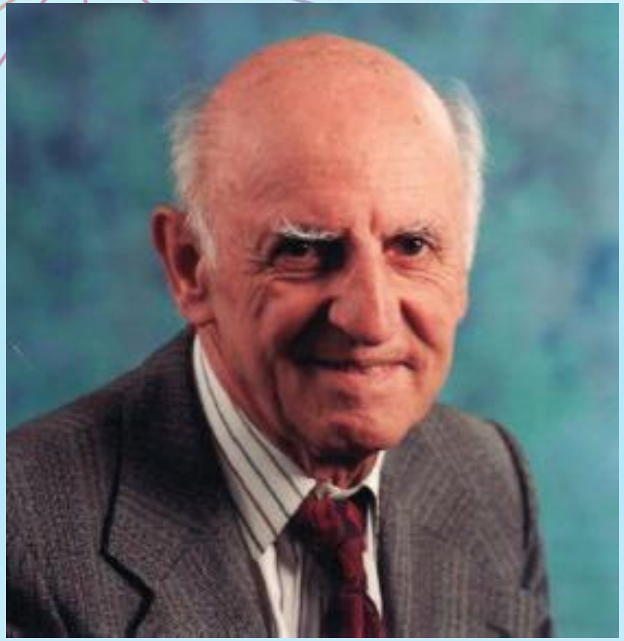
Neutron spin

as a measuring probe

(the case of nuclear scattering with a touch of magnetic scattering)

Wojciech Zając

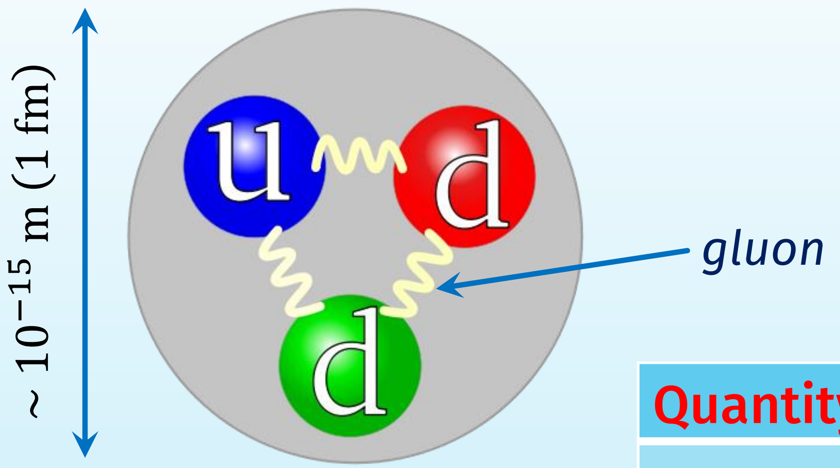
In memory of professor dr Otto Schärpf (1929–2019)



Otto Schärpf, a brilliant physicist, experimenter, a demanding teacher, a critical mind and a warm-hearted, optimistic person. He was an original, of which there are few left today because the scientific system promotes conventional behaviour.

I. Introduction

The neutron



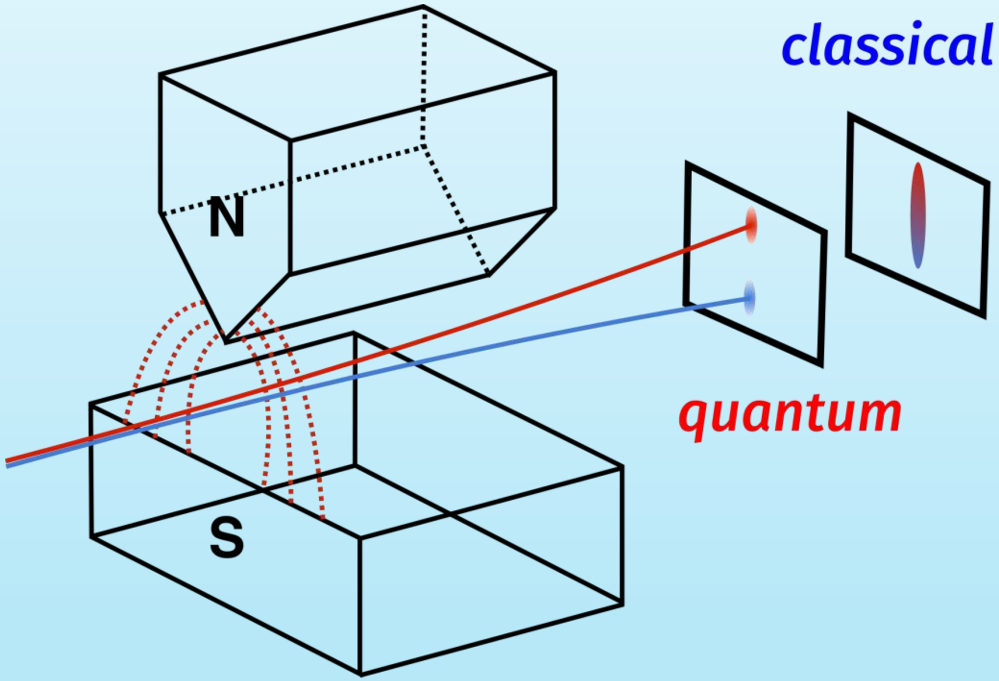
Hadron comprised of three quarks; no net charge

