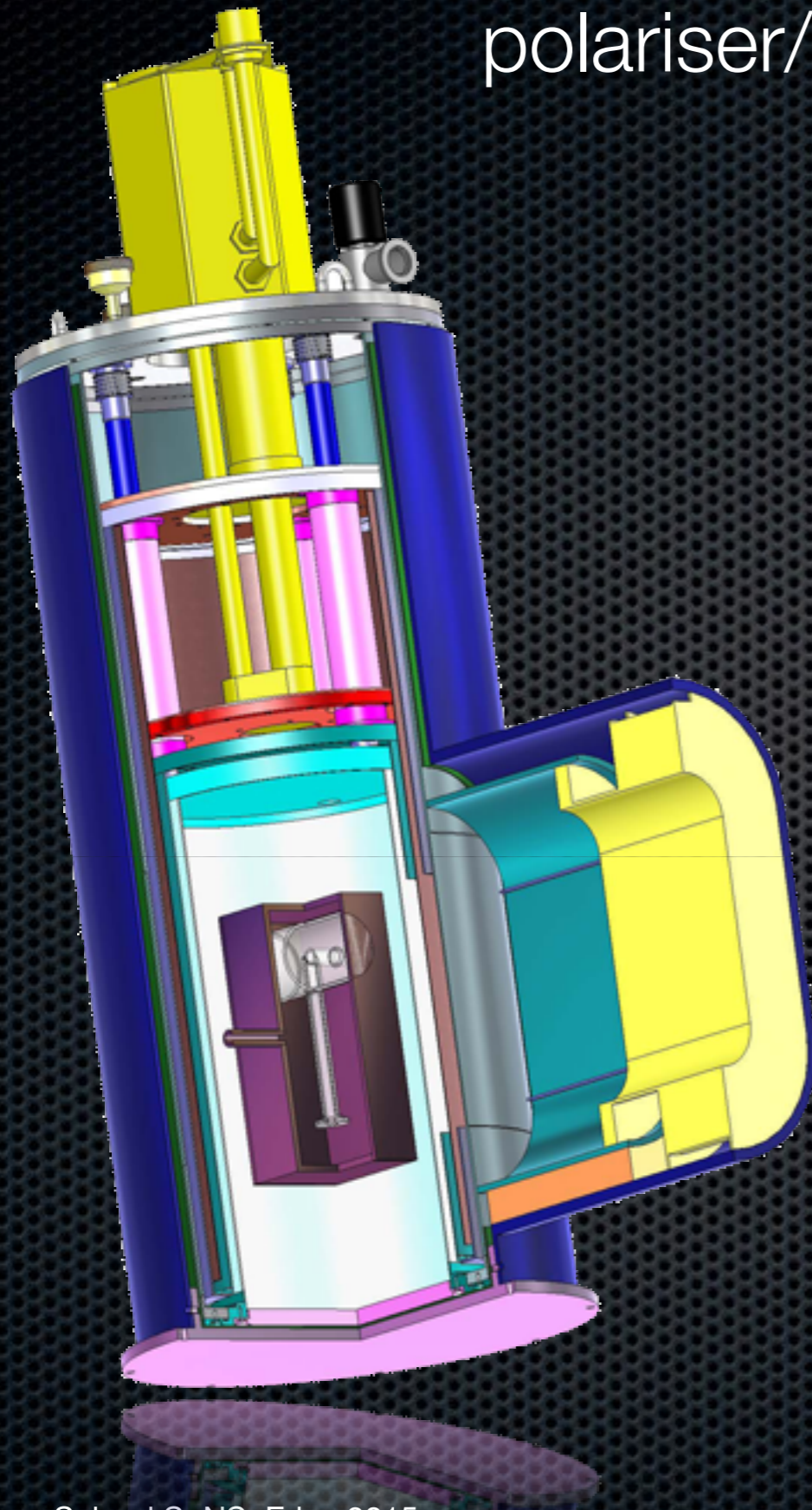
^3He polarisation maintained
with homogeneous field
trapped in Meißner cylinder

polarisation flipped
using non-adiabatic transition
(i.e. Cryoflipper)



Polarised neutron diffraction (powder)

polariser/flipper used on D20, D1B



Cryopol

99.9 % flipping
efficiency above
 0.3 \AA in 400 G

$T_1 > 180$ hours
at 1 bar



Polarised neutron diffraction (powder)

polariser/flipper used on D20, D1B



Polarised neutron diffraction (powder)

magnetisation of systems
with no anisotropy, low magnetisation

- The incident beam polarisation is determined continuously using two monitors placed before and after the spin filter:

$$\epsilon = \sqrt{1 - \frac{(M_{20}/M_{10})^2}{(M_2/M_1)^2}}$$
$$\sigma_{\epsilon}^2 = \frac{M_1^3 M_{20}^3 [M_1 M_2 (M_{10} + M_{20}) + M_{10} M_{20} (M_1 + M_2)]}{M_{10}^3 M_2^3 (M_{10}^2 M_2^2 - M_1^2 M_{20}^2)}$$

M_{10} and M_{20} are measured for $P_{3\text{He}} = 0$

Polarised neutron diffraction (powder)

magnetisation of systems
with no anisotropy, low magnetisation

- The [+] and [-] spectra are corrected for the time-dependent transmission and efficiency of the filter:

$$P_{3He} = \frac{V_0}{p N_a \ell \sigma_a \lambda} \ln \left(\sqrt{\frac{1 + \epsilon}{1 - \epsilon}} \right)^2$$
$$\tau = \exp \left(-\frac{p N_a \ell \sigma_a \lambda}{V_0} \right) \cosh \left(\frac{p N_a \ell \sigma_a \lambda P_{3He}}{V_0} \right)$$

- The spectra are then averaged at each temperature and applied magnetic field.

Polarised neutron diffraction (powder)

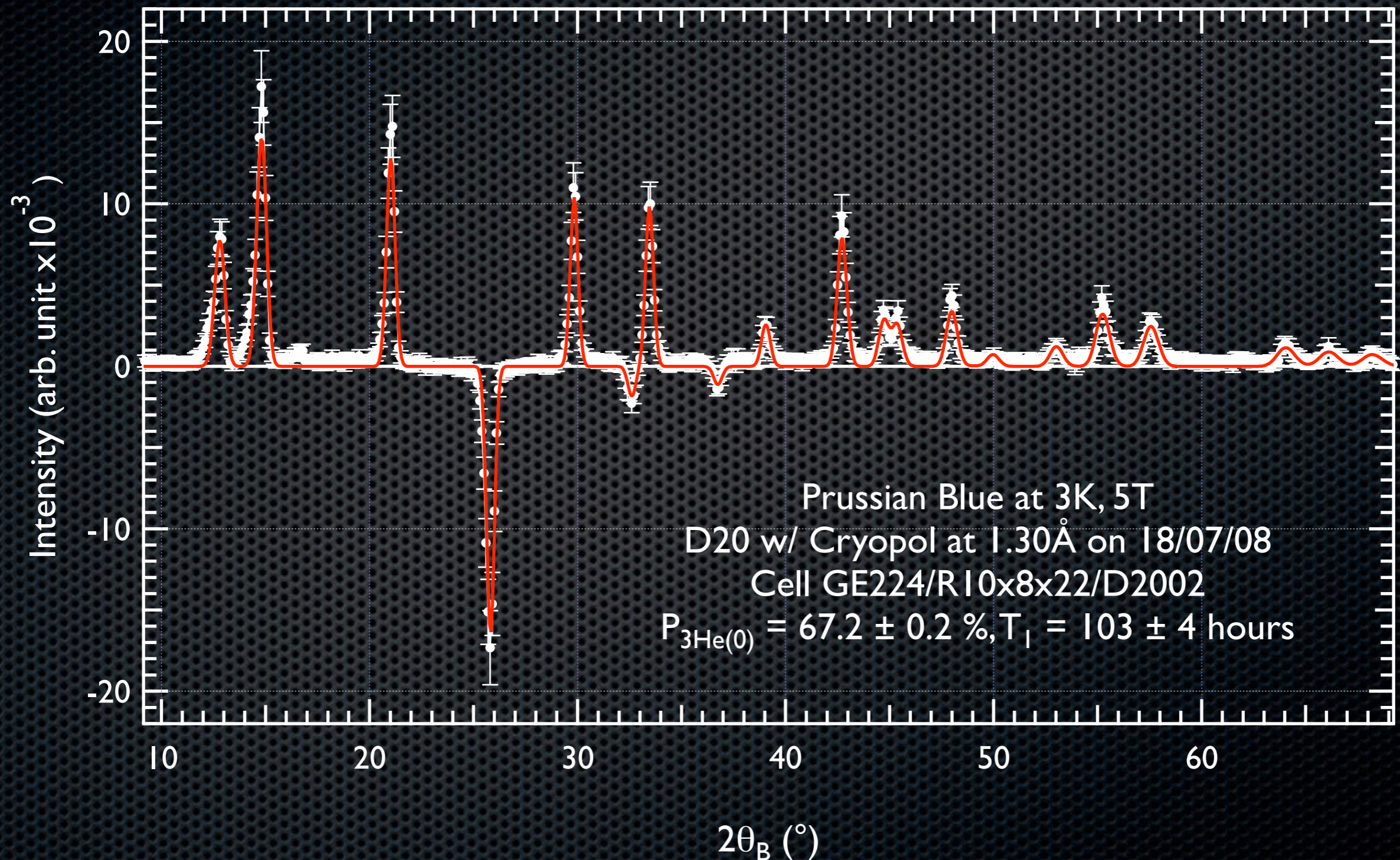
magnetisation of systems
with no anisotropy, low magnetisation

- The scale factor is determined from the refinement of the non-polarised measurements (spin filter removed - flux x3).
- The scale factor is then corrected for the transmission of the glass of the cell T_G and the depolarisation in the sample D_S :

$$4P_i N M_{\perp} \propto \frac{1}{T_G D_S} \frac{1}{N} \sum_{j=1}^N \left(\frac{1}{\epsilon(t_j) \tau(t_j)} I_{\Delta}(t_j) \right)$$

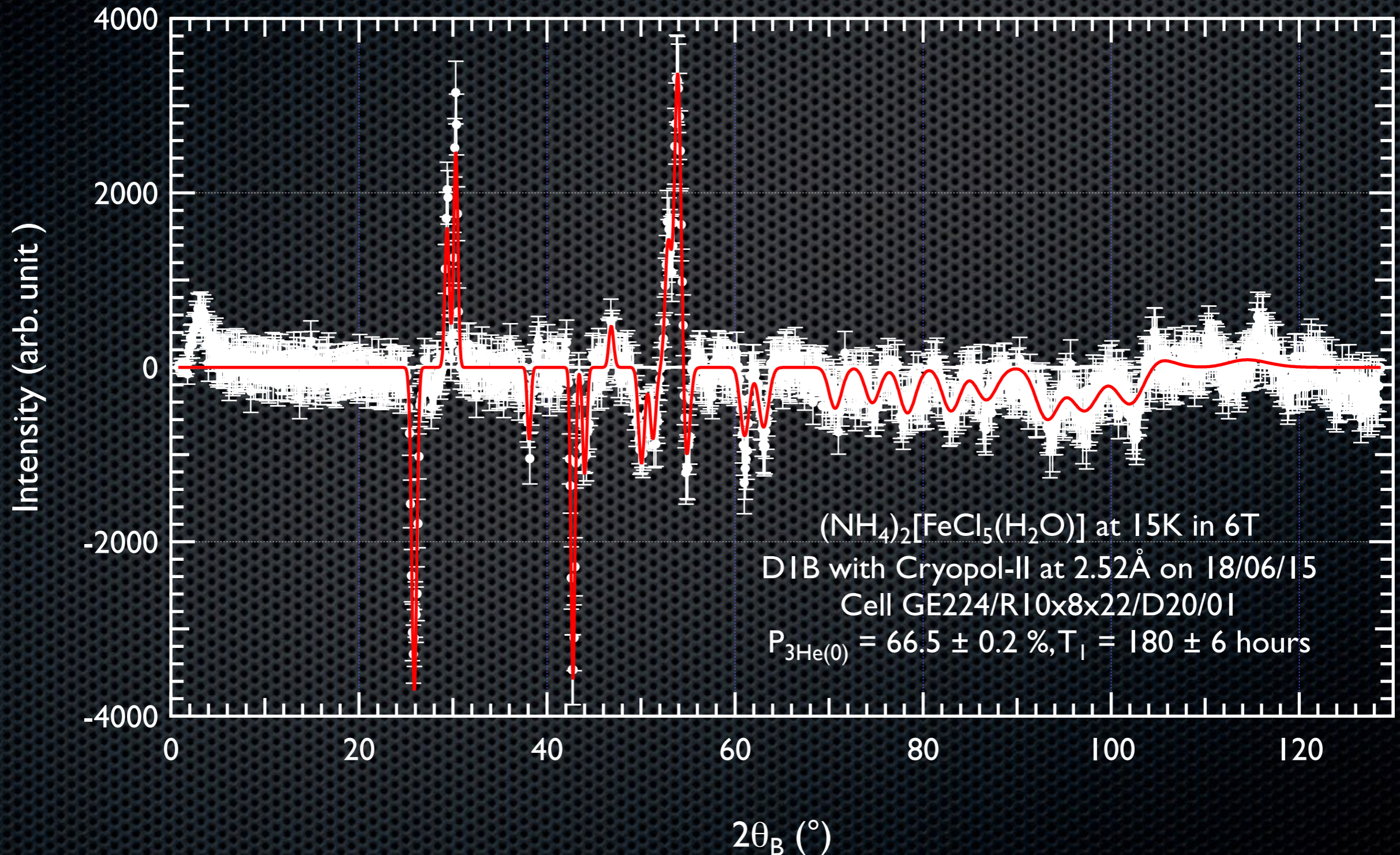
Polarised neutron diffraction (powder)

Example #1: deuterated Prussian Blue



Polarised neutron diffraction (powder)

Example #2: $(\text{NH}_4)_2[\text{FeCl}_5(\text{H}_2\text{O})]$



Polarised neutron diffraction (Xtal)

magnetisation of single crystals
under applied magnetic field

- Method: flipping ratio

$$\frac{\partial \sigma}{\partial \Omega} = NN^* + \vec{M}_{\perp} \cdot \vec{M}_{\perp}^* + 2\vec{P}_i \cdot (\vec{M}_{\perp}^* \wedge \vec{M}_{\perp}) + 2\vec{P}_i \cdot \Re(N^* \vec{M}_{\perp})$$

➡ We exploit the interference term to enhance the sensitivity

$$\|\vec{M}_{\perp}\| \propto \frac{1}{10}N \text{ and } \vec{P}_i = 0 \Rightarrow I \propto N^2 + \underline{0.01N^2}$$

$$\|\vec{M}_{\perp}\| \propto \frac{1}{10}N \text{ and } \vec{P}_i = \pm \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \Rightarrow R = \frac{I_+}{I_-} \propto \frac{3}{2}$$

Polarised neutron diffraction (Xtal)

magnetisation of single crystals
under applied magnetic field

- Method: flipping ratio

$$\frac{\partial \sigma}{\partial \Omega} = NN^* + \vec{M}_{\perp} \cdot \vec{M}_{\perp}^* + \cancel{i\vec{P}_i \cdot (\vec{M}_{\perp}^* \wedge \vec{M}_{\perp})} + 2\vec{P}_i \cdot \Re(N^* \vec{M}_{\perp})$$

For a ferromagnetically aligned sample, we measure:

$$R = \frac{I_+}{I_-} = \frac{N^2 + \sin^2(\alpha) M_{\perp}^2 + 2p_+ \sin^2(\alpha) N \cdot M_{\perp}}{N^2 + \sin^2(\alpha) M^2 + 2p_- \sin^2(\alpha) N \cdot M_{\perp}}$$

where p_+ and p_- are the incident polarisations, α is the angle between \vec{Q} and \vec{B} .

Polarised neutron diffraction (Xtal)

magnetisation of single crystals
under applied magnetic field

- Method: flipping ratio

$$\frac{\partial \sigma}{\partial \Omega} = NN^* + \vec{M}_{\perp} \cdot \vec{M}_{\perp}^* + \cancel{i\vec{P}_i \cdot (\vec{M}_{\perp}^* \wedge \vec{M}_{\perp})} + 2\vec{P}_i \cdot \Re(N^* \vec{M}_{\perp})$$

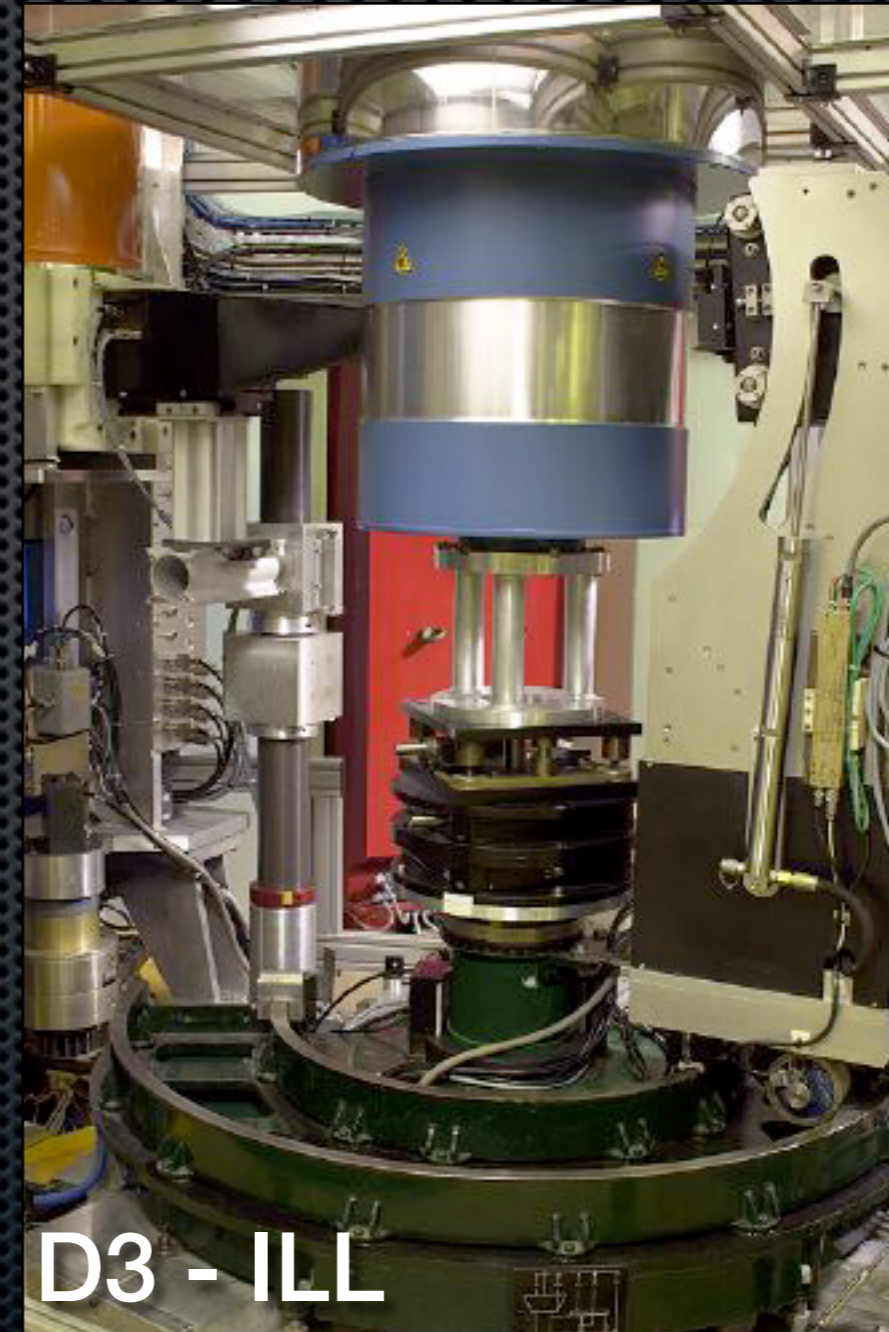
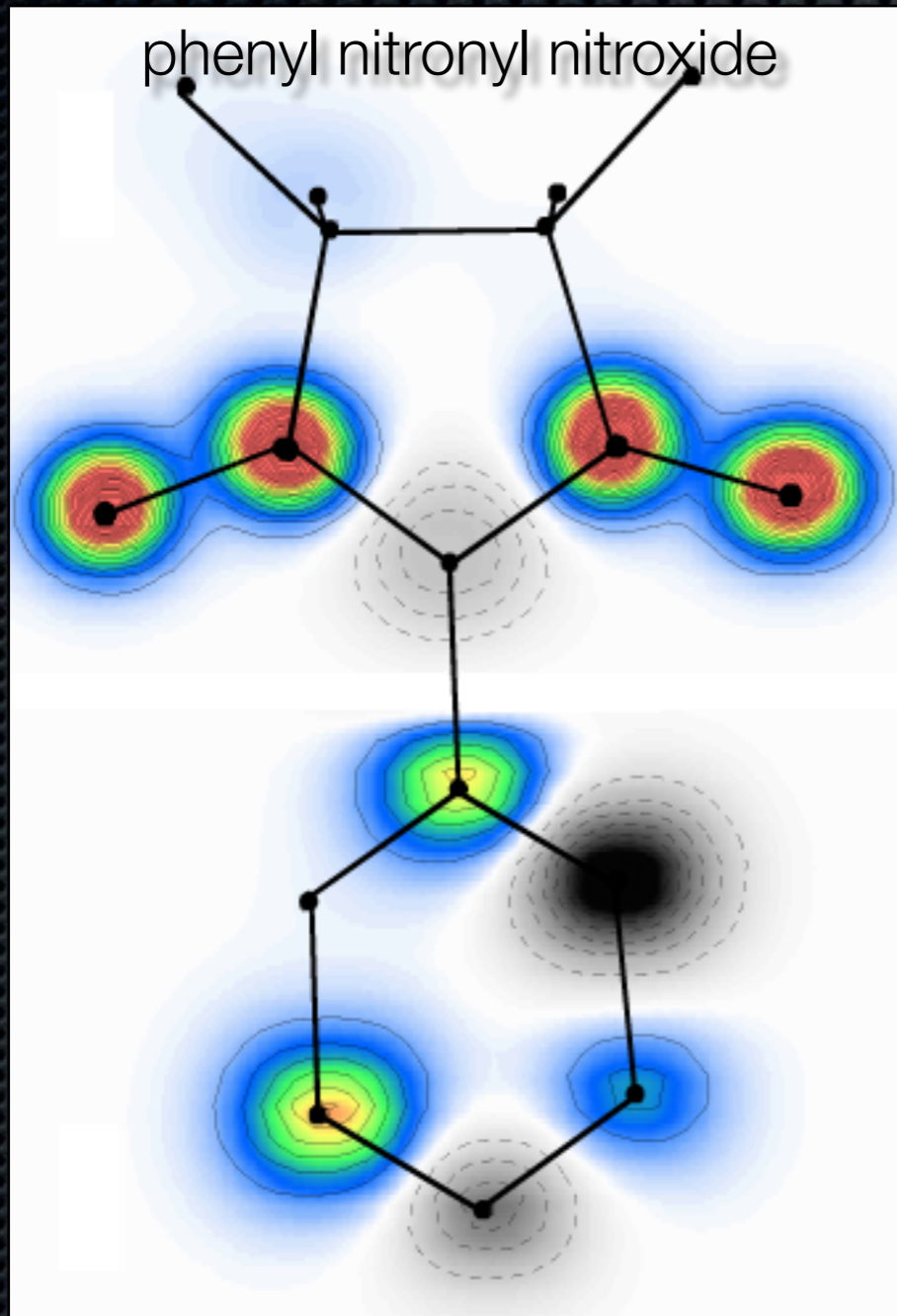
We deduce M from the equation:

$$\gamma = \frac{R+1}{R-1} \pm \sqrt{\left(\frac{R+1}{R-1}\right)^2 - \sin^2(\alpha)}$$

where γ is the ratio M/N . The distribution in real space is obtained by Fourier transformation (max. Entropy).

Polarised neutron diffraction (Xtal)

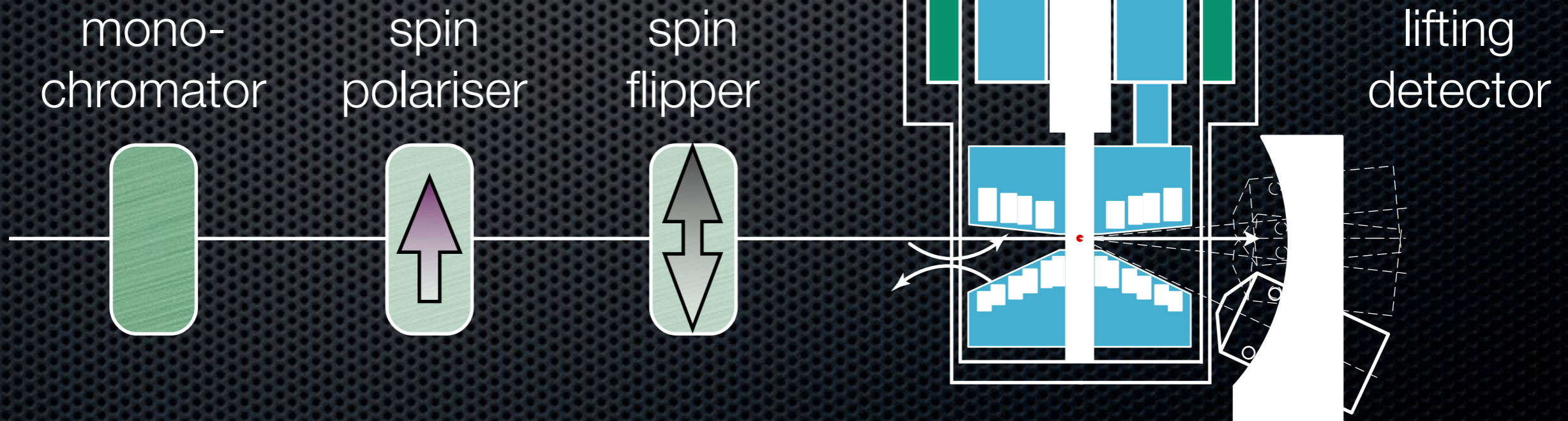
magnetisation of single crystals
under applied magnetic field



Polarised neutron diffraction (Xtal)

magnetisation of single crystals
under applied magnetic field

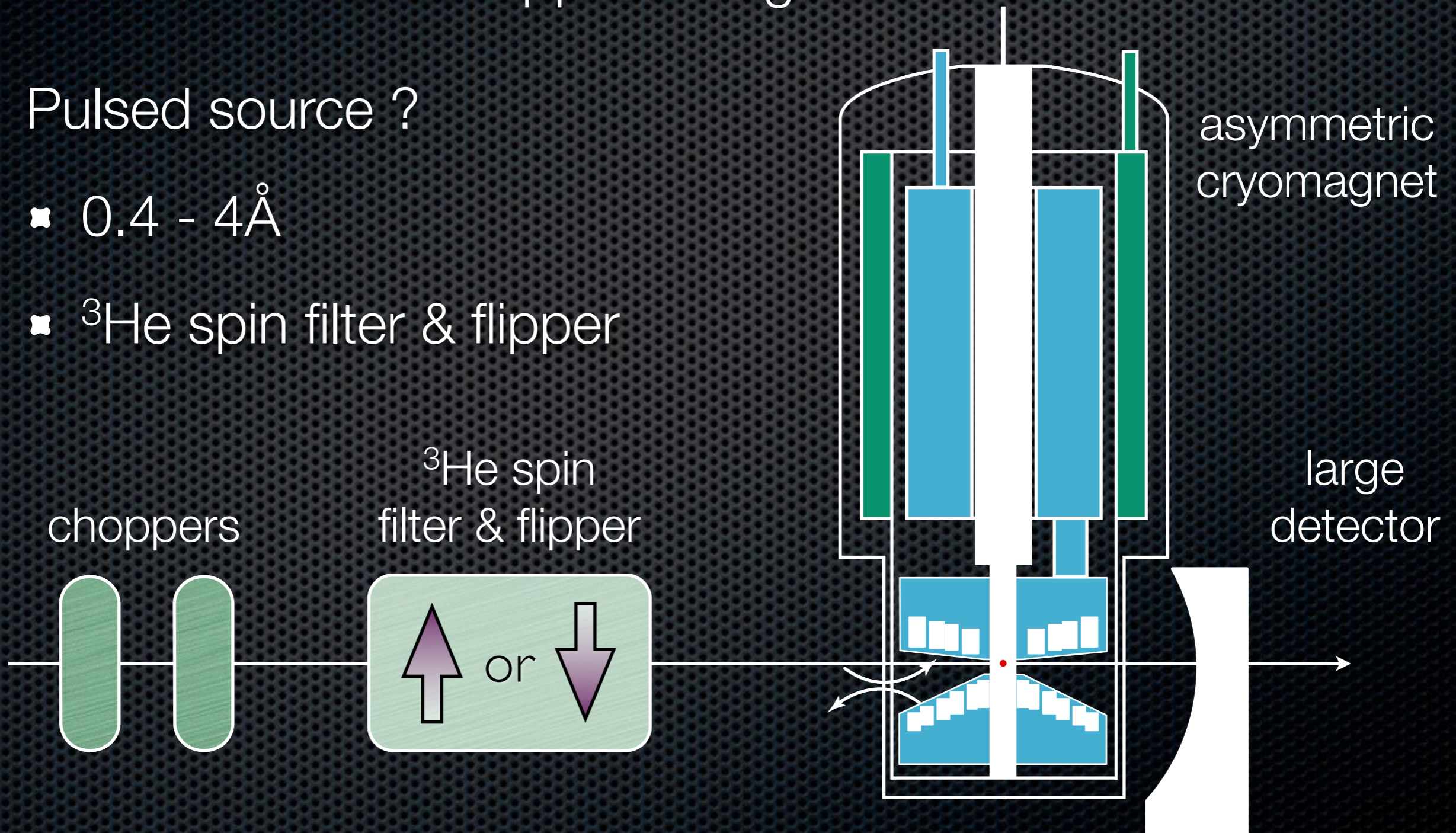
- ✦ Steady-state source
 - ✦ 0.4 - 4Å
 - ✦ Heusler + (cryo)flipper



Polarised neutron diffraction (Xtal)

magnetisation of single crystals
under applied magnetic field

- ✦ Pulsed source ?
 - ✦ 0.4 - 4Å
 - ✦ ^3He spin filter & flipper



Content

- ✦ Beam polarisation vector
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- ✦ Cross-section & scattered polarisation vector
- ✦ **PND — Polarised neutron diffraction (powder, crystal)**
- ✦ UPA - Uniaxial polarisation analysis
- ✦ SNP - Spherical neutron polarimetry
- ✦ PNSE — Polarimetric neutron spin-echo

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Uniaxial polarisation analysis

for separating the nuclear and magnetic contributions

- The incident polarisation is set adiabatically in any direction \vec{z} or \vec{Q} :

$$\sigma_{+,+} = N_0 \frac{(2\pi)^3}{v_0} |N + M_{\perp,z}|^2$$

$$\sigma_{-,-} = N_0 \frac{(2\pi)^3}{v_0} |N - M_{\perp,z}|^2$$

$$\sigma_{+,-} = N_0 \frac{(2\pi)^3}{v_0} |M_{\perp,x} + iM_{\perp,y}|^2$$

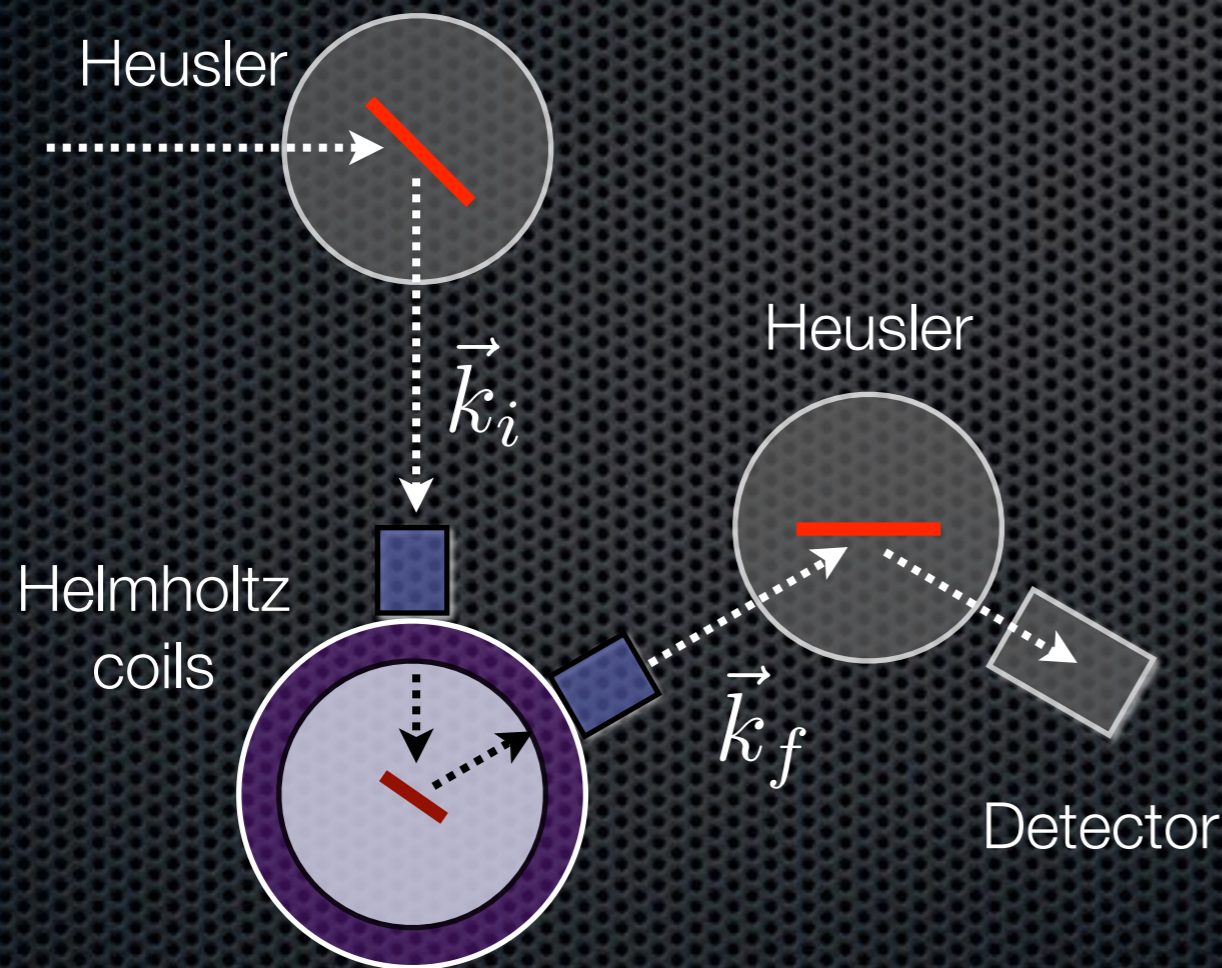
$$\sigma_{-,+} = N_0 \frac{(2\pi)^3}{v_0} |M_{\perp,x} - iM_{\perp,y}|^2$$

- If the polarisation is parallel to the scattering vector \vec{Q} , only the nuclear contribution participates to the non-spin-flip cross-section.

Uniaxial polarisation analysis

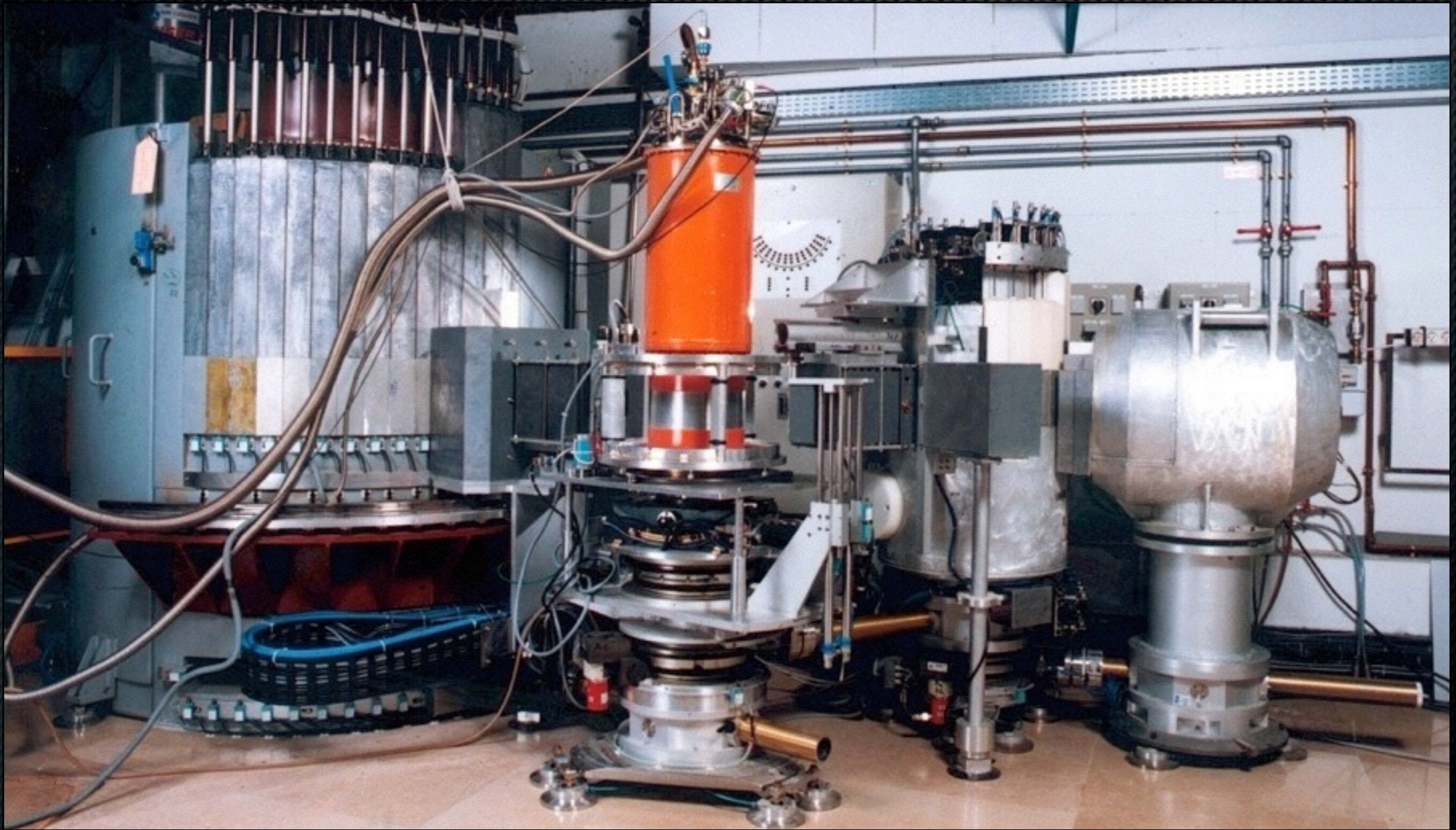
for separating the nuclear and magnetic contributions

- On three-axis spectrometers



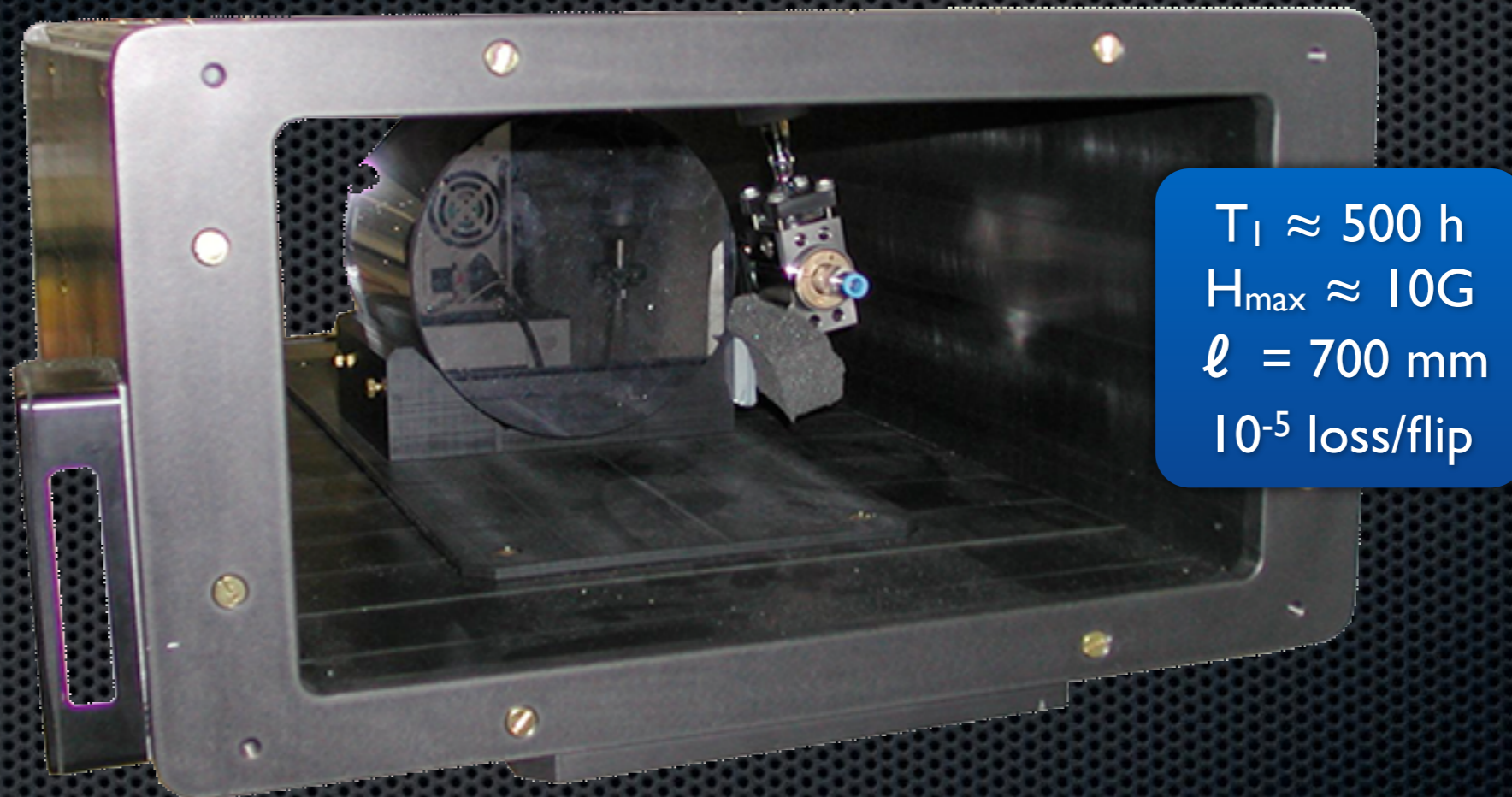
Uniaxial polarisation analysis

for separating the nuclear and
magnetic contributions



Uniaxial polarisation analysis

for separating the nuclear and magnetic contributions on SANS, Reflectometers



$T_1 \approx 500$ h
 $H_{\max} \approx 10$ G
 $\ell = 700$ mm
 10^{-5} loss/flip

Ø140 Si-windowed cell, pneumatic valve,
permanent static field, flipper included.