Quantity	Symbol	Value
Rest mass	m_n	$1.674927211(84) \times 10^{-27}$ kg
		1.00866491597(43) at.u.
	$m_n c^2$	939.565346(23) MeV
Spin	I	½
Charge		0
Magnetic moment	μ_n	$-0.96623641 \cdot 10^{-27}$ J·T
		$-1.04187565 \cdot 10^{-3}\ \mu_B$
		$-1.91304276\ \mu_N$
Mean life time (free)	τ	879.9±0.9 s (very recent value by [6])

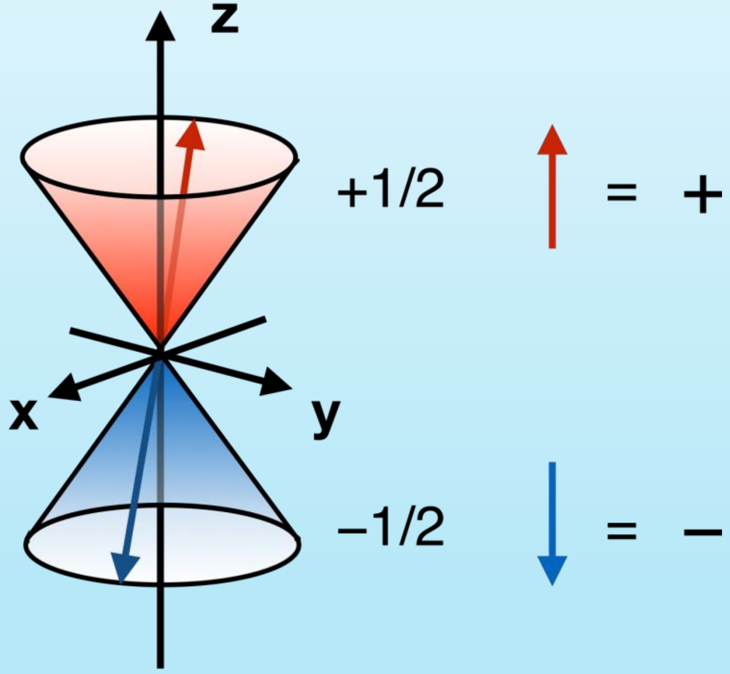
Spin and magnetic moment are oppositely oriented, complicating what "up" and "down" mean with respect to an applied field.

The neutron magnetic moment

The neutrons possesses an inherent magnetic moment related to its spin-angular momentum.



Stern, Gerlach (1922)



Neutron interaction with the scattering system

Let s_i, s_f and λ_i, λ_f be the initial and final states of the neutron and of the scattering system, respectively. Then, in the Born approximation the scattering cross section contains this matrix element:

$$\langle s_f \lambda_f | \, V(\mathbf{Q}) \, | \, s_i \lambda_i \rangle$$

where $V(\mathbf{Q})$ is the Fourier transform of the interaction potential $V(\mathbf{r})$:

$$V(\mathbf{Q}) = \int V(\mathbf{r}) \; e^{i\mathbf{R}\cdot\mathbf{r}} \, d^3r$$

In general, the potential $V(\mathbf{Q})$ can be written as a sum of spin-inependent and vector-type terms:

$$V(\mathbf{Q}) = \frac{2\pi\hbar}{m_n} [V_{si}(\mathbf{Q}) + V_v(\mathbf{Q})]$$

Neutron interaction with the scattering system

For convenience, both components are sometimes represented in this way:

	$V_{si}(\mathbf{Q})$	$V_v(\mathbf{Q})$
Nuclear	$\sum_j A_j \exp(i\mathbf{Q}\cdot\mathbf{r}_j)$	$\frac{1}{2}\sum_j B_j \mathbf{I}_j \exp(i\mathbf{Q}\cdot\mathbf{r}_j)$
Magnetic	0	$\frac{\gamma r_0}{2\mu_B}\mathbf{M}_\perp(\mathbf{Q})$
Electric*)	$\frac{\gamma r_0}{2}\frac{m_e}{m_n}n(\mathbf{Q})$	$\frac{\gamma r_0}{2}\frac{m_e}{m_n}n(\mathbf{Q})i\cot\left(\frac{\phi}{2}\right)\hat{\mathbf{z}}$

*) Electric interactions:

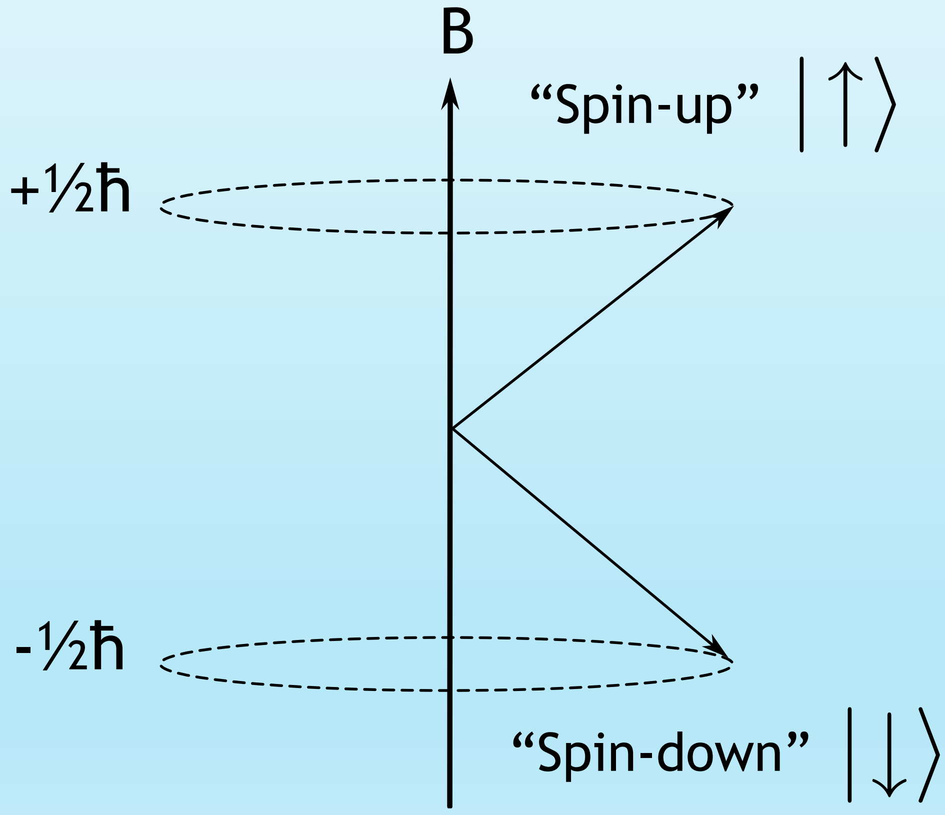
- spin-orbit coupling
- Foldy interaction due to the existence of internal electric fields within the neutron

II. Neutron in a magnetic field

Neutron in a static magnetic field

Quantum mechanics:

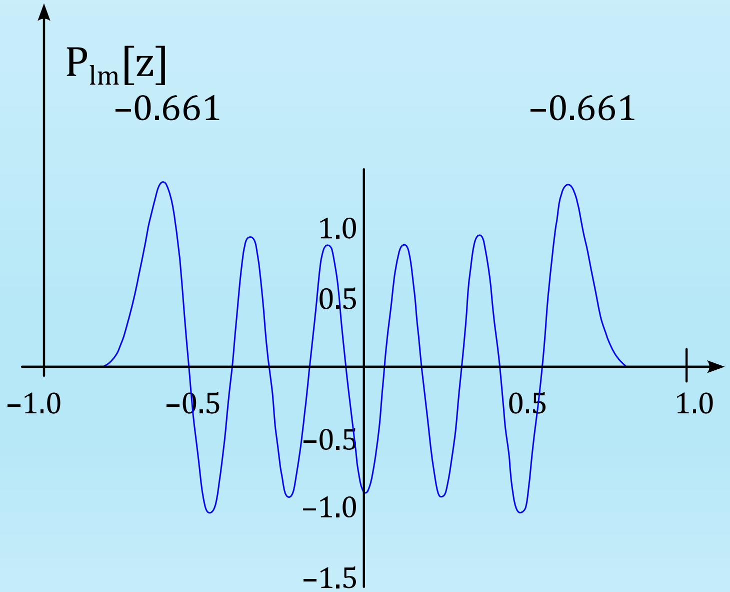
- Probability density of finding a particle in a state of particular orbital angular momentum, spin, and total angular momentum
- Nothing about the motion of the particle on its orbit, nor about the coordinates of the axis of rotation.

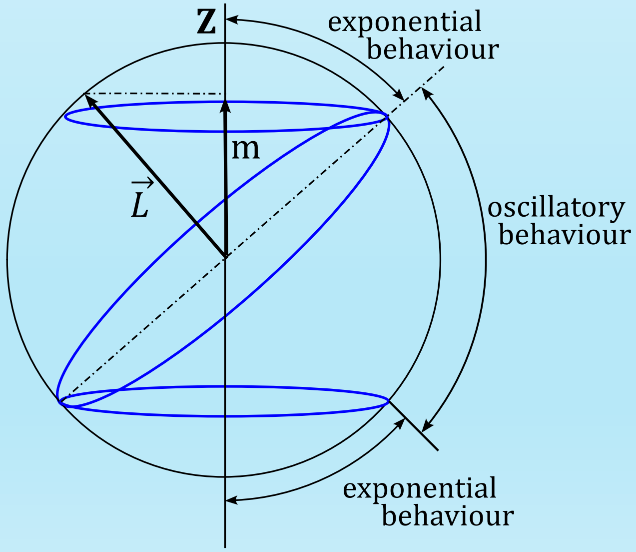


All we can say:

- can be visualized as if the orbit "precessed" in an unobservable way about the z-axis, what could be described by a precession cone of the total $\vec{J}, \vec{L},$ or $\vec{S}$.
- as for the neutron spin, we know only that the particle has an internal angular momentum of $\hbar/2$, and that the three components s_x, s_y, s_z obey the commutation relations $[s_x, s_y] = i\hbar s_z$, or generally, $[s_i, s_j] = i\hbar s_k \epsilon_{ijk}$, with $i, j, k = x, y, z$, but no probability density regarding orbit or the spin directions or something similar is given.