Uniaxial polarisation analysis

XYZ Method — Generalisation to PSD detector
 applies only to isotropic magnetisation

- Separation of the nuclear coherent, magnetic, spin incoherent and isotope incoherent contributions

$$\begin{aligned}
 \alpha &= \widehat{\vec{Q}_{\perp \vec{z}}, \vec{x}} \\
 &= \frac{1}{2} \operatorname{atan} \left(\frac{\sigma_{x+y}^{sf} - \sigma_{x-y}^{sf}}{\sigma_x^{sf} - \sigma_y^{sf}} \right) \\
 &= \frac{1}{2} \operatorname{atan} \left(\frac{\sigma_{x-y}^{nsf} - \sigma_{x+y}^{nsf}}{\sigma_y^{nsf} - \sigma_x^{nsf}} \right)
 \end{aligned}
 \quad
 \begin{aligned}
 \gamma &= \widehat{\vec{Q}_{// \vec{z}}, \vec{Q}} \\
 \sin^2 \gamma &= \frac{1-r}{(1+r) \cdot \cos^2 \alpha - 2r + 1} \\
 \text{with } r &= \frac{\sigma_x^{sf} - \sigma_z^{sf}}{\sigma_y^{sf} - \sigma_z^{sf}} \\
 &= \frac{\sigma_z^{nsf} - \sigma_x^{nsf}}{\sigma_z^{nsf} - \sigma_y^{nsf}}
 \end{aligned}$$

Uniaxial polarisation analysis

XYZ Method — Generalisation to PSD detector
applies only to isotropic magnetisation

- Separation of the nuclear coherent, magnetic, spin incoherent and isotope incoherent contributions

$$\sigma_x^{sf} = \frac{1}{2} (1 + \sin^2 \gamma \cdot \cos^2 \alpha) \sigma_{mag} + \frac{2}{3} \sigma_{si}$$

$$\sigma_x^{nsf} = \frac{1}{2} (1 - \sin^2 \gamma \cdot \cos^2 \alpha) \sigma_{mag} + \frac{1}{3} \sigma_{si} + \sigma_{nc} + \sigma_{ii}$$

$$\sigma_y^{sf} = \frac{1}{2} (1 + \sin^2 \gamma \cdot \sin^2 \alpha) \sigma_{mag} + \frac{2}{3} \sigma_{si}$$

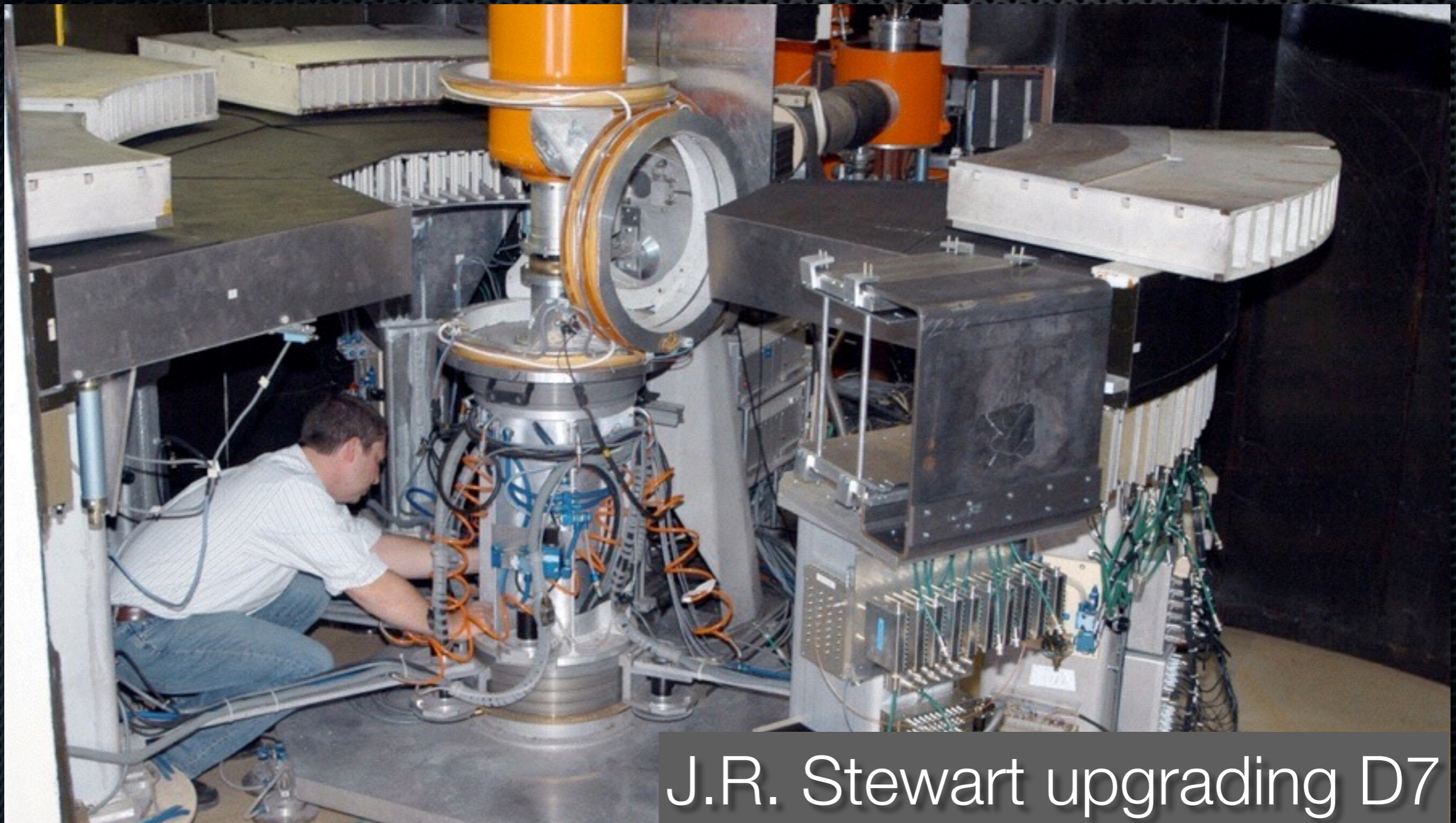
$$\sigma_y^{nsf} = \frac{1}{2} (1 - \sin^2 \gamma \cdot \sin^2 \alpha) \sigma_{mag} + \frac{1}{3} \sigma_{si} + \sigma_{nc} + \sigma_{ii}$$

$$\sigma_z^{sf} = \frac{1}{2} (1 + \cos^2 \gamma) \sigma_{mag} + \frac{2}{3} \sigma_{si}$$

$$\sigma_z^{nsf} = \frac{1}{2} (1 - \cos^2 \gamma) \sigma_{mag} + \frac{1}{3} \sigma_{si} + \sigma_{nc} + \sigma_{ii}$$

Uniaxial polarisation analysis

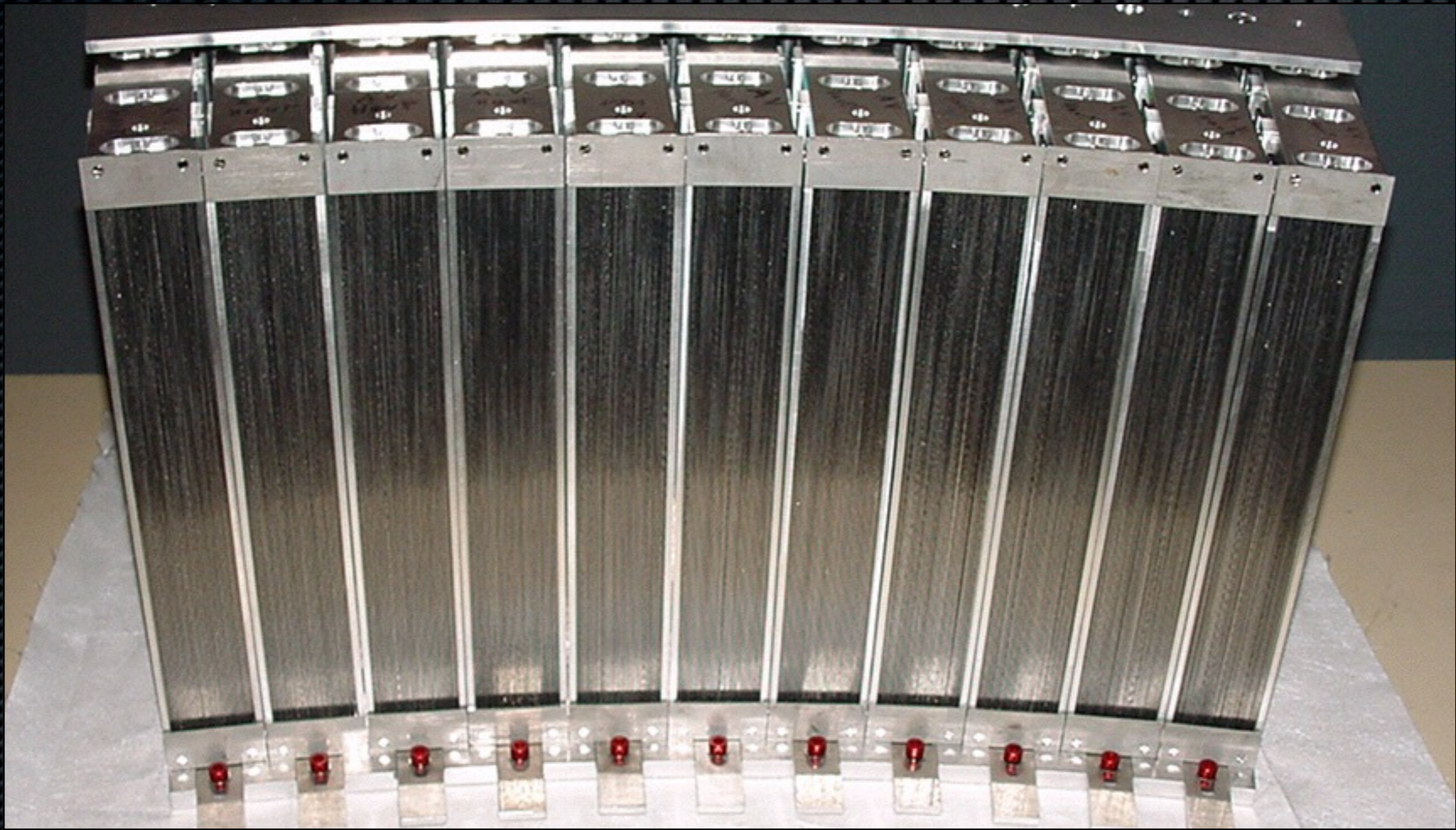
XYZ Method: generalisation to PSD detector



J.R. Stewart upgrading D7

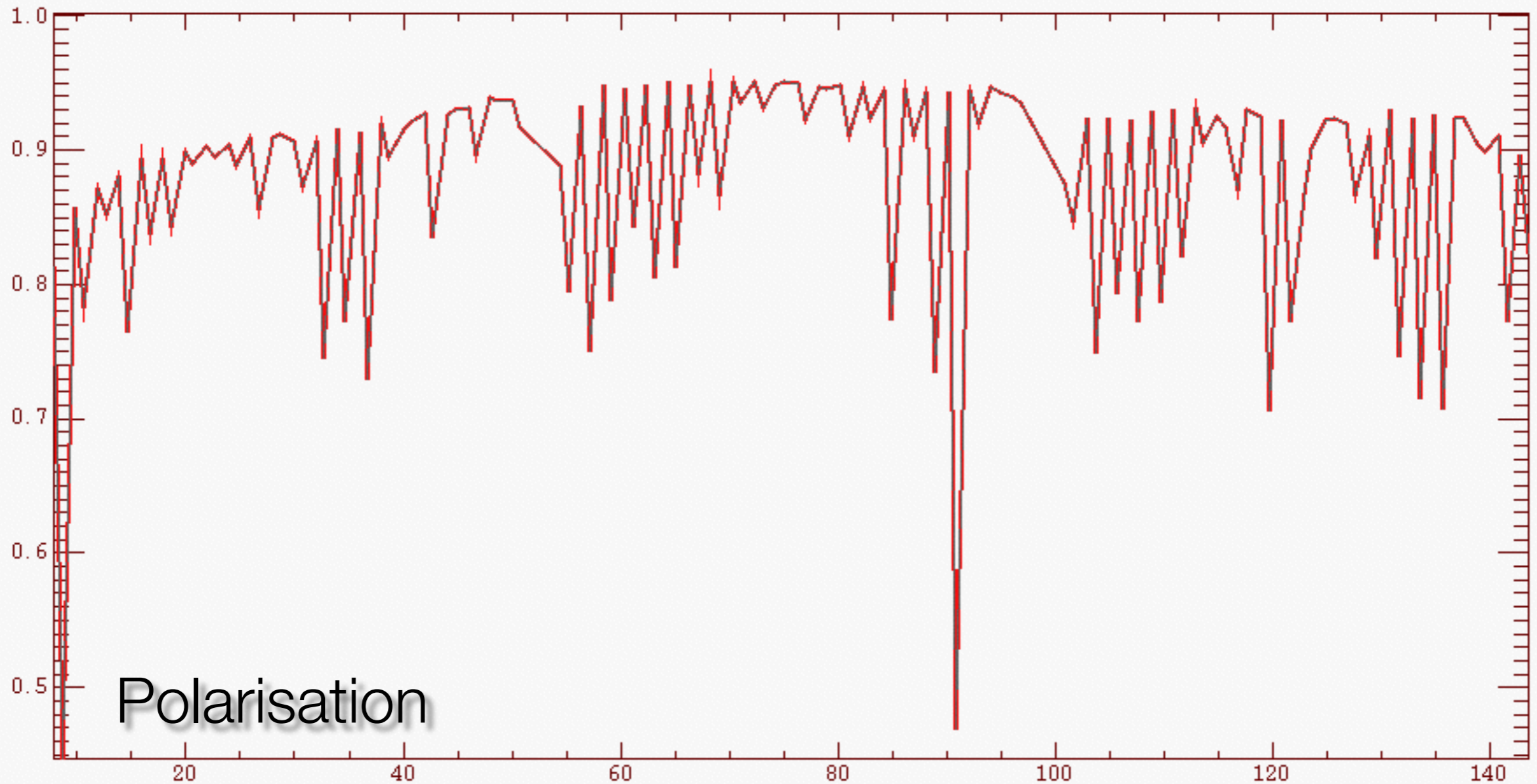
Uniaxial polarisation analysis

XYZ Method — Generalisation to PSD detector



Uniaxial polarisation analysis

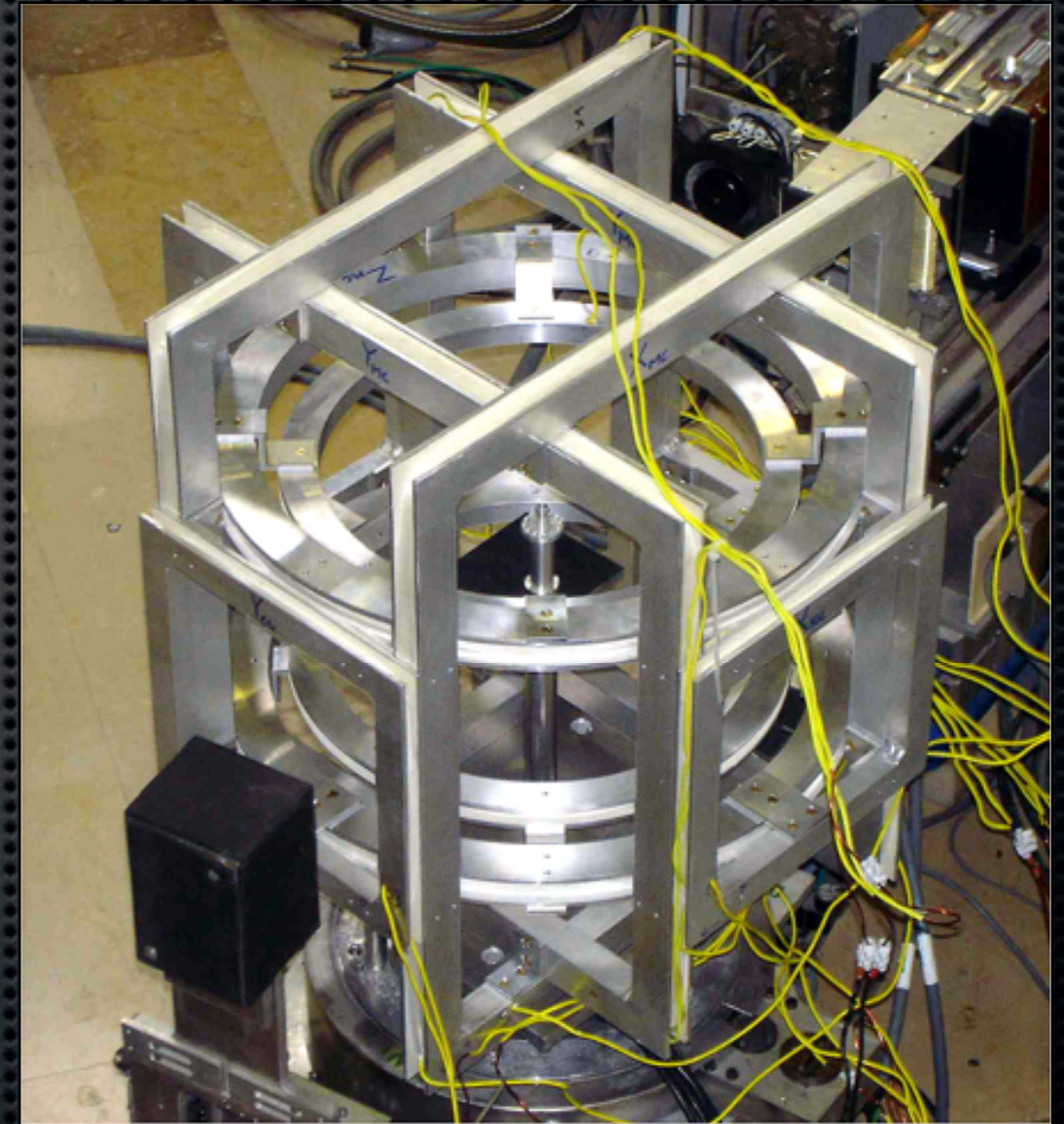
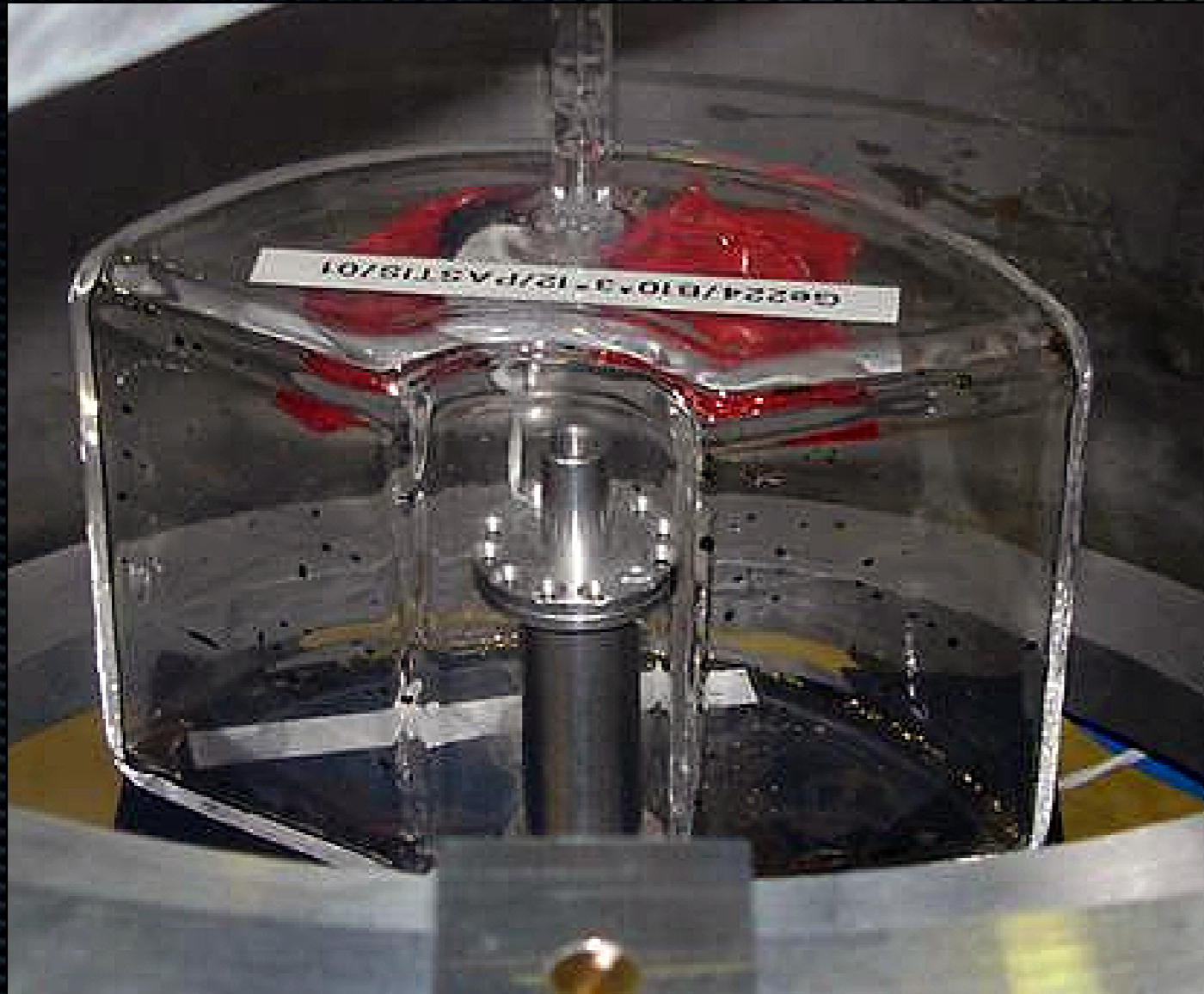
XYZ Method — Generalisation to PSD detector



50 60 70 80 90 100 110 120 130 140

Uniaxial polarisation analysis

XYZ Polarisation Analysis



PASTIS 1.0 - $T_1 \approx 100$ hours

Uniaxial polarisation analysis

XYZ Polarisation Analysis

- ✦ PASTIS 2.0:
 - Ø 700 mm
 - $T_1 \approx 70$ to 110 hours
 - Ø40 mm sample at 1.5 K
 - No dark angle
 - Perfect with graphite monochromator/analyser at steady-state source



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Spherical neutron polarimetry

$$P_{i,j} = \frac{P_i \mathbb{P}_{i,j} + P_j^\dagger}{\|\vec{P}_f\|} \text{ with } (i,j) \in \{x,y,z\}$$

A useful strategy is to measure the scattered polarisation with incident polarisation parallel to each of the polarisation axes in turn.

$$\mathbb{P} = \begin{bmatrix} N.N^* - \vec{M}_\perp.\vec{M}_\perp^* & 2\Im(NM_{\perp,z}^*) & -2\Im(NM_{\perp,y}^*) \\ -2\Im(NM_{\perp,z}^*) & N.N^* - \vec{M}_\perp.\vec{M}_\perp^* + 2\Re(M_{\perp,y}M_{\perp,y}^*) & 2\Re(M_{\perp,y}M_{\perp,z}^*) \\ 2\Im(NM_{\perp,y}^*) & 2\Re(M_{\perp,y}M_{\perp,z}^*) & N.N^* - \vec{M}_\perp.\vec{M}_\perp^* + 2\Re(M_{\perp,z}M_{\perp,z}^*) \end{bmatrix}$$

$$\vec{P}_i^\dagger \sigma = \begin{bmatrix} 2\Im(M_{\perp,y}M_{\perp,z}^*) \\ 2\Re(NM_{\perp,y}^*) \\ 2\Re(NM_{\perp,z}^*) \end{bmatrix} \text{ with } \sigma = N.N^* + \vec{M}_\perp.\vec{M}_\perp^* + P_i. \begin{bmatrix} 2\Im(M_{\perp,y}M_{\perp,z}^*) \\ 2\Re(NM_{\perp,y}^*) \\ 2\Re(NM_{\perp,z}^*) \end{bmatrix}$$

Spherical neutron polarimetry

A lot of directional information is lost when only intensities are measured.

$$\frac{\partial \sigma}{\partial \Omega} = NN^* + \vec{M}_\perp \cdot \vec{M}_\perp^* + i\vec{P}_i \cdot (\vec{M}_\perp^* \wedge \vec{M}_\perp) + 2\vec{P}_i \cdot \Re(N^* \vec{M}_\perp)$$


The vector properties of the neutron polarisation provide a way of recovering some of this information.

$$\vec{P}_f \frac{\partial \sigma}{\partial \Omega} = \vec{P}_i NN^* - \vec{P}_i (\vec{M}_\perp \cdot \vec{M}_\perp^*) + 2\Re(\vec{M}_\perp (\vec{P}_i \cdot \vec{M}_\perp^*)) + i(\vec{M}_\perp \wedge \vec{M}_\perp^*) + 2\Re(N^* \vec{M}_\perp) + 2\vec{P}_i \wedge \Im(N^* \vec{M}_\perp)$$

Spherical neutron polarimetry

Antiferromagnetic single crystals
with non-zero propagation vector

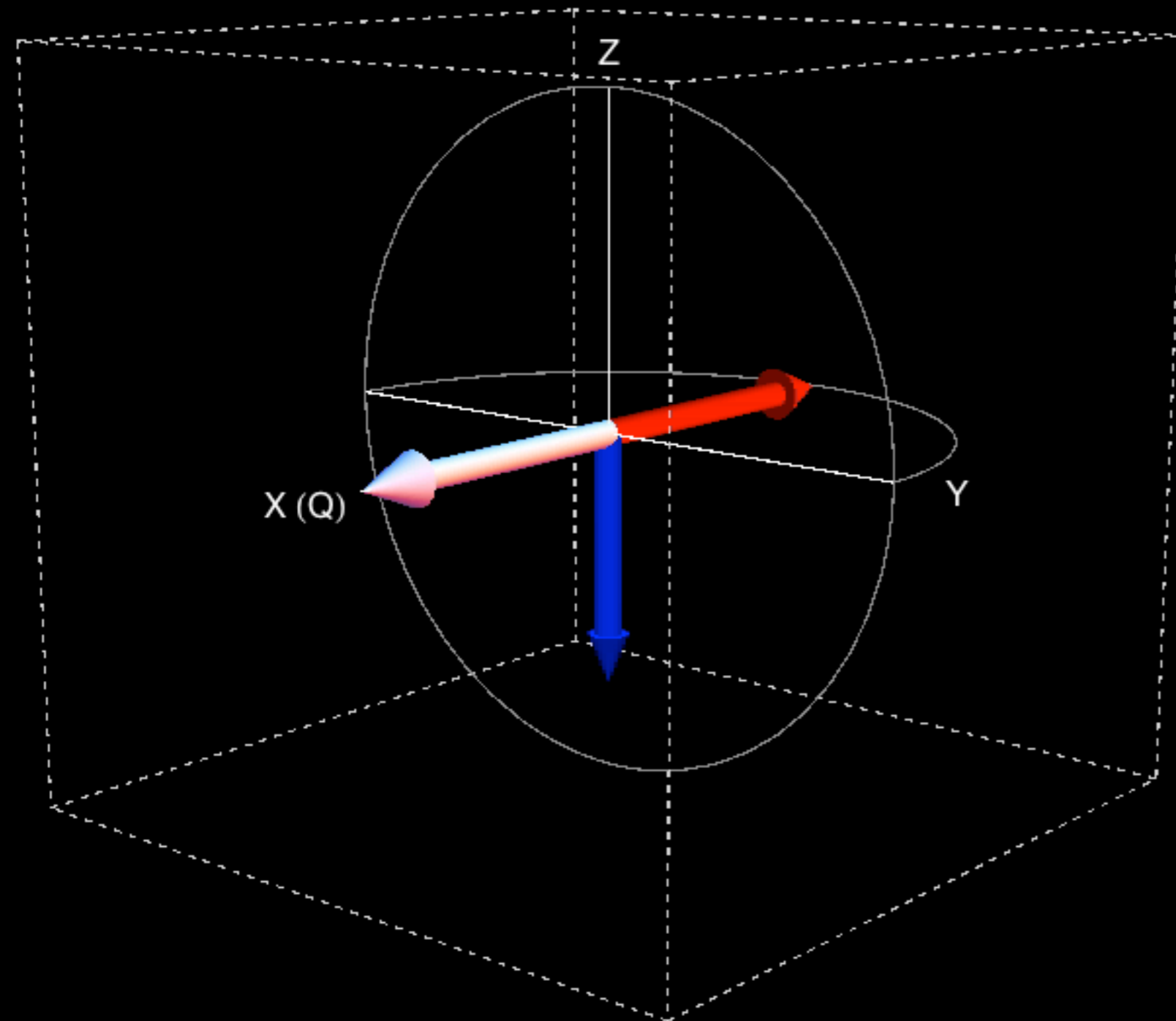
$$\frac{\partial \sigma}{\partial \Omega} = \cancel{N N^*} + \vec{M}_\perp \cdot \vec{M}_\perp^* + \cancel{i \vec{P}_i \cdot (\vec{M}_\perp^* \wedge \vec{M}_\perp)} + \cancel{2 \vec{P}_i \cdot \Re(N^* \vec{M}_\perp)}$$

When \vec{M}_\perp is purely real or imaginary, the polarisation rotates around \vec{M}_\perp by 180° - not a spin flip ! 

$$\vec{P}_f \frac{\partial \sigma}{\partial \Omega} = \cancel{\vec{P}_i N N^*} - \vec{P}_i (\vec{M}_\perp \cdot \vec{M}_\perp^*) + 2 \Re(\vec{M}_\perp (\vec{P}_i \cdot \vec{M}_\perp^*)) + \cancel{i (\vec{M}_\perp \wedge \vec{M}_\perp^*)} + \cancel{2 \Re(N^* \vec{M}_\perp)} + \cancel{2 \vec{P}_i \wedge \Im(N^* \vec{M}_\perp)}$$

Spherical neutron polarimetry

Antiferromagnetic single crystals: $\tau \neq 0$



Nuclear Structure Factor

real part

imaginary part

Magnetic Structure Factor

real part, $\theta = -180^\circ$

imaginary part, $\theta = 180^\circ$

Pure
Magnetic
Signal

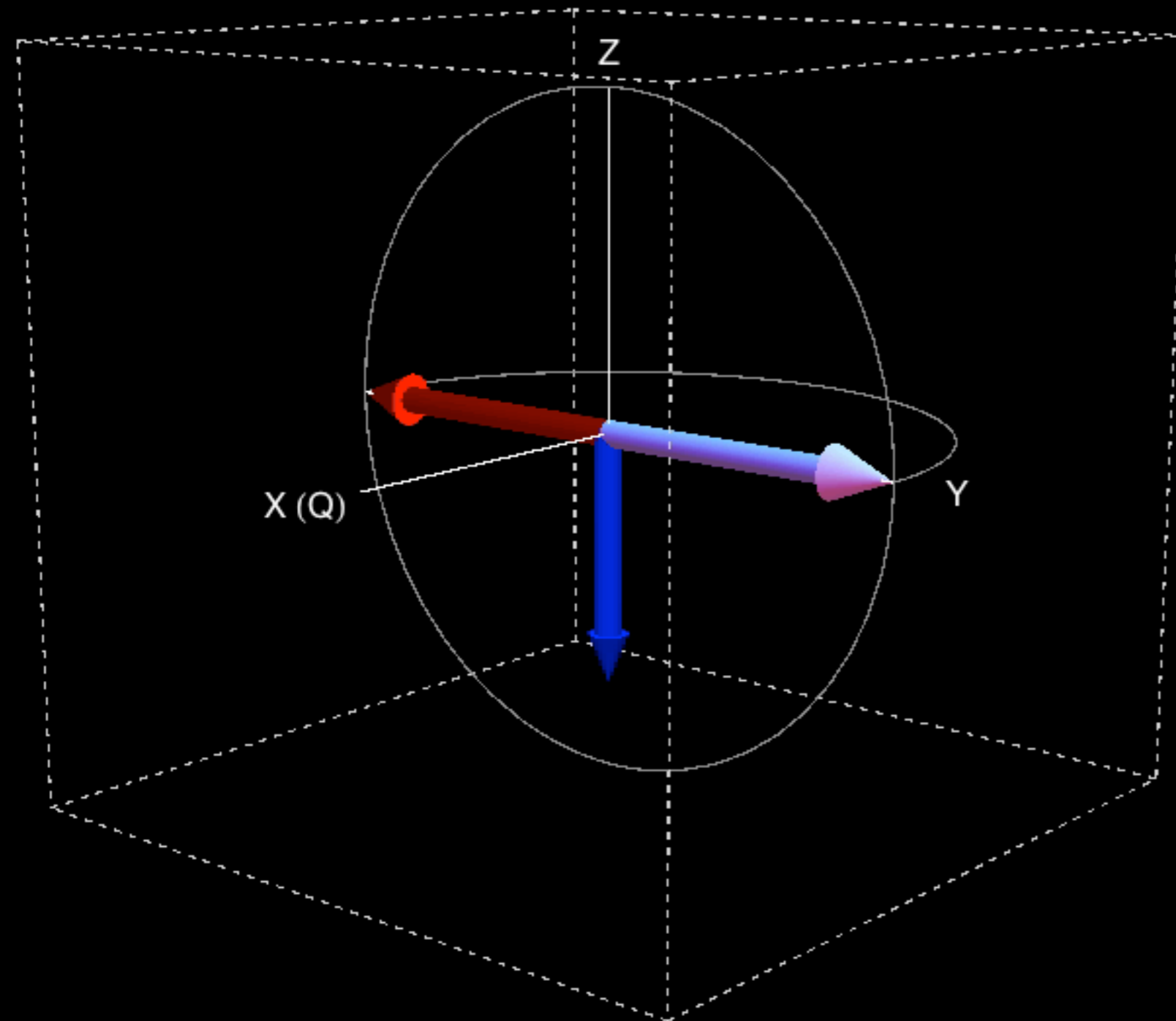
Cross Section



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Spherical neutron polarimetry

Antiferromagnetic single crystals: $\tau \neq 0$



Nuclear Structure Factor

real part

imaginary part

Magnetic Structure Factor

real part, $\theta = -180^\circ$

imaginary part, $\theta = 0^\circ$

Pure
Magnetic
Signal

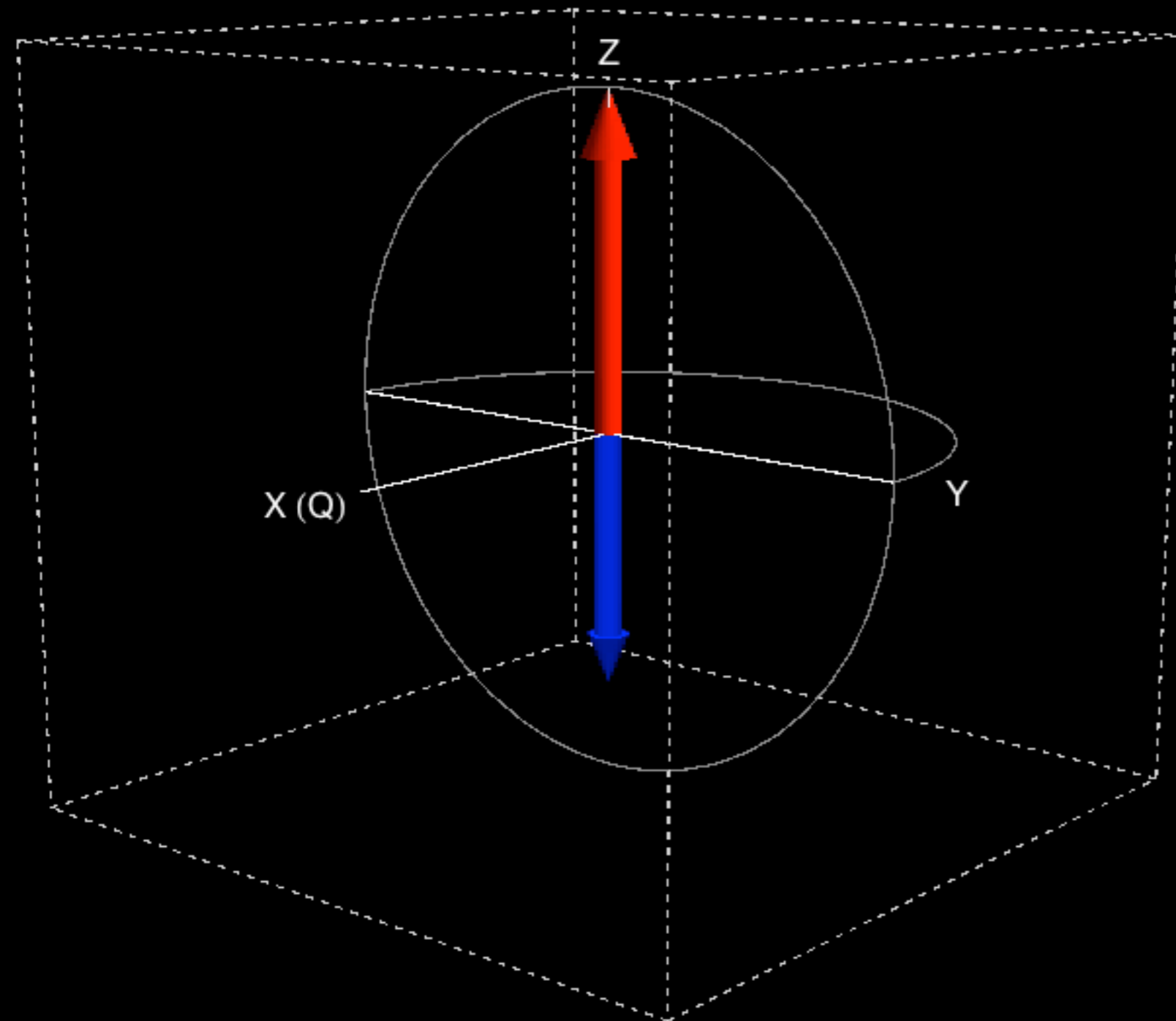
Cross Section



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Spherical neutron polarimetry

Antiferromagnetic single crystals: $\tau \neq 0$



Nuclear Structure Factor

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real part, $\theta = -180^\circ$

imaginary part, $\theta = 180^\circ$

Pure
Magnetic
Signal

Cross Section



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Spherical neutron polarimetry

Antiferromagnetic single crystals
with non-zero propagation vector

$$\frac{\partial \sigma}{\partial \Omega} = \cancel{N N^*} + \vec{M}_\perp \cdot \vec{M}_\perp^* + i \vec{P}_i \cdot (\vec{M}_\perp^* \wedge \vec{M}_\perp) + \cancel{2 \vec{P}_i \cdot \Re(N^* \vec{M}_\perp)}$$

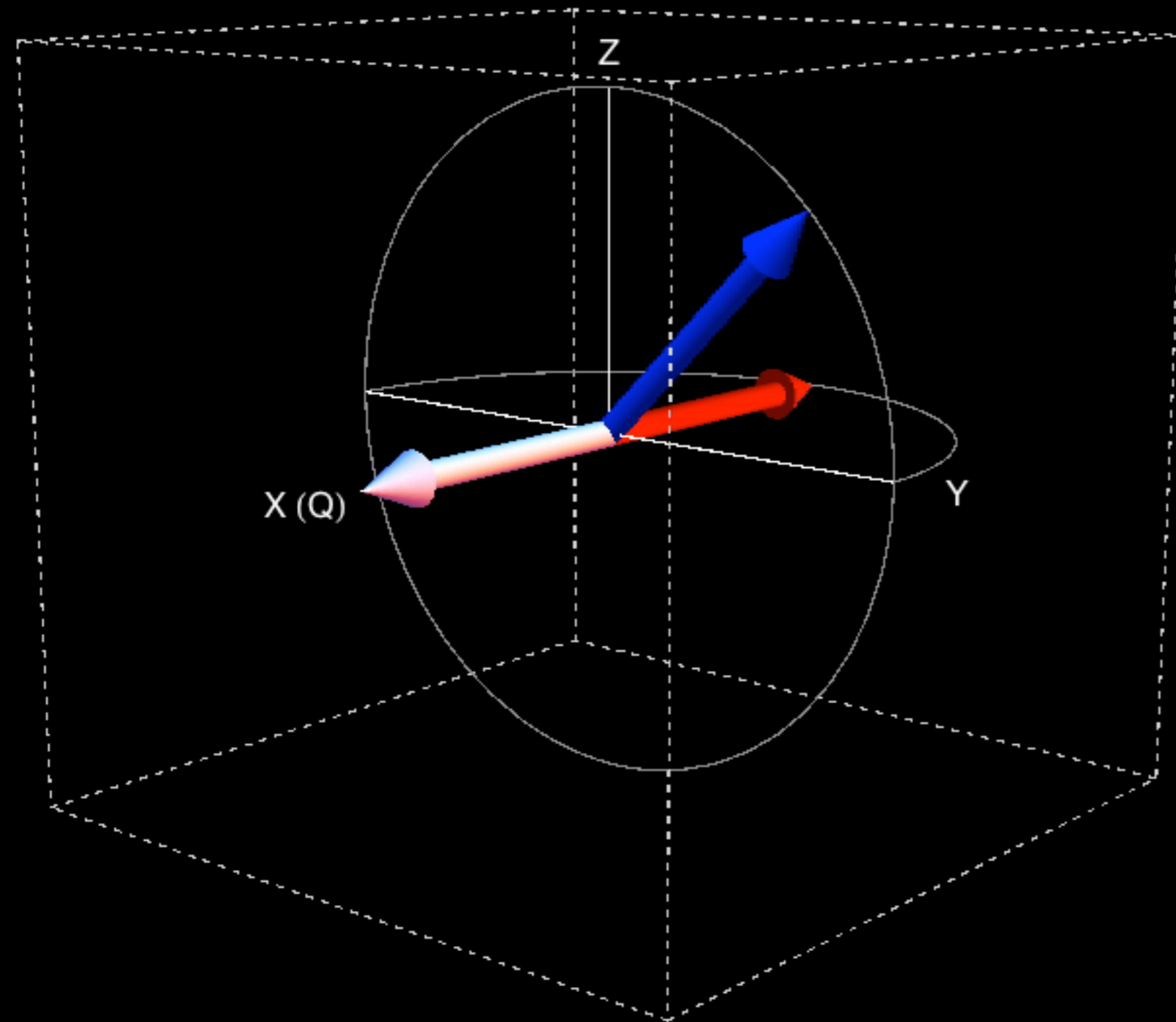
When \vec{M}_\perp is complex, the polarisation rotates by 90°
and its final orientation depends on $\|\vec{M}_\perp\|/N$.