Left: Oscillatory behaviour of the associated Legendre polynomial $P_{lm}(z)$ for $-\sqrt{1-\mu^2} < z < \sqrt{1-\mu^2}$ and exponential behaviour for $1 < |z| < \sqrt{1-\mu^2}$ as obtained for $l = 40,\ m = 30, \mu = m/l$.
Right: hypothetical orbit of a particle of quantum numbers $l = 40$ and $m = 30$, "precessing" about the z-axis. The particle then moves in the "classically allowed" region with the oscillatory behaviour and stays out of the region where $P_{lm}(z)$ behaves exponentially. The y scale is divided by 10^{46}.





Neutron wave function

The state of a free neutron, i.e. a particle with spin $\frac{1}{2}$, interacting with a magnetic field **B** is described by a nonrelativistic Schrödinger equation, also referred to as the *Pauli equation*, whose solution is a two dimensional spinor wave function of the neutron:

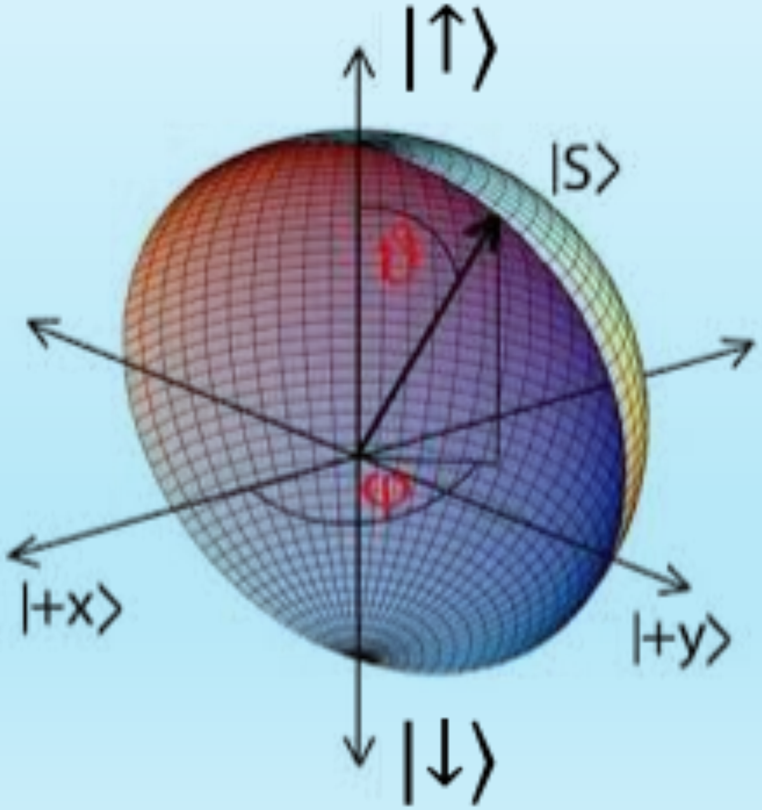
$$\psi(\mathbf{r}) = \begin{pmatrix} \psi_+(\mathbf{r}) \\ \psi_-(\mathbf{r}) \end{pmatrix} = \phi(\mathbf{r})|S\rangle$$

with spatial wave function $\phi(\mathbf{r})$. The state vector for the spin eigenstates $|\uparrow\rangle$ and $|\downarrow\rangle$ is given by :

$$|S\rangle = a|\uparrow\rangle + b|\downarrow\rangle$$

or using the conventional notation of the *Bloch sphere* (or *Poincaré sphere*):

$$|S\rangle = \cos\frac{\vartheta}{2}|\uparrow\rangle + e^{i\varphi}\sin\frac{\vartheta}{2}b|\downarrow\rangle$$



Spinors

A constant spinor:

$$|+\rangle = \begin{pmatrix}1\\0\end{pmatrix} = \chi_+$$

$$|-\rangle = \begin{pmatrix}0\\1\end{pmatrix} = \chi_-$$

$$\langle +| = (1 \quad 0) = \chi_+^\dagger$$

$$\langle -| = (0 \quad 1) = \chi_-^\dagger$$

$$\chi = c_+\chi_+ + c_-\chi_- = \begin{pmatrix}c_+\\c_-\end{pmatrix}$$

The relationship between cartesian space: $\vec{s} = (s_x, s_y, s_z)$ and the spinor space is provided via the Pauli matrices:

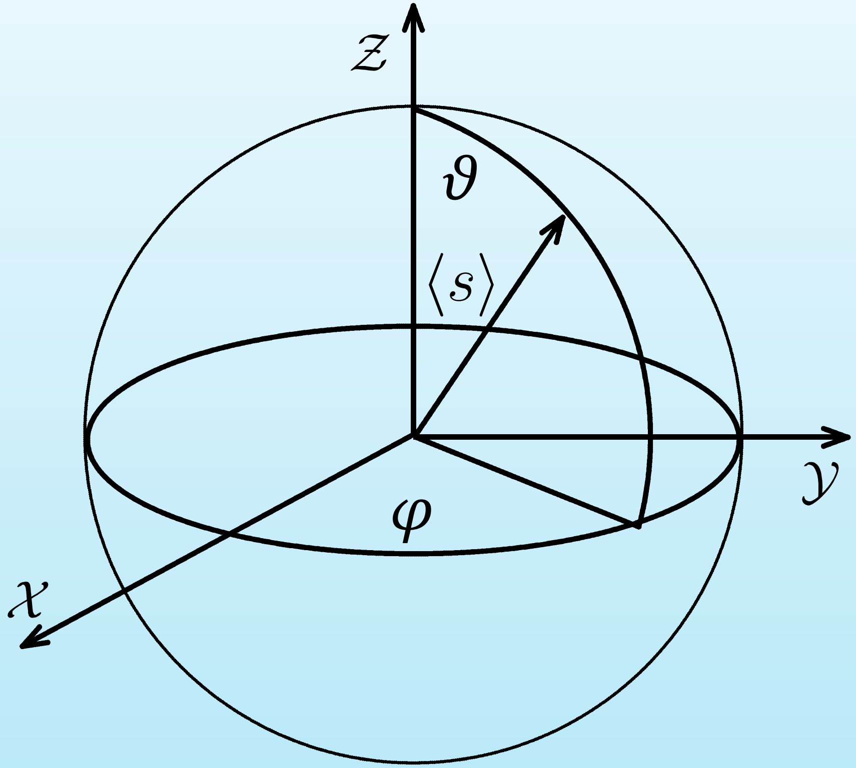
$$\sigma_x = \begin{pmatrix}0 & 1\\1 & 0\end{pmatrix} \qquad \sigma_y = \begin{pmatrix}0 & -i\\i & 0\end{pmatrix} \qquad \sigma_z = \begin{pmatrix}1 & 0\\0 & -1\end{pmatrix}$$

$$(\langle s_x\rangle, \langle s_y\rangle, \langle s_z\rangle) = \frac{\hbar}{2}(\chi^\dagger\sigma_x\chi, \quad \chi^\dagger\sigma_y\chi, \quad \chi^\dagger\sigma_z\chi)$$

Note, that the above relation is defined for $(\langle s_x\rangle, \langle s_y\rangle, \langle s_z\rangle)$, and not for (s_x, s_y, s_z).

For example:

$$\left(\langle s_x\rangle, \langle s_y\rangle, \langle s_z\rangle\right) = \frac{\hbar}{2}\left(\cos\varphi\sin\vartheta,\ \ \sin\varphi\sin\vartheta,\ \ \cos\vartheta\right)$$



$$\chi = \begin{pmatrix} \cos\frac{\vartheta}{2}\ e^{-i\frac{\varphi}{2}} \\ \sin\frac{\vartheta}{2}\ e^{i\frac{\varphi}{2}} \end{pmatrix}$$

Let's check it for the *x*-component:

$$\left(\cos\frac{\vartheta}{2}\ e^{-i\frac{\varphi}{2}},\ \ \sin\frac{\vartheta}{2}\ e^{i\frac{\varphi}{2}}\right)\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} \cos\frac{\vartheta}{2}\ e^{-i\frac{\varphi}{2}} \\ \sin\frac{\vartheta}{2}\ e^{i\frac{\varphi}{2}} \end{pmatrix} = \sin\vartheta\cos\varphi$$

q.e.d.

Neutron wave function, cntd.

By the way of digression:

the formal equation describing the motion a free neutron, interacting with a magneticeld **B** is described by a nonrelativistic time-dependent Schrödinger equation:

$$\widehat{H}\psi(\mathbf{r},t) = -\left(\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2 - \mu\boldsymbol{\sigma}\mathbf{B}(\mathbf{r},t)\right)\psi(\mathbf{r},t) = i\hbar\frac{\partial}{\partial t}\psi(\mathbf{r},t)$$

Where m and μ are the mass and magnetic moment of the neutron, respectively. $\boldsymbol{\sigma}$ is the Pauli vector operator.