$$\vec{P}_f \frac{\partial \sigma}{\partial \Omega} = \cancel{\vec{P}_i N N^*} - \vec{P}_i (\vec{M}_\perp \cdot \vec{M}_\perp^*) + 2 \Re(\vec{M}_\perp (\vec{P}_i \cdot \vec{M}_\perp^*)) +$$

$$i (\vec{M}_\perp \wedge \vec{M}_\perp^*) + \cancel{2 \Re(N^* \vec{M}_\perp)} + \cancel{2 \vec{P}_i \wedge \Im(N^* \vec{M}_\perp)}$$

Spherical neutron polarimetry

Antiferromagnetic single crystals: $\tau \neq 0$



Nuclear Structure Factor

real part

imaginary part

Magnetic Structure Factor

real part, $\theta = -45^\circ$

imaginary part, $\theta = -135^\circ$

Pure
Magnetic
Signal

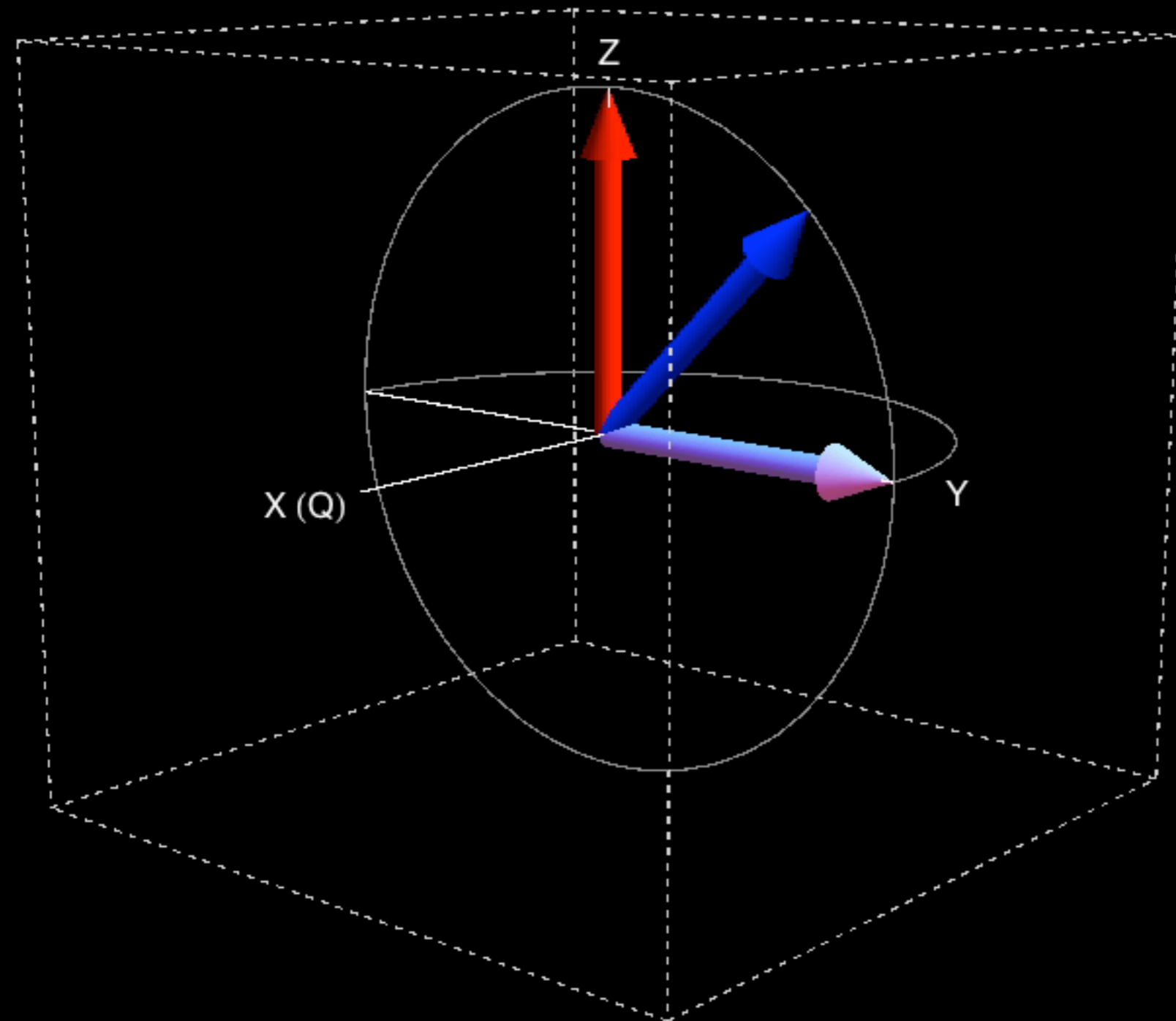
Cross Section



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Spherical neutron polarimetry

Antiferromagnetic single crystals: $\tau \neq 0$



Nuclear Structure Factor

real part

imaginary part

Magnetic Structure Factor

real part, $\theta = -45^\circ$

imaginary part, $\theta = -135^\circ$

Pure
Magnetic
Signal

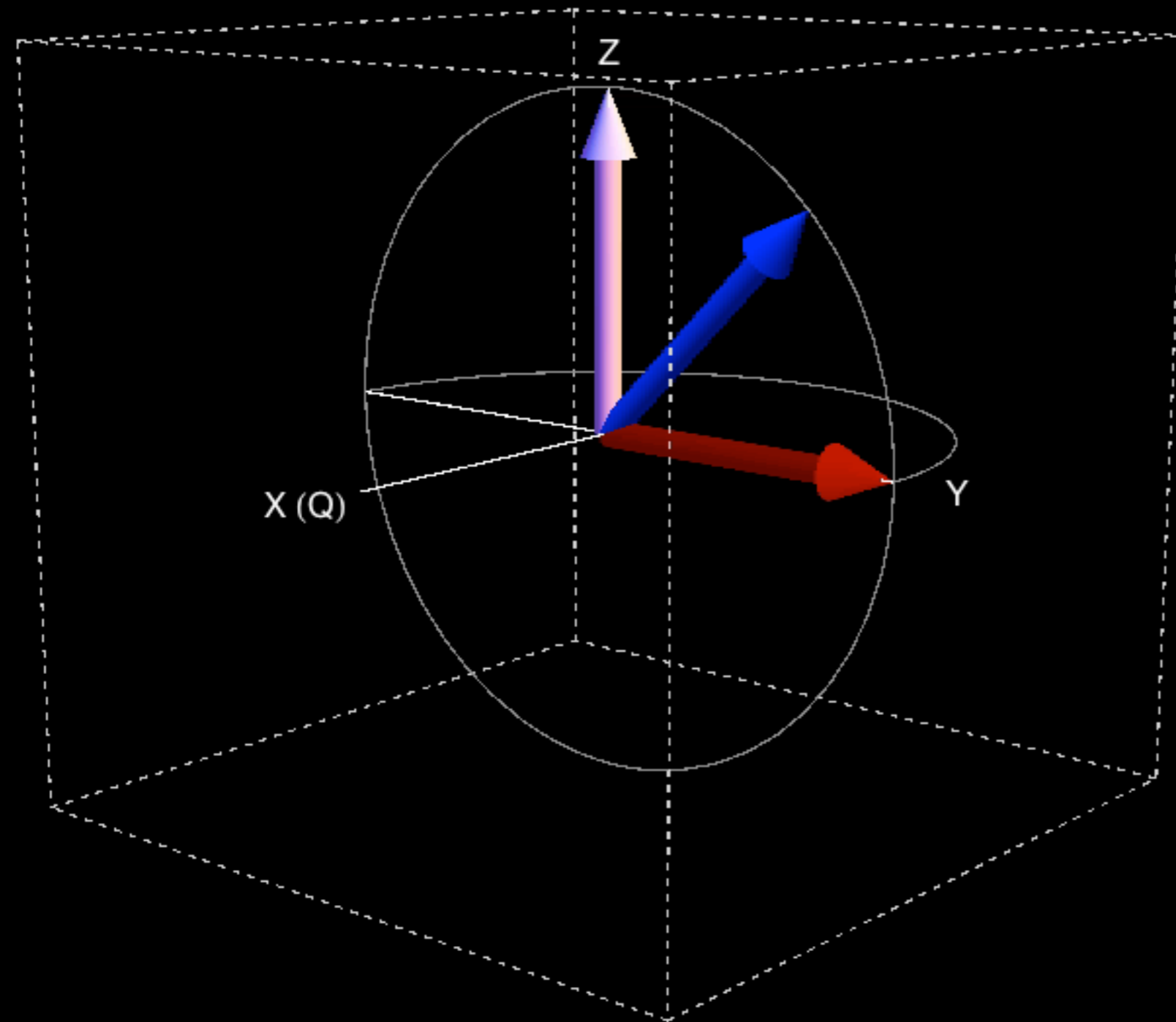
Cross Section



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Spherical neutron polarimetry

Antiferromagnetic single crystals: $\tau \neq 0$



Nuclear Structure Factor

real part

imaginary part

Magnetic Structure Factor

real part, $\theta = -45^\circ$

imaginary part, $\theta = -135^\circ$

Pure
Magnetic
Signal

Cross Section



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Spherical neutron polarimetry

Antiferromagnetic single crystals
with zero propagation vector

$$\frac{\partial \sigma}{\partial \Omega} = \underbrace{NN^*}_{\text{orange}} + \vec{M}_\perp \cdot \vec{M}_\perp^* + \underbrace{i\vec{P}_i \cdot (\vec{M}_\perp^* \wedge \vec{M}_\perp)}_{\text{blue, crossed out}} + \underbrace{2\vec{P}_i \cdot \Re(N^* \vec{M}_\perp)}_{\text{green, orange}}$$

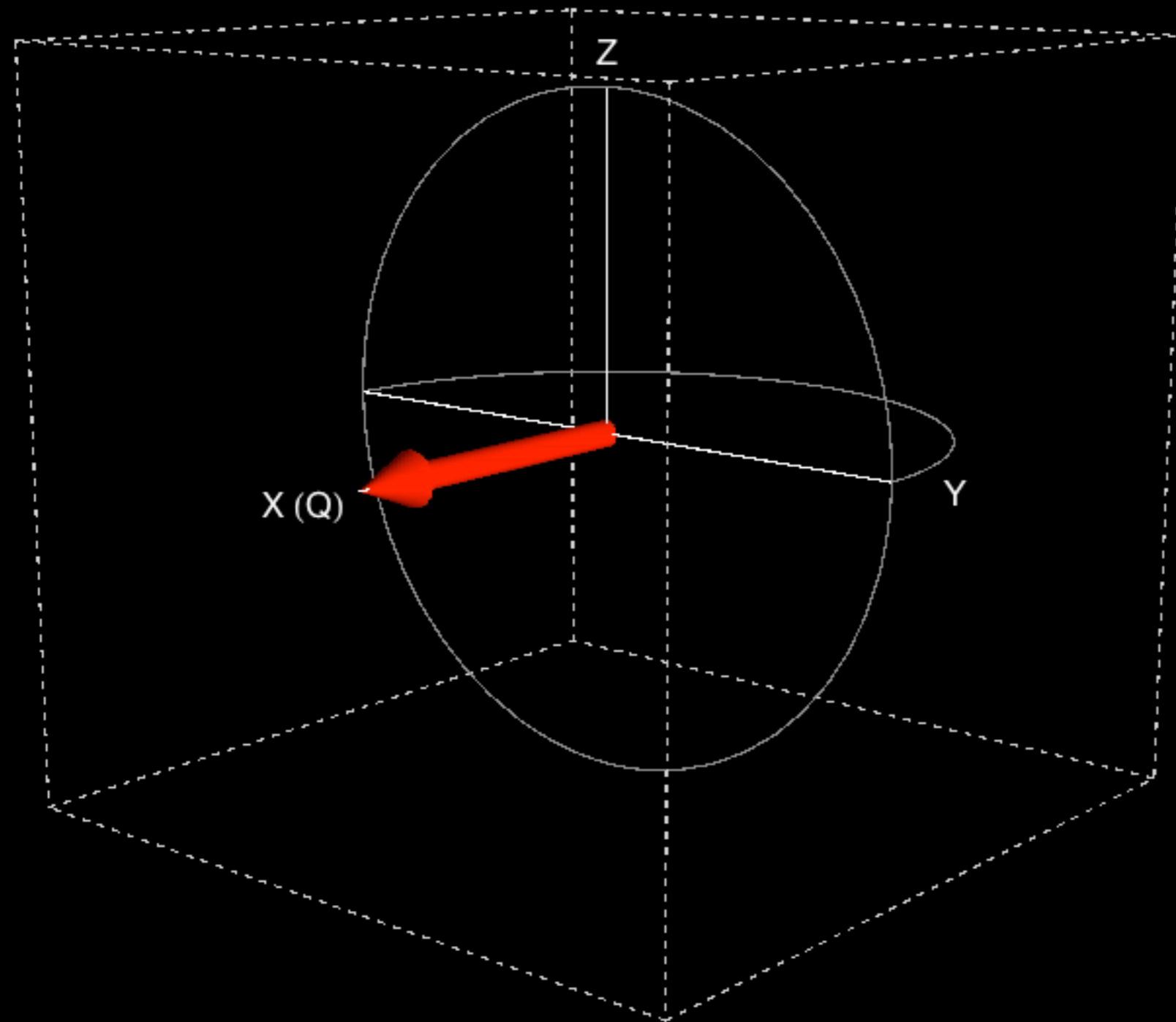
When \vec{M}_\perp is real, the polarisation rotates toward \vec{M}_\perp
by an angle depending on $\|\vec{M}_\perp\|/N$.

$$\vec{P}_f \frac{\partial \sigma}{\partial \Omega} = \underbrace{\vec{P}_i NN^*}_{\text{orange}} - \underbrace{\vec{P}_i (\vec{M}_\perp \cdot \vec{M}_\perp^*)}_{\text{grey}} + \underbrace{2\Re(\vec{M}_\perp (\vec{P}_i \cdot \vec{M}_\perp^*))}_{\text{grey}} +$$

$$\underbrace{i(\vec{M}_\perp \wedge \vec{M}_\perp^*)}_{\text{blue, crossed out}} + \underbrace{2\Re(N^* \vec{M}_\perp)}_{\text{green, orange}} + \underbrace{2\vec{P}_i \wedge \Im(N^* \vec{M}_\perp)}_{\text{green, orange}}$$

Spherical neutron polarimetry

Antiferromagnetic single crystals: $\tau=0$



Nuclear Structure Factor

real part

imaginary part

Magnetic Structure Factor

real part, $\theta=-90^\circ$

imaginary part, $\theta=0^\circ$

Nuclear
Magnetic
in Phase

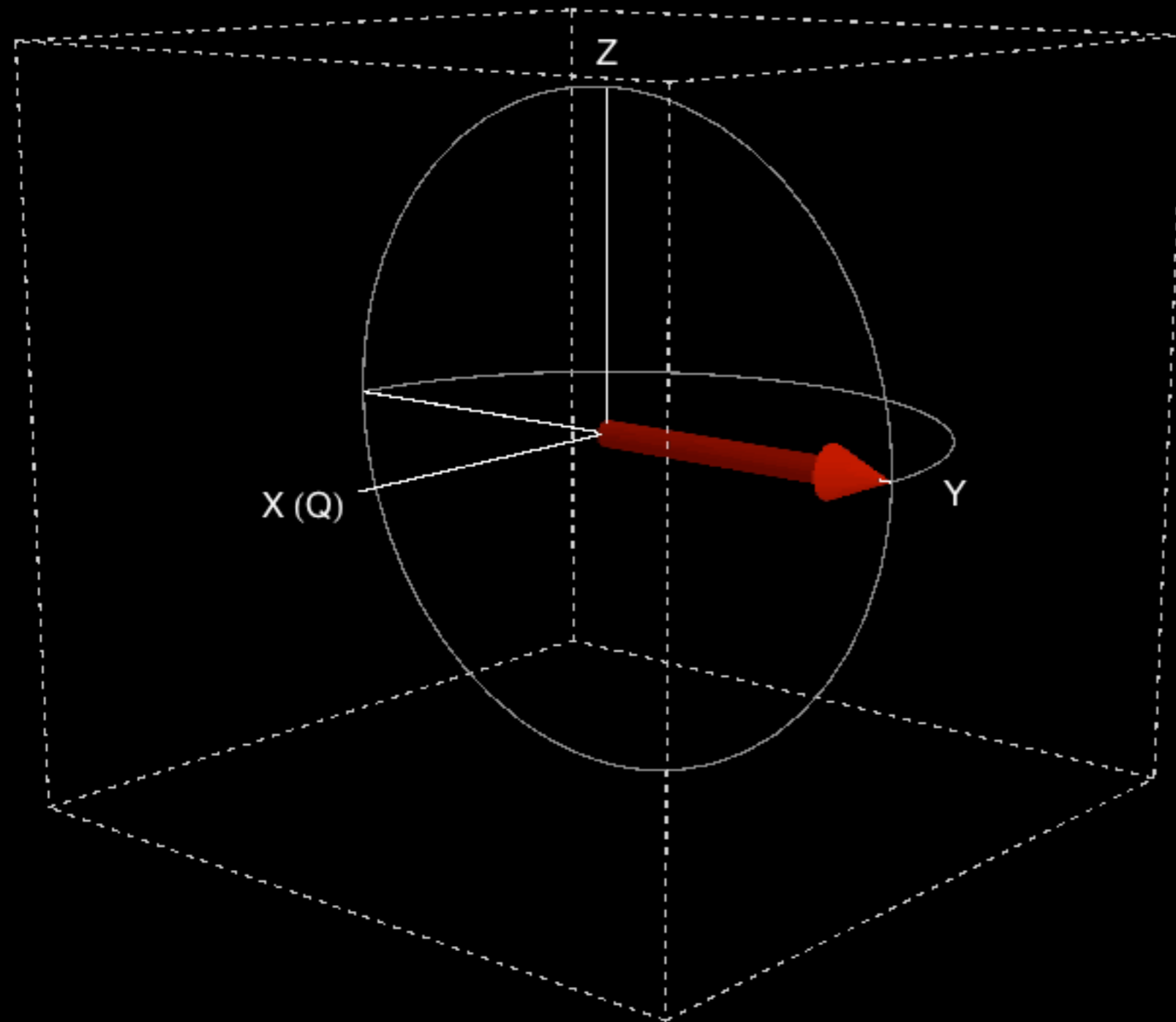
Cross Section



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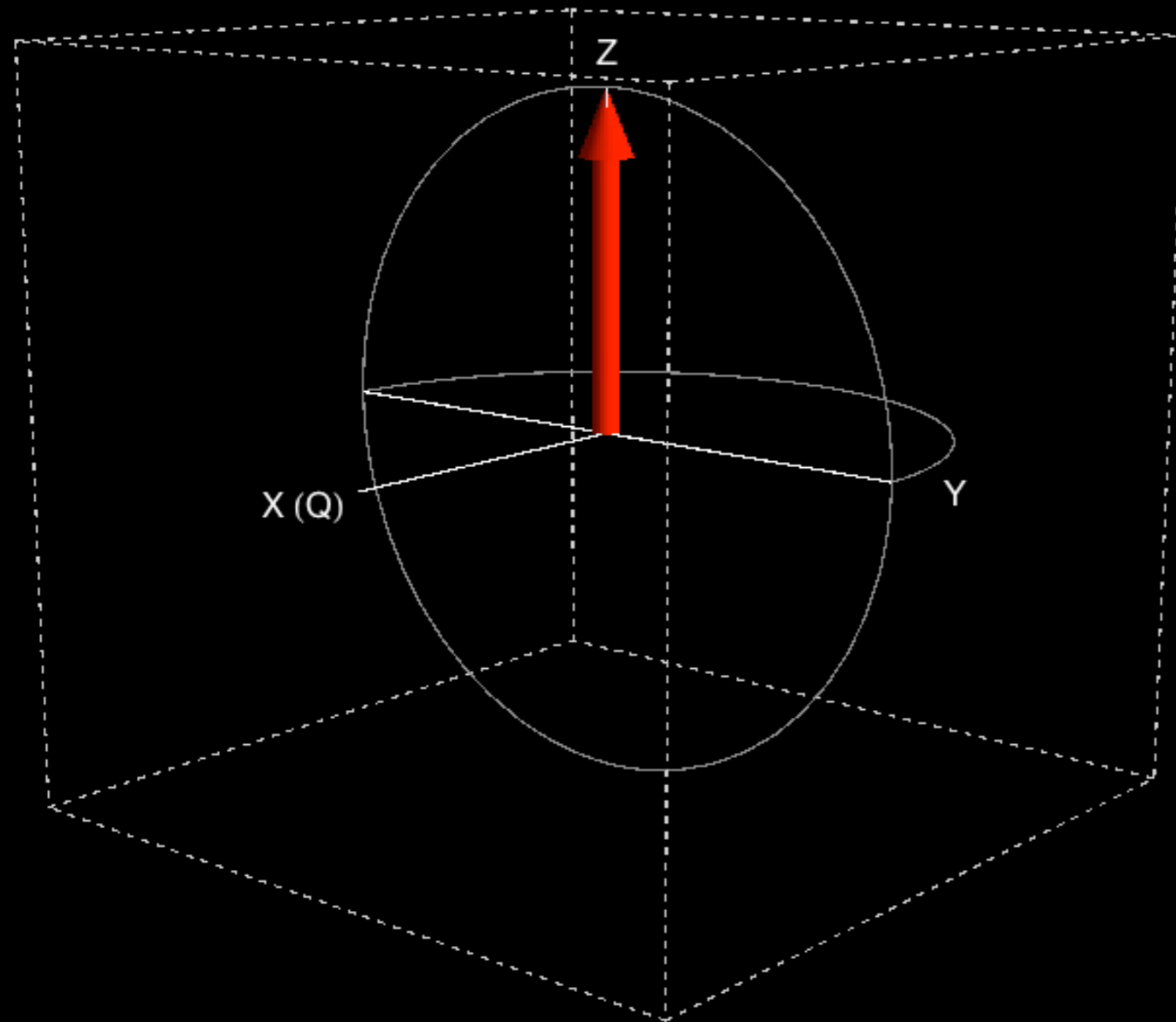
Cross Section