The time-dependent solution is then:

$$\psi(\mathbf{r},t) = \begin{pmatrix}\psi_+(\mathbf{r},t)\\ \psi_-(\mathbf{r},t)\end{pmatrix} = \phi(\mathbf{r},t)|S\rangle$$

Neutron polarization

Let's recall: the state vector for the spin eigenstates $|\uparrow\rangle$ and $|\downarrow\rangle$ is given by :

$$|S\rangle = a|\uparrow\rangle + b|\downarrow\rangle$$

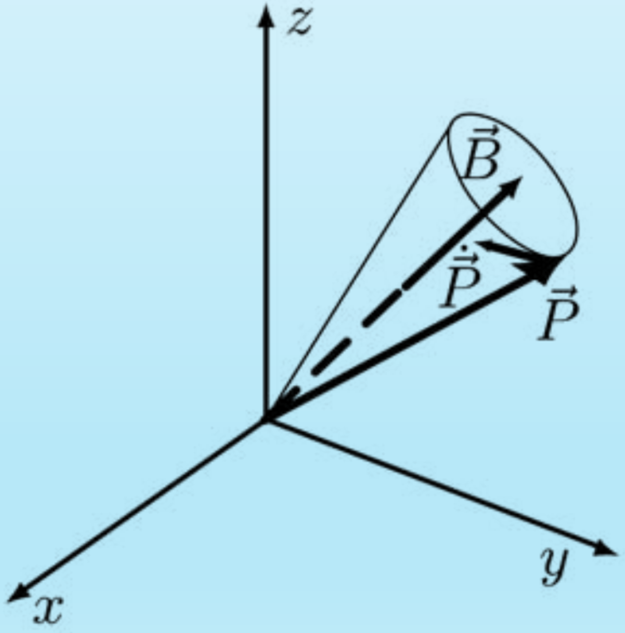
The neutron polarization vector, $\mathbf{P}$ is defined as the expectation value of the Pauli spin matrices:

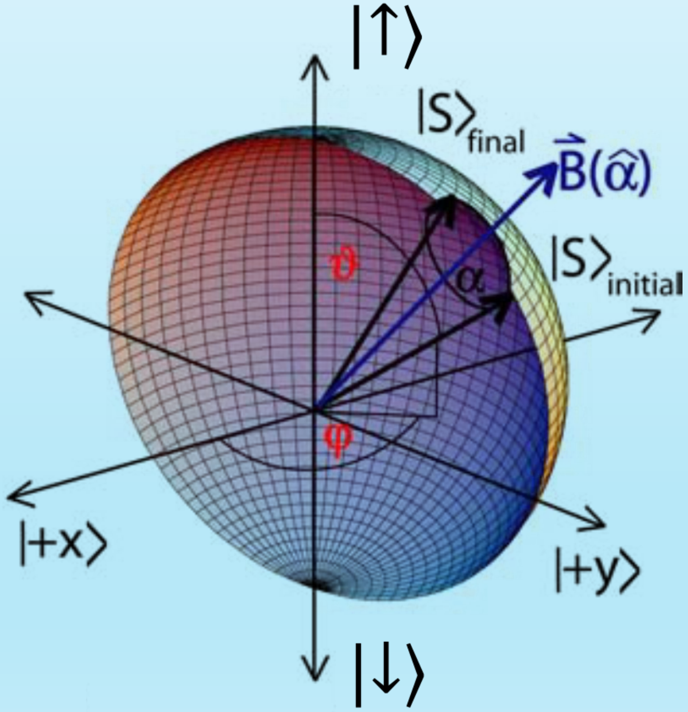
$$\mathbf{P} = \langle S|\boldsymbol{\sigma}|S\rangle$$

$$\mathrm{P}_x = \langle S|\sigma_x|S\rangle = 2\,\mathrm{Re}(a * b)$$

$$\mathrm{P}_y = \langle S|\sigma_y|S\rangle = 2\,\mathrm{Im}(a * b)$$

$$\mathrm{P}_z = \langle S|\sigma_z|S\rangle = |a|^2 - |b|^2$$





Neutron in the magnetic field

The neutron couples via its permanent magnetic dipole moment $\boldsymbol{\mu}$ to the magnetic field:

$$H_{mag} = -\boldsymbol{\mu} \cdot \boldsymbol{B} = -\mu\, \boldsymbol{\sigma} \cdot \boldsymbol{B}$$

Magnetic fields are used e.g. to perform arbitrary spinor rotations in particular neutron transport tasks (cf. *neutron optics*).

When a neutron „non-adiabatically” travels through a magnetic field (stationary or time-dependent), its polarization vector performs ***Larmor precession***, described by the Bloch equation:

$$\frac{d\mathbf{P}}{dt} = \mathbf{P} \times \gamma_N \mathbf{B}$$

Larmor precession

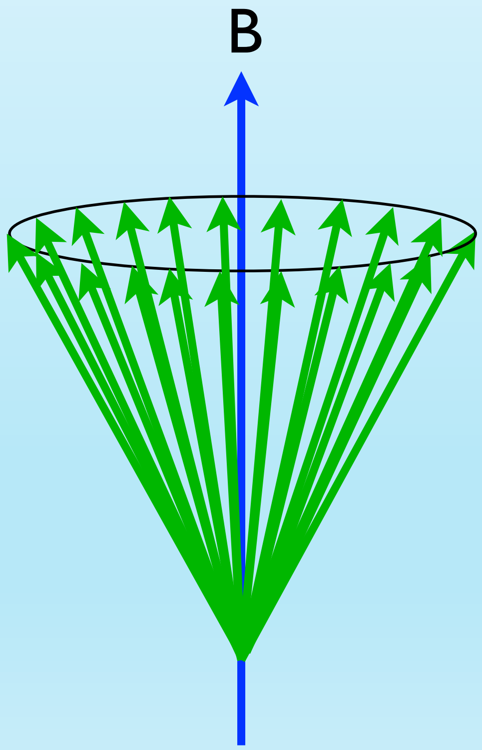
Angular momentum of a spin in a magnetic field (in the z-direction):