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Spherical neutron polarimetry

Antiferromagnetic single crystals
with zero propagation vector

$$\frac{\partial \sigma}{\partial \Omega} = \underbrace{NN^*}_{\text{orange}} + \vec{M}_\perp \cdot \vec{M}_\perp^* + \underbrace{i\vec{P}_i \cdot (\vec{M}_\perp^* \wedge \vec{M}_\perp)}_{\text{blue, crossed out}} + \underbrace{2\vec{P}_i \cdot \Re(N^* \vec{M}_\perp)}_{\text{green, orange}}$$

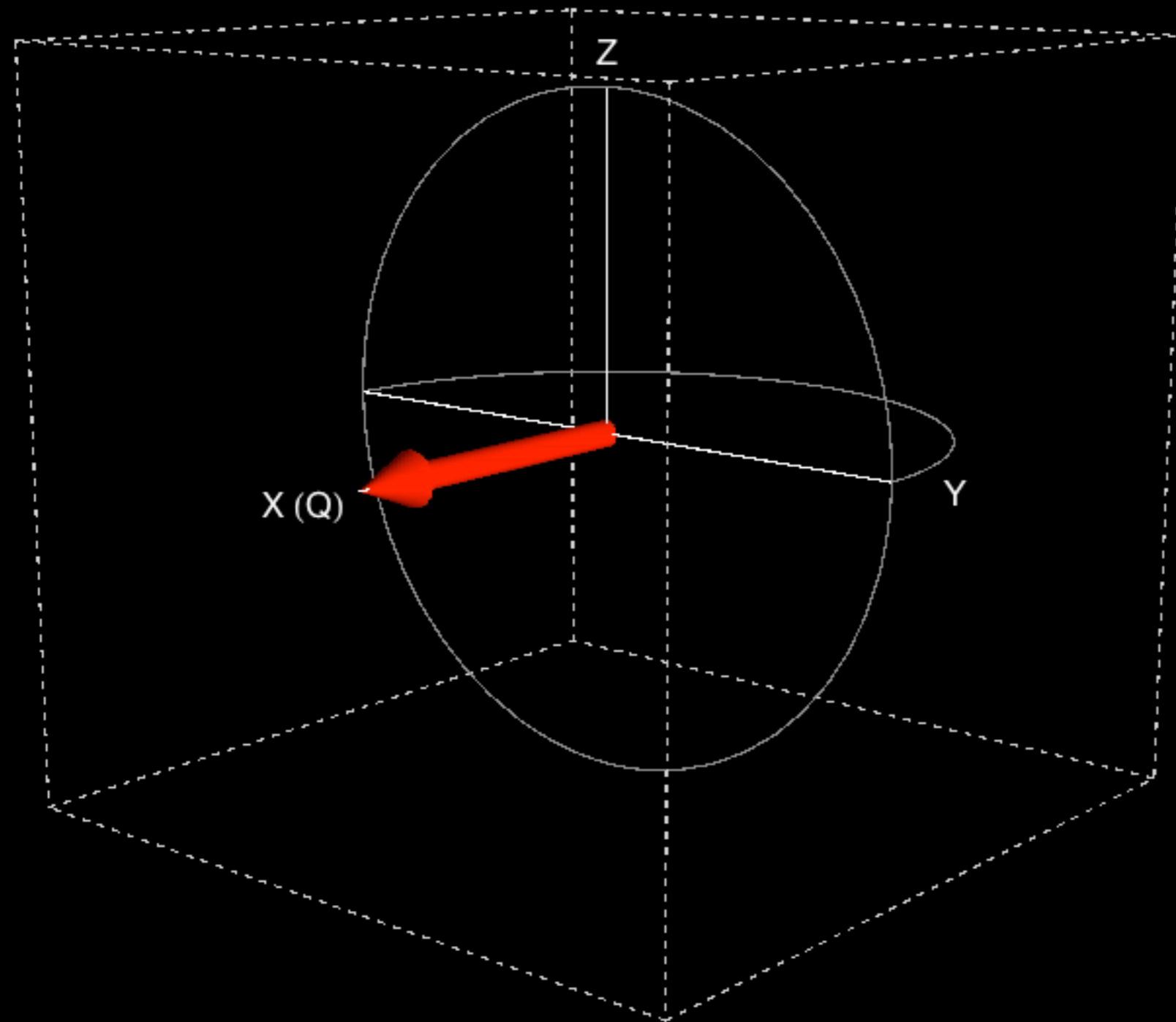
When \vec{M}_\perp is imaginary, the polarisation rotates
around \vec{M}_\perp by an angle depending on $\|\vec{M}_\perp\|/N$.

$$\vec{P}_f \frac{\partial \sigma}{\partial \Omega} = \underbrace{\vec{P}_i NN^*}_{\text{orange}} - \underbrace{\vec{P}_i (\vec{M}_\perp \cdot \vec{M}_\perp^*)}_{\text{grey}} + \underbrace{2\Re(\vec{M}_\perp (\vec{P}_i \cdot \vec{M}_\perp^*))}_{\text{grey}} +$$

$$\underbrace{i(\vec{M}_\perp \wedge \vec{M}_\perp^*)}_{\text{blue, crossed out}} + \underbrace{2\Re(N^* \vec{M}_\perp)}_{\text{green, orange}} + \underbrace{2\vec{P}_i \wedge \Im(N^* \vec{M}_\perp)}_{\text{green, orange}}$$

Spherical neutron polarimetry

Antiferromagnetic single crystals: $\tau=0$



Nuclear Structure Factor

real part

imaginary part

Magnetic Structure Factor

real part, $\theta=0^\circ$

imaginary part, $\theta=90^\circ$

Nuclear
Magnetic
in Quadrature

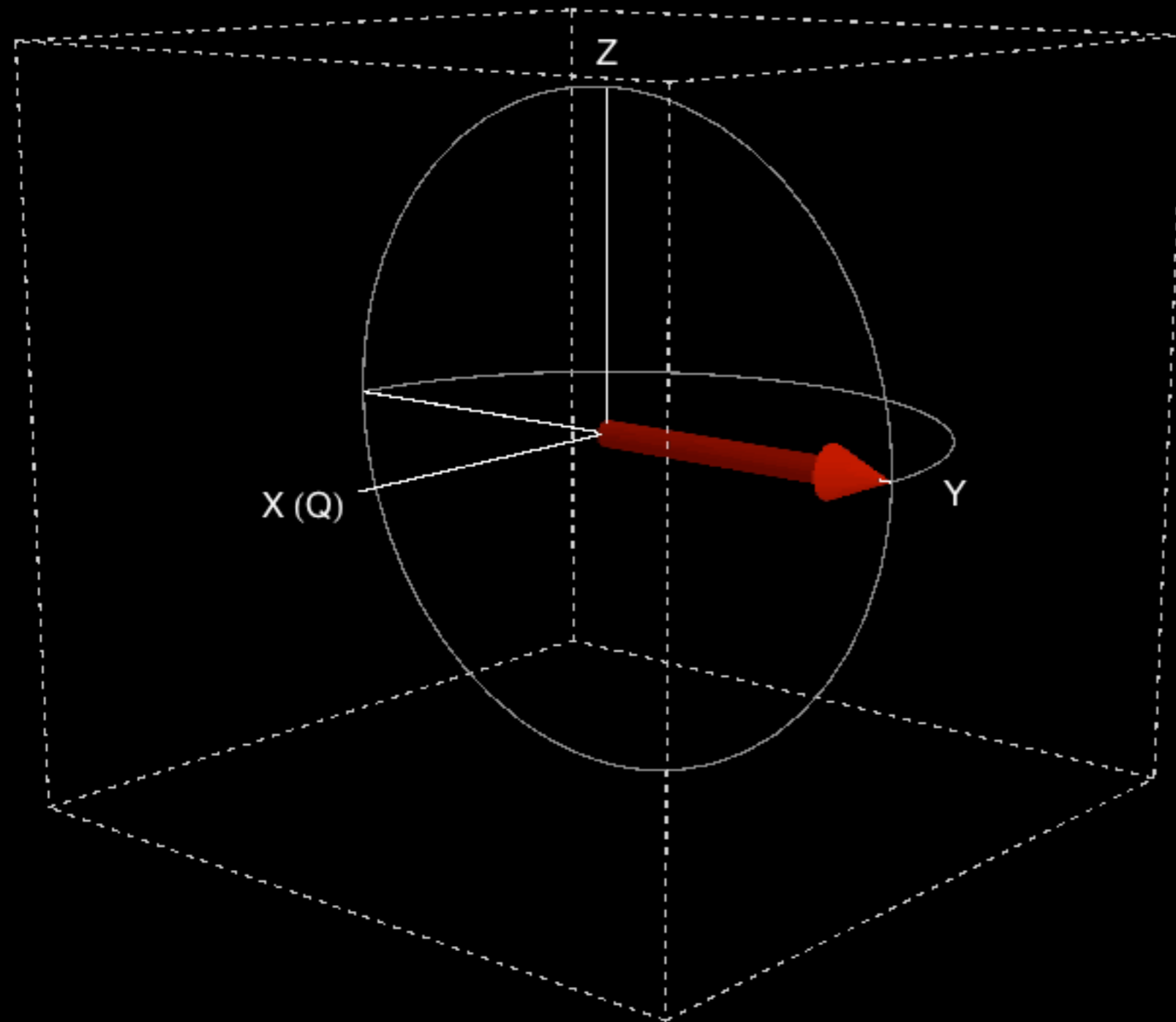
Cross Section



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Spherical neutron polarimetry

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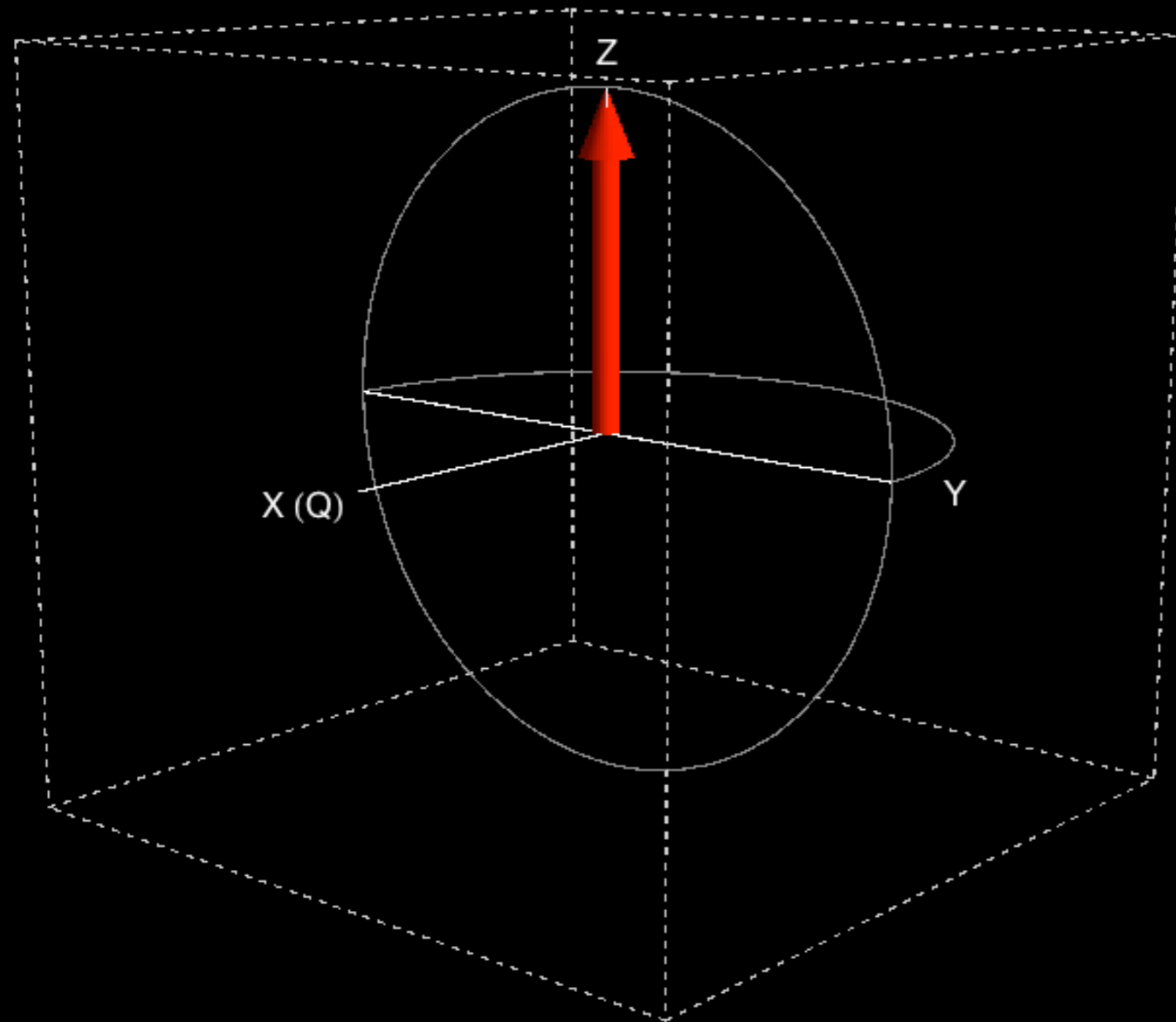
Cross Section



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Spherical neutron polarimetry

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Magnetic Structure Factor

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imaginary part, $\theta=90^\circ$

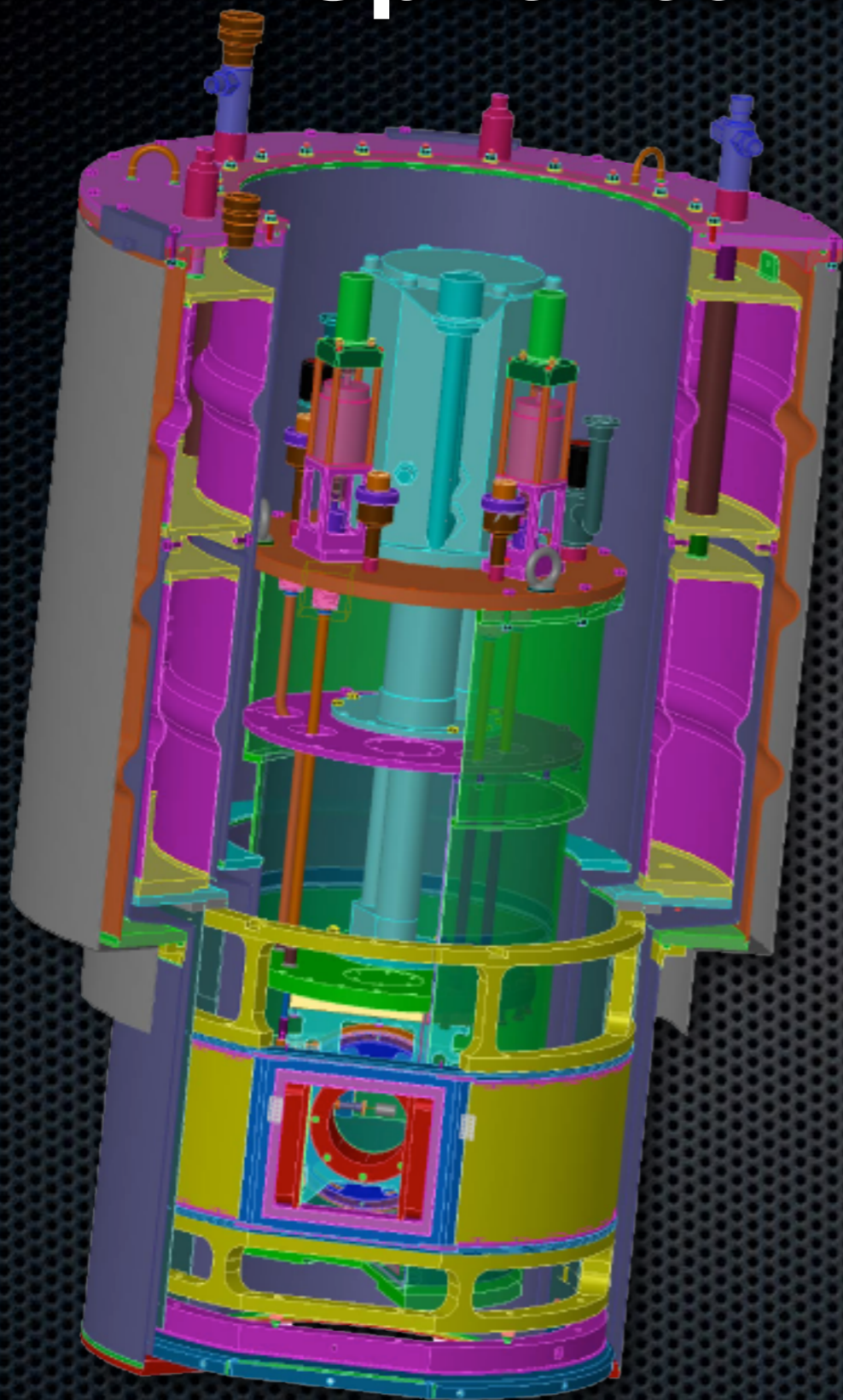
Nuclear
Magnetic
in Quadrature

Cross Section

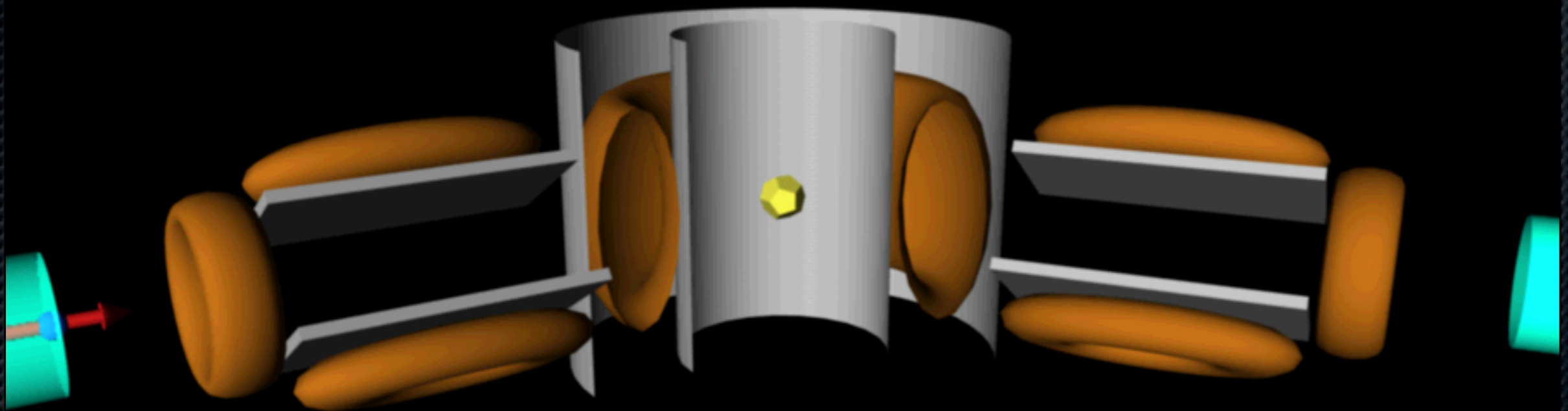


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Spherical neutron polarimetry