$$\frac{\hbar d\mathbf{I}}{dt} = \mu \times \mathbf{B} \qquad \text{or} \qquad \frac{d\mu}{dt} = \gamma_n \mu \times \mathbf{B}$$

γ_N is the gyromagnetic ratio, i.e. the ratio of the magnetic moment to the angular momentum.

The solutions are:

$$\mu_x = |\mu| \cos(\omega_L t) \qquad \mu_y = -|\mu| \sin(\omega_L t)$$

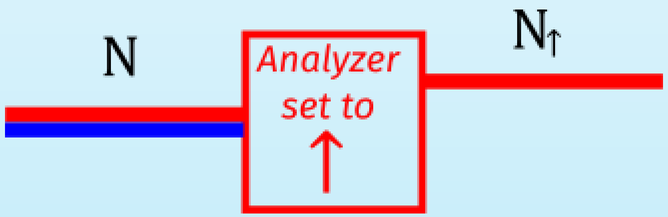


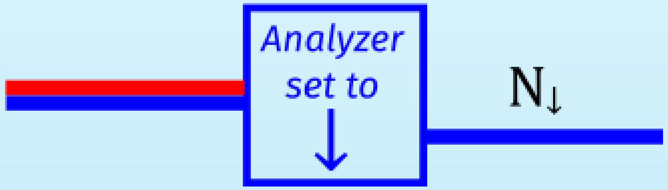
These are oscillatory solutions with the Larmor frequency of:

$$\omega_L = \gamma_n B$$

Neutron **beam** polarization

In a magnetic field, the polarization of a beam is a vector pointing in the direction of the field, with the length of the vector defined as the **scalar polarization**:





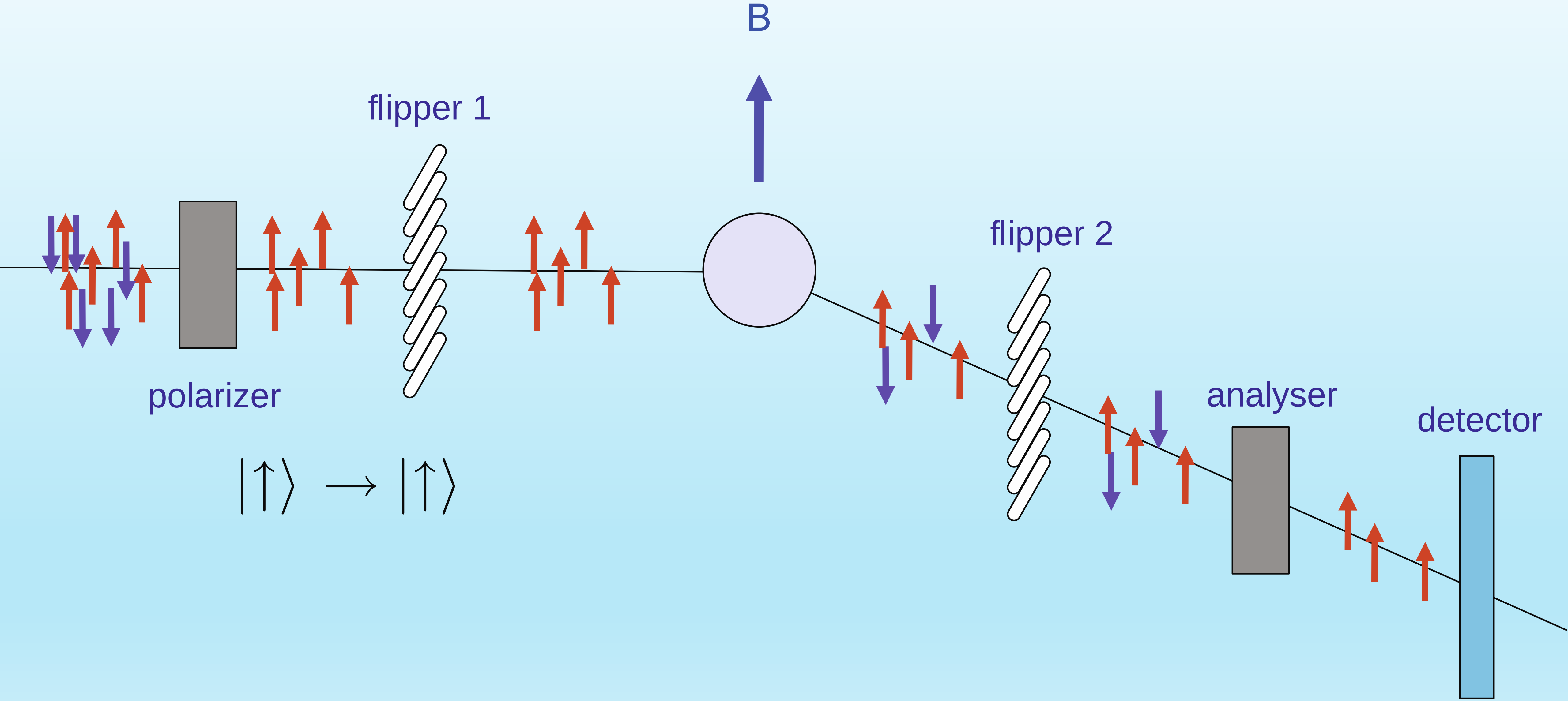
$$P = \frac{N_\uparrow - N_\downarrow}{N_\uparrow + N_\downarrow} = \frac{F - 1}{F + 1}$$