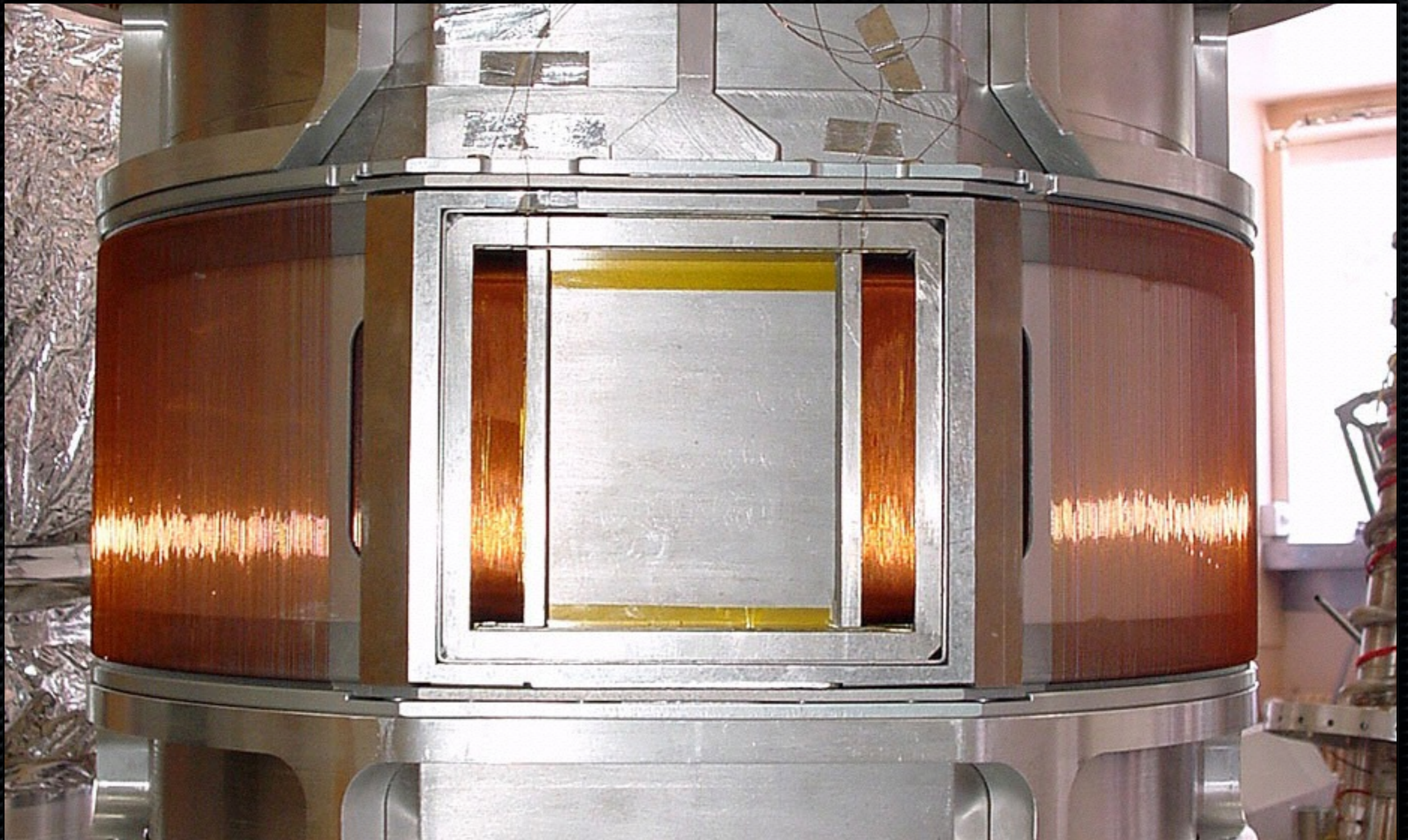
Spherical neutron polarimetry



Cryopad - < 2mG in sample chamber

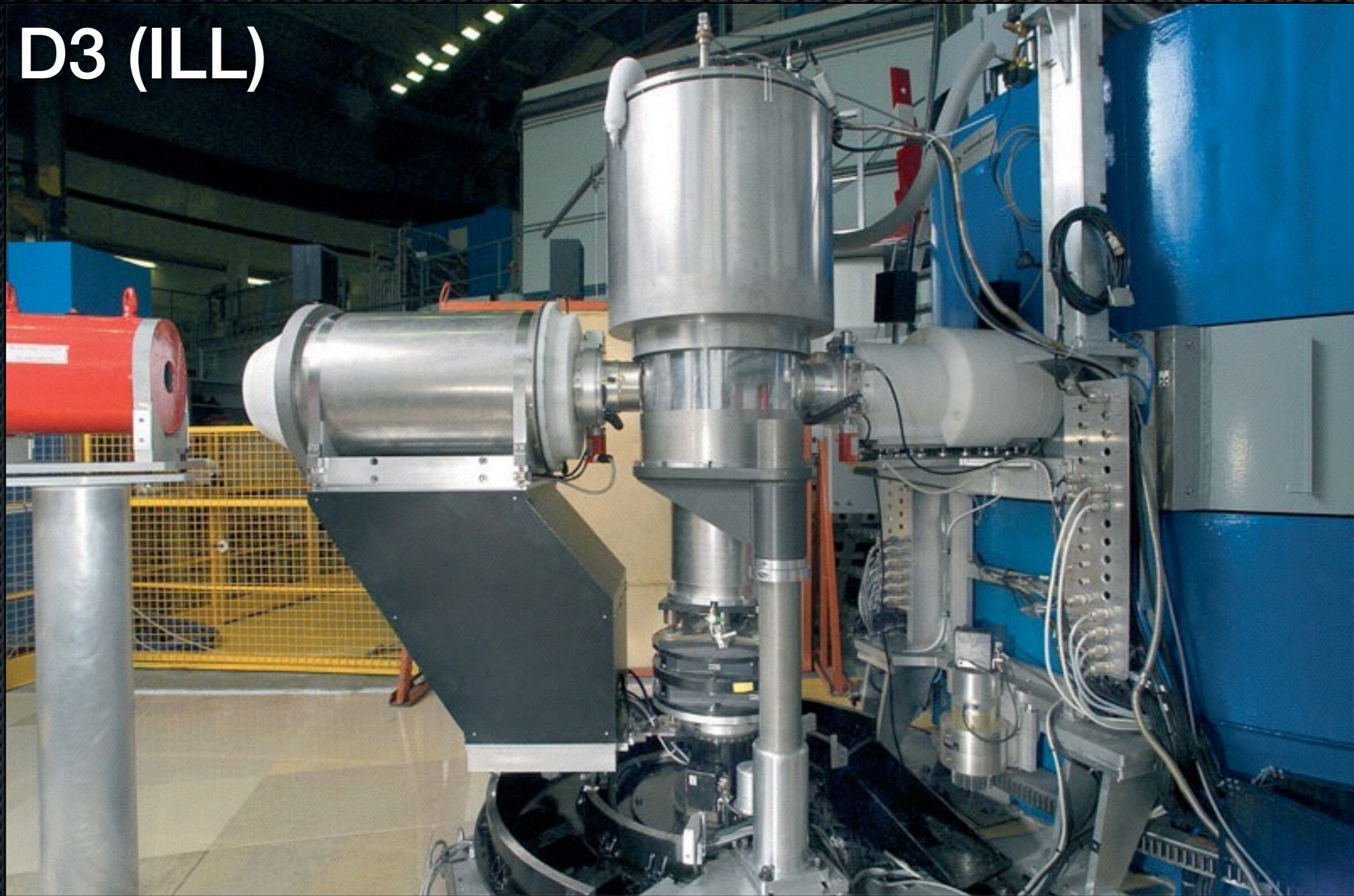


Spherical neutron polarimetry



Spherical neutron polarimetry

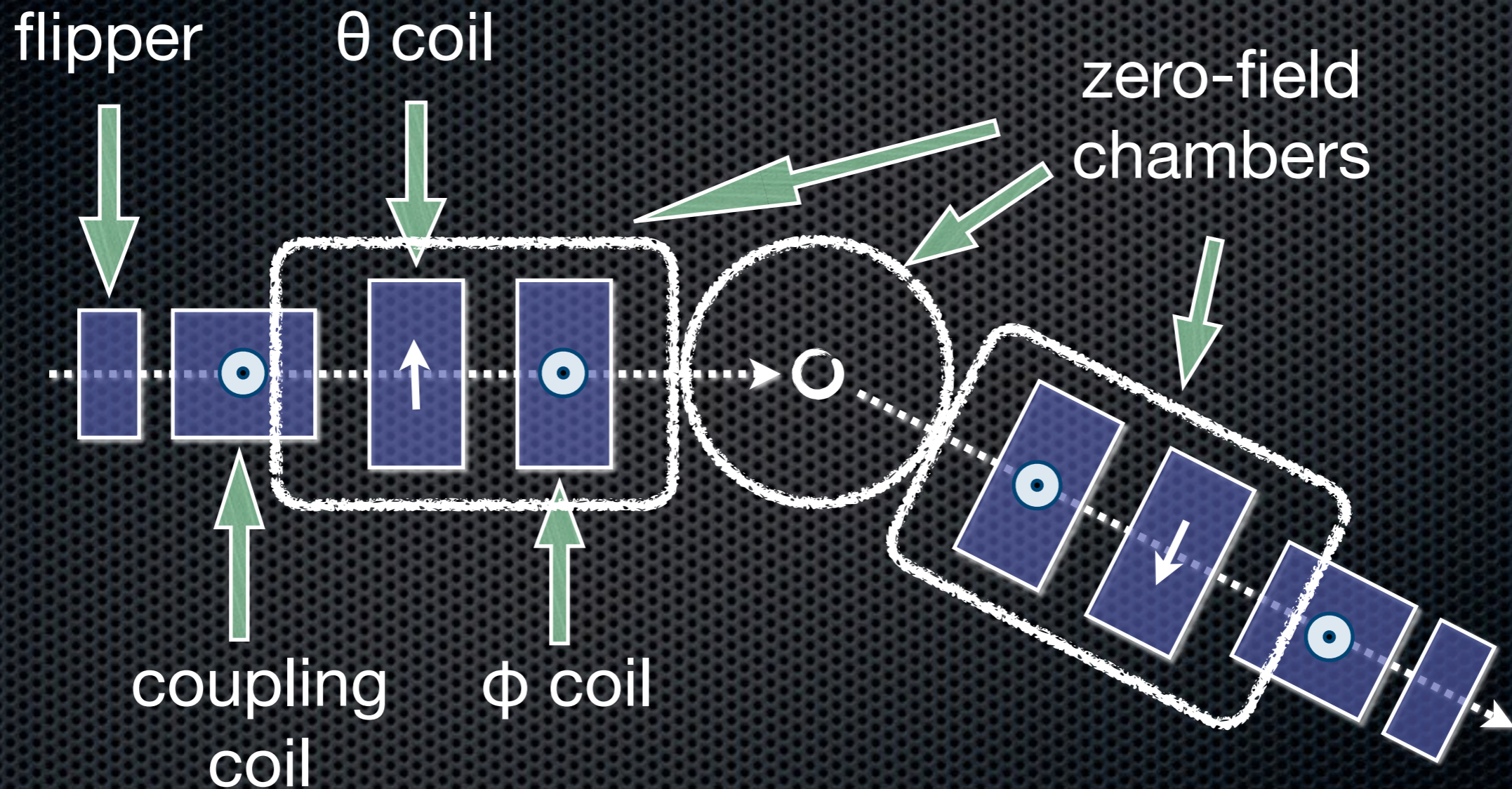
D3 (ILL)



Spherical neutron polarimetry

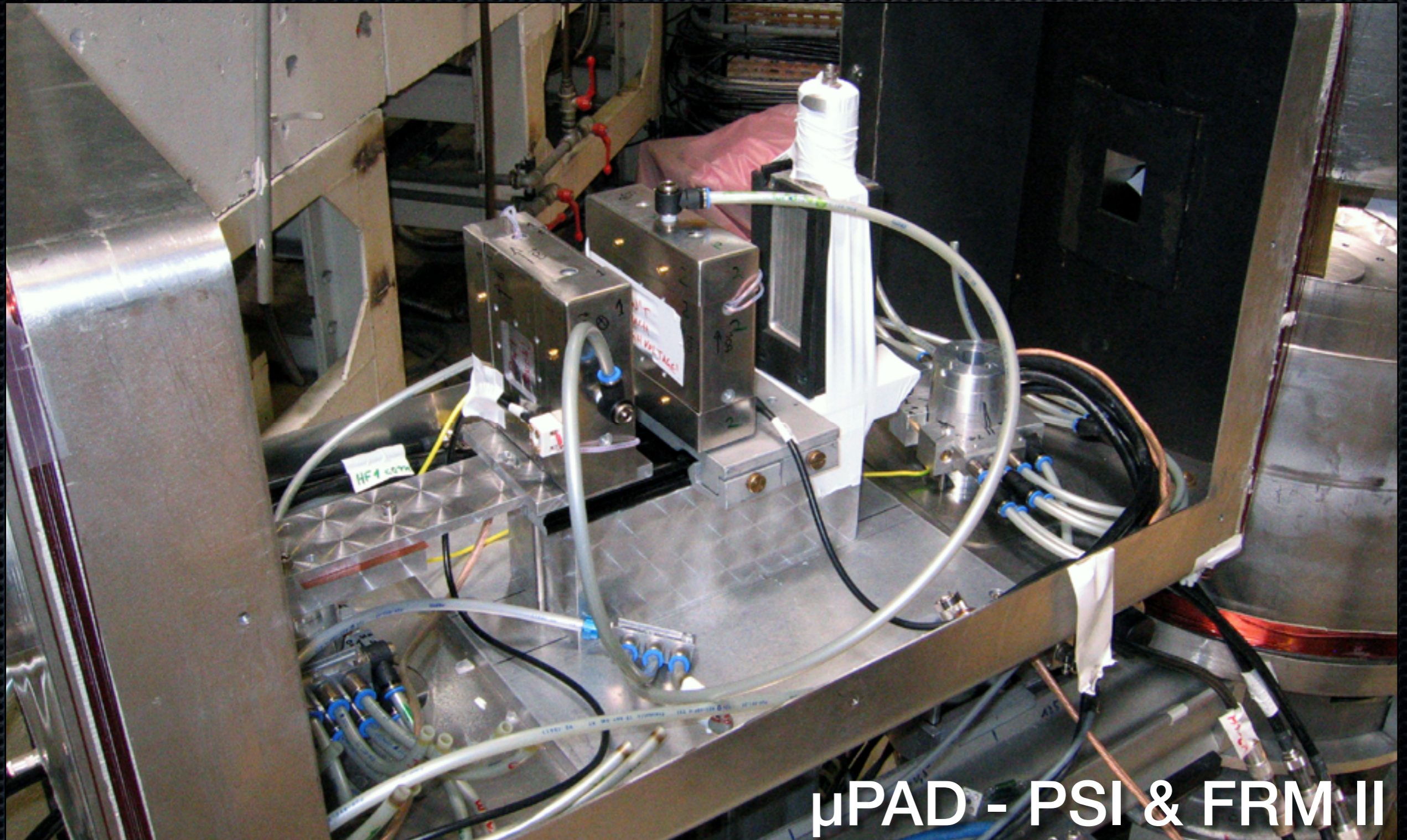


Spherical neutron polarimetry



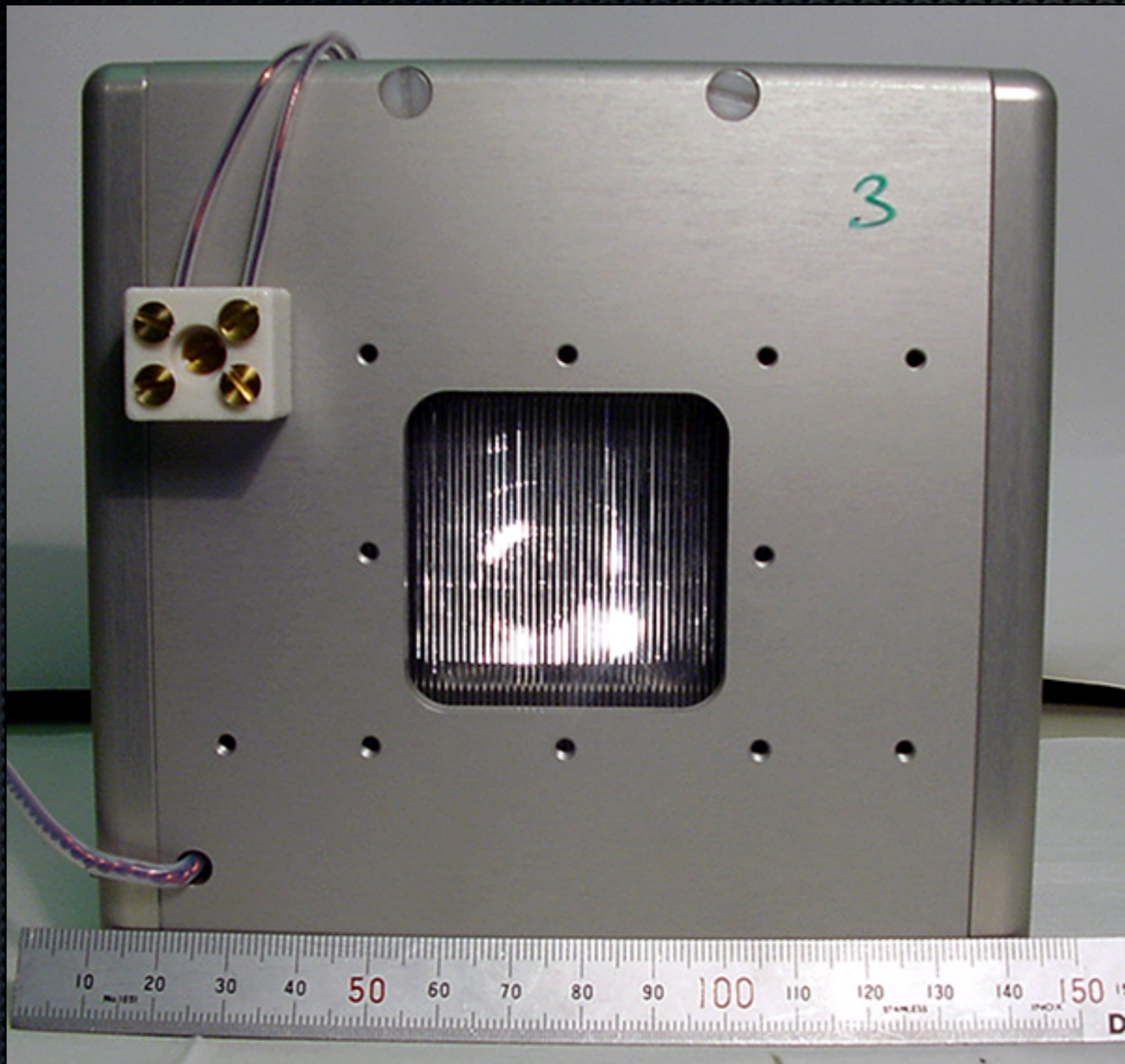
μ PAD - PSI & FRM II

Spherical neutron polarimetry



μ PAD - PSI & FRM II

Spherical neutron polarimetry



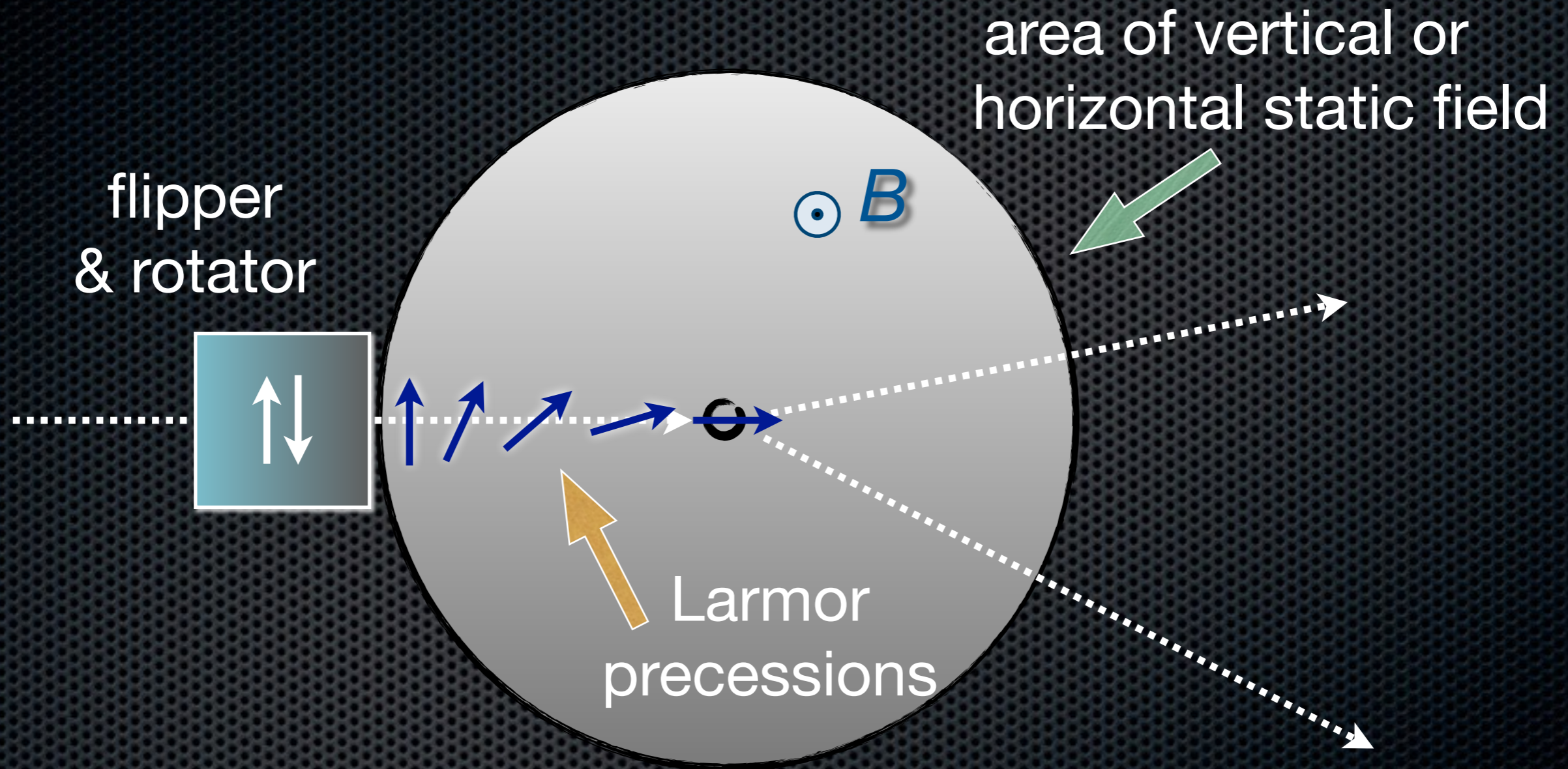
μ PAD works but...

problem of leakage
at high field i.e. for
short wavelengths

problem with zero-
field chamber at long
wavelength because
of field environment

μ -metal “pumps”
external fields

Spherical neutron polarimetry



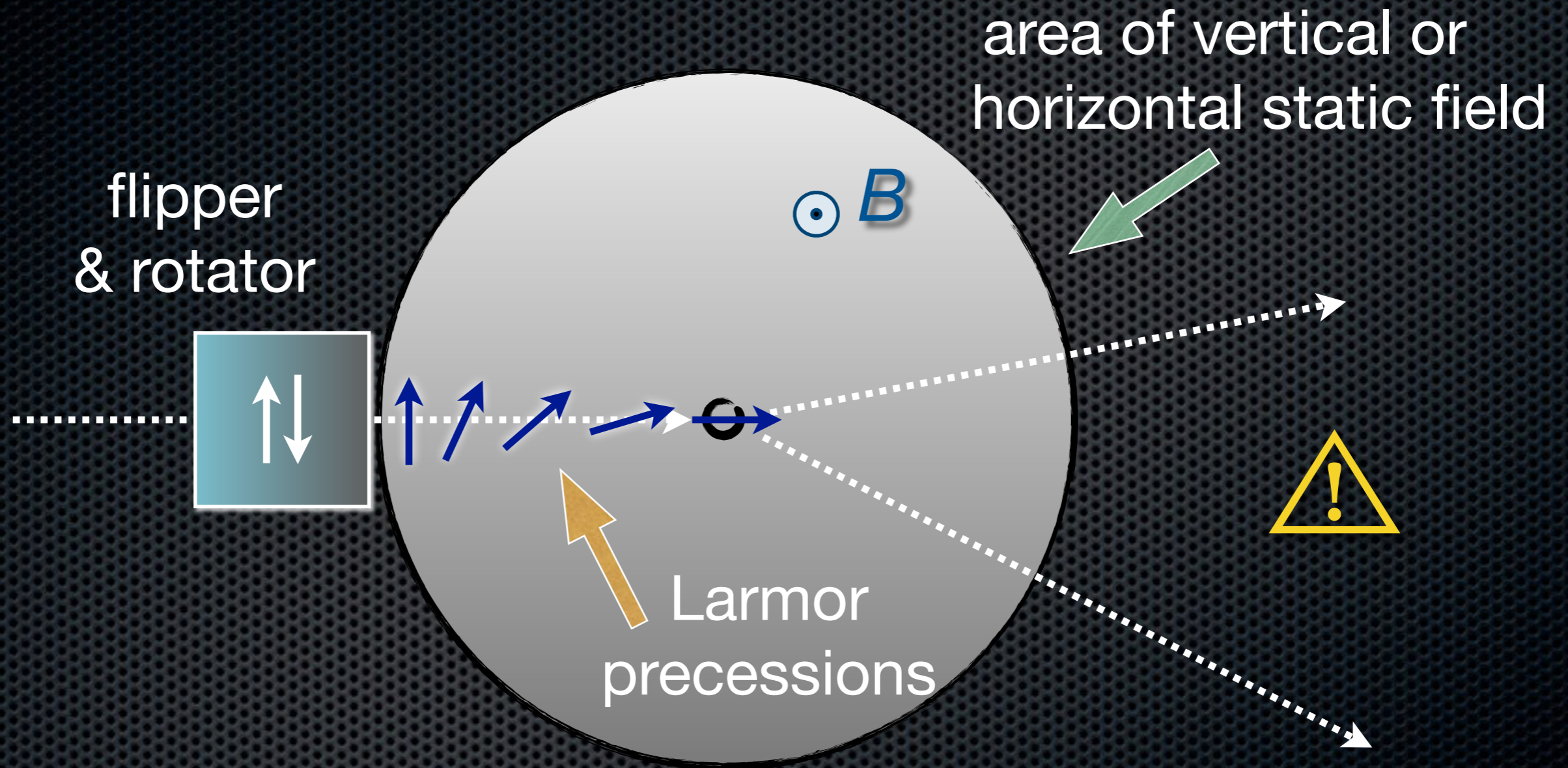
dnsPAD: the incident direction of polarisation is controlled with the field applied around the sample area.

Spherical neutron polarimetry



Cr_2O_3 test experiment carried out on DNS...

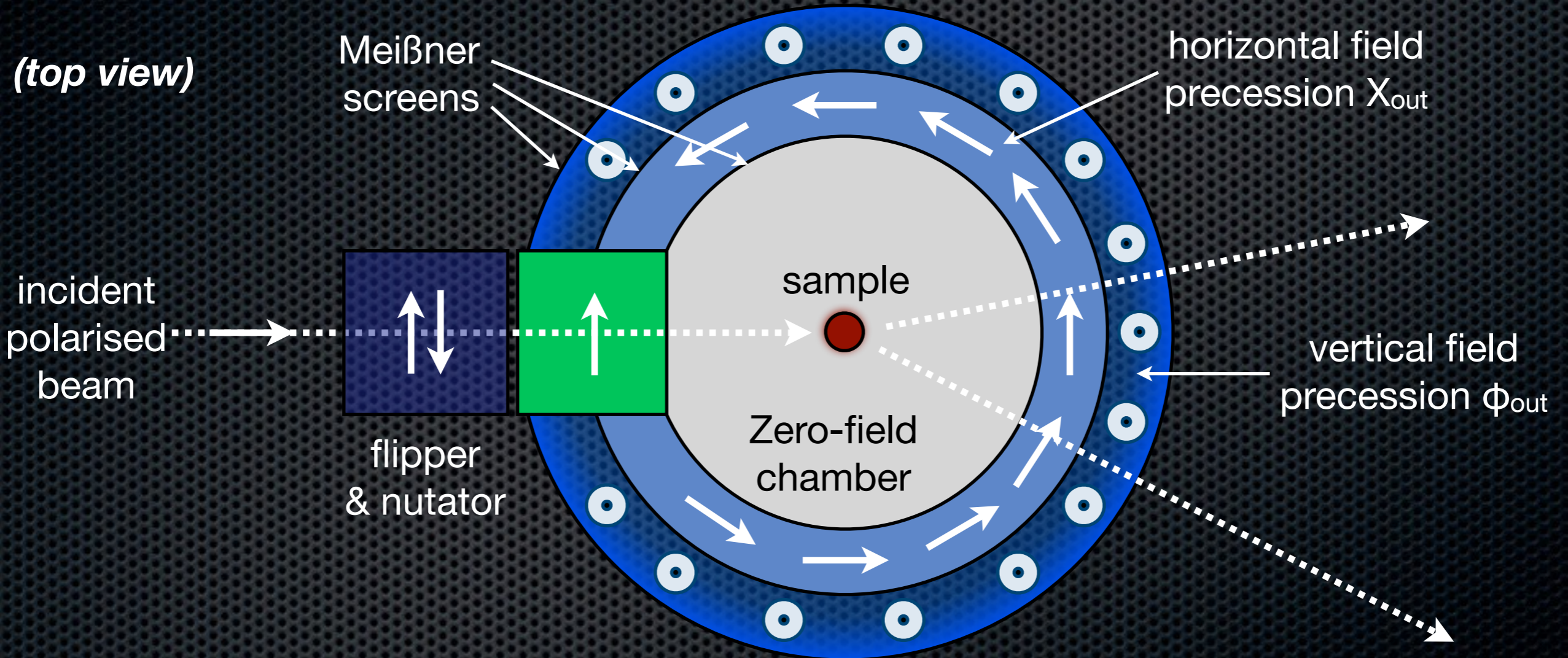
Spherical neutron polarimetry



dnsPAD: the applied field decreases the resolution with which the orientation of the polarisation is set.

Spherical neutron polarimetry

Time of Flight Polarimetry?



Solution proposed with a ^3He spin filter as analyser...

Content

- ✦ Beam polarisation vector
- ✦ Spin flippers and Spin filters
- ✦ Cross-section & scattered polarisation vector
- ✦ PND — Polarised neutron diffraction (powder, crystal)
- ✦ UPA — Uniaxial polarisation analysis
- ✦ **SNP — Spherical neutron polarimetry**
- ✦ PNSE — Polarimetric neutron spin-echo

Content

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Polarimetric Neutron Spin Echo

Spin-Echo Spectrometer

paramagnetic

high-resolution spectroscopy with relatively low flux reduction

Cryostat

π rotation in sample

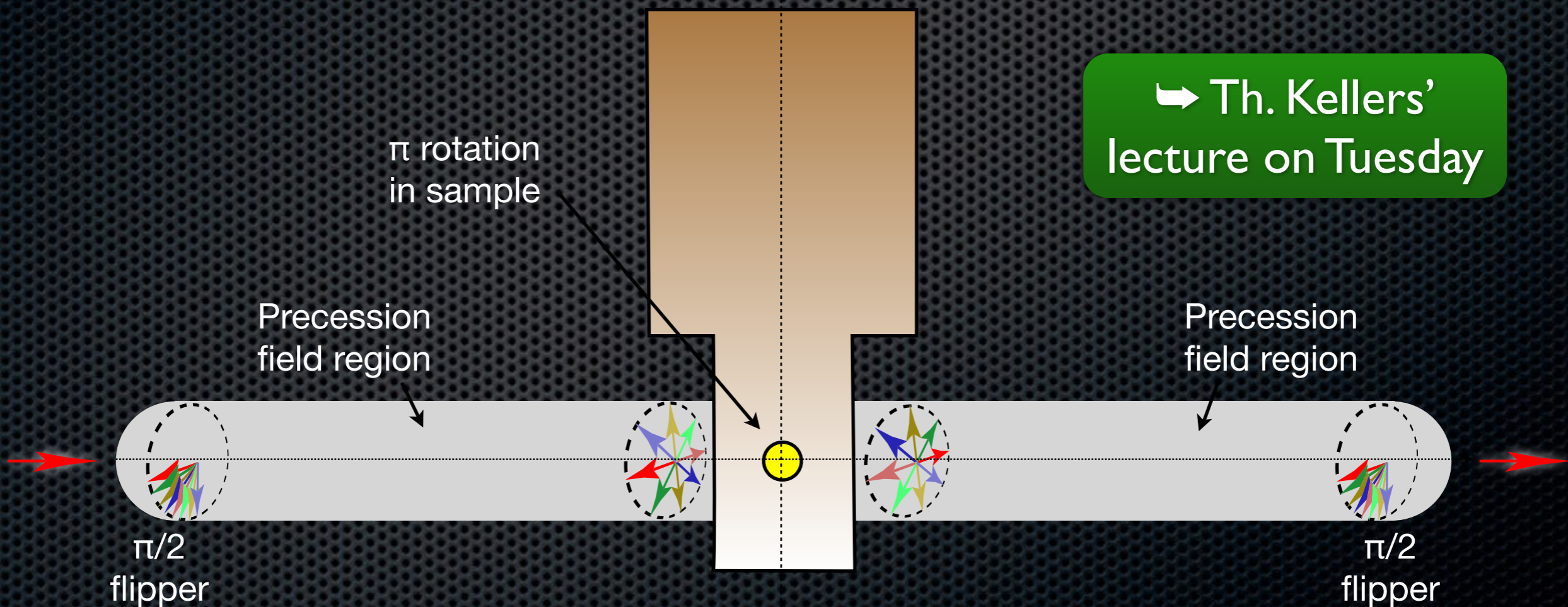
Th. Kellers' lecture on Tuesday

Precession field region

Precession field region

$\pi/2$ flipper

$\pi/2$ flipper

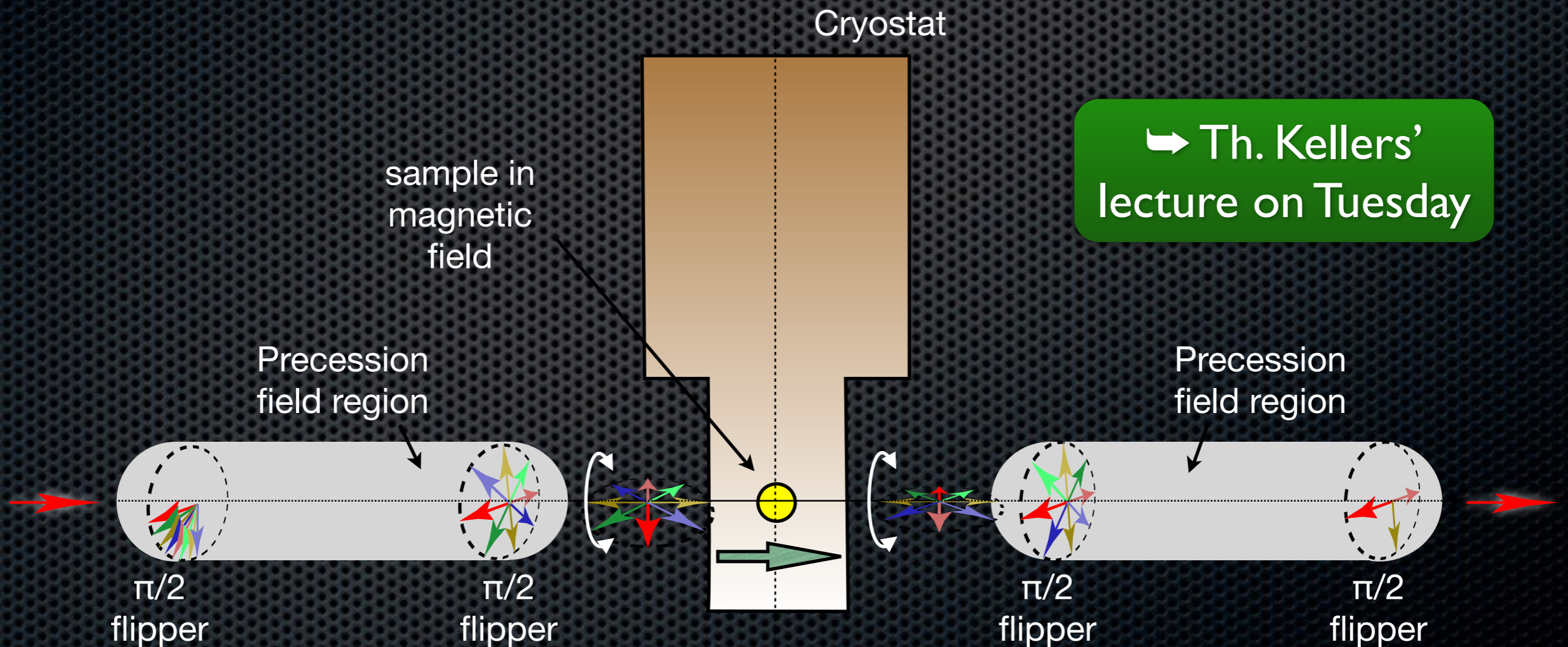


Polarimetric Neutron Spin Echo

Spin-Echo Spectrometer

ferromagnetic

one component is lost,
intensity divided by 2

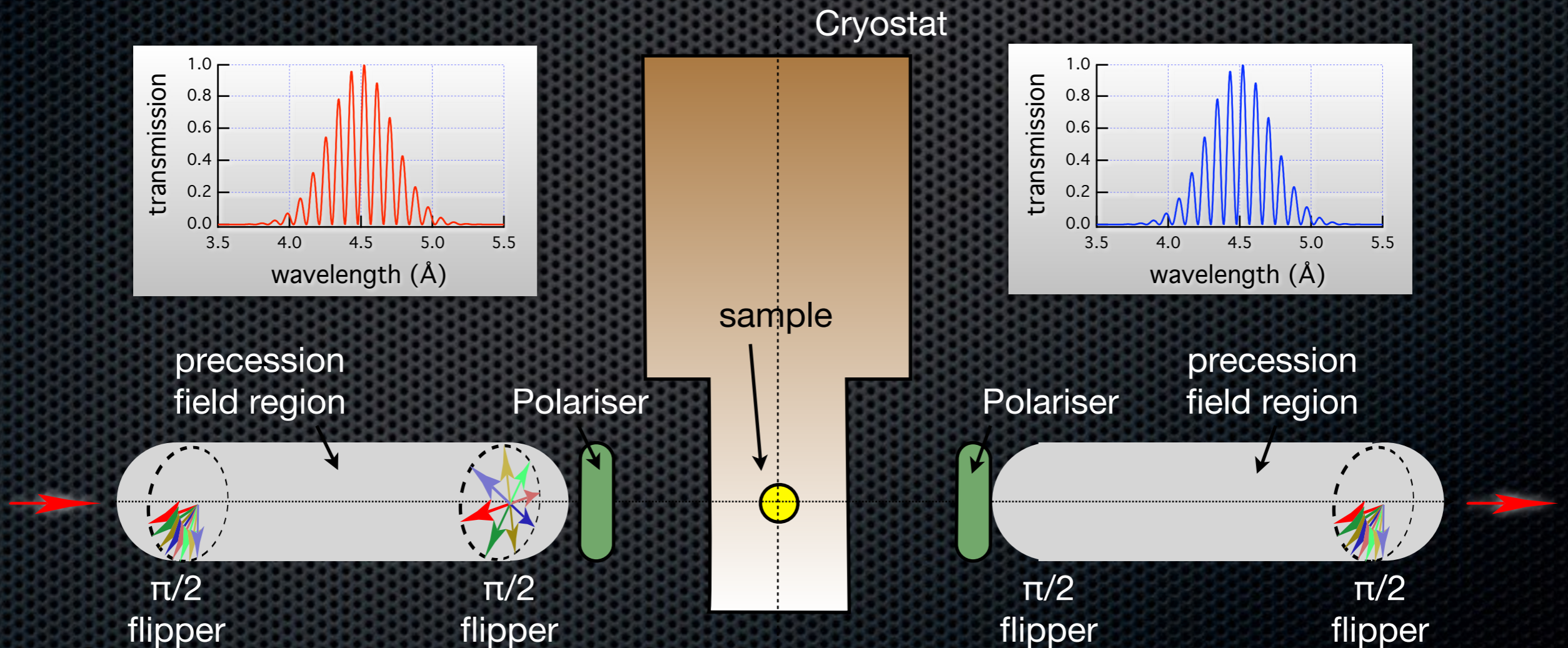


Polarimetric Neutron Spin Echo

Spin-Echo Spectrometer

intensity modulated

ferromagnets in low field,
intensity divided by 4

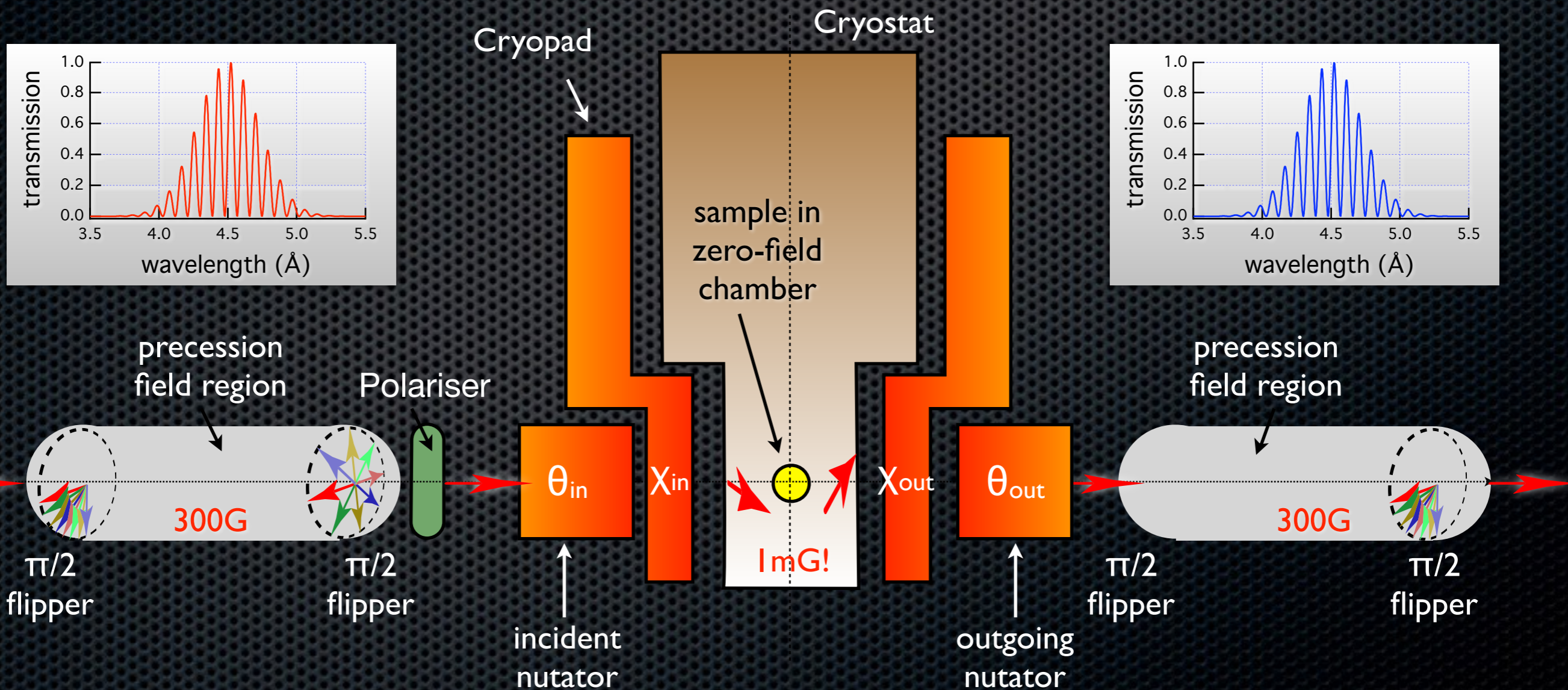


Polarimetric Neutron Spin Echo

Spin-Echo Spectrometer

polarimetric mode

antiferromagnets in zero-field, intensity divided by 4



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**Many thanks
for your attention**