$$F = \frac{N_\uparrow}{N_\downarrow}$$

*F is known as the **flipping ratio**. The flipping ratio is a frequently measured quantity (in fact, in every neutron scattering experiment with polarization analysis).*

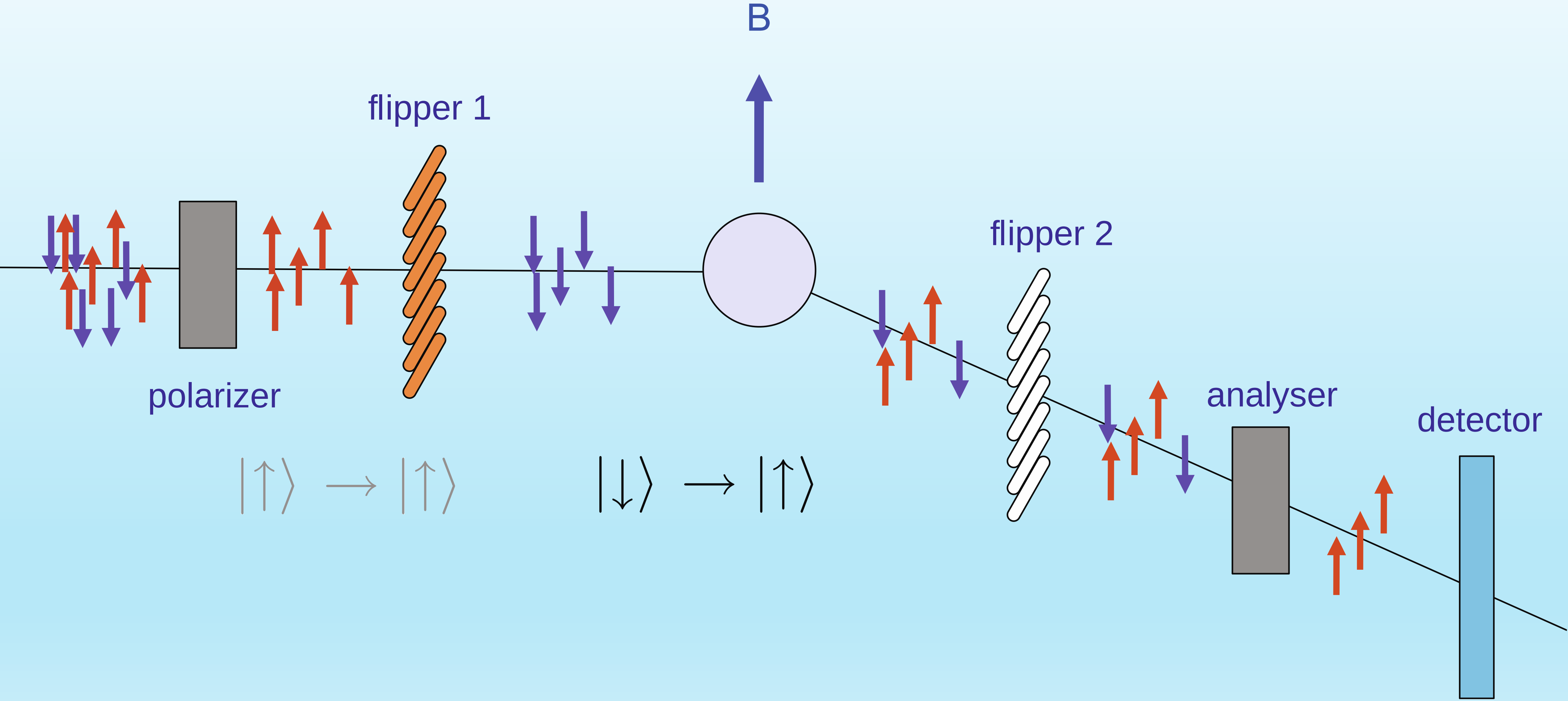
III. Uniaxial polarization experiment

Uniaxial Polarization analysis experiment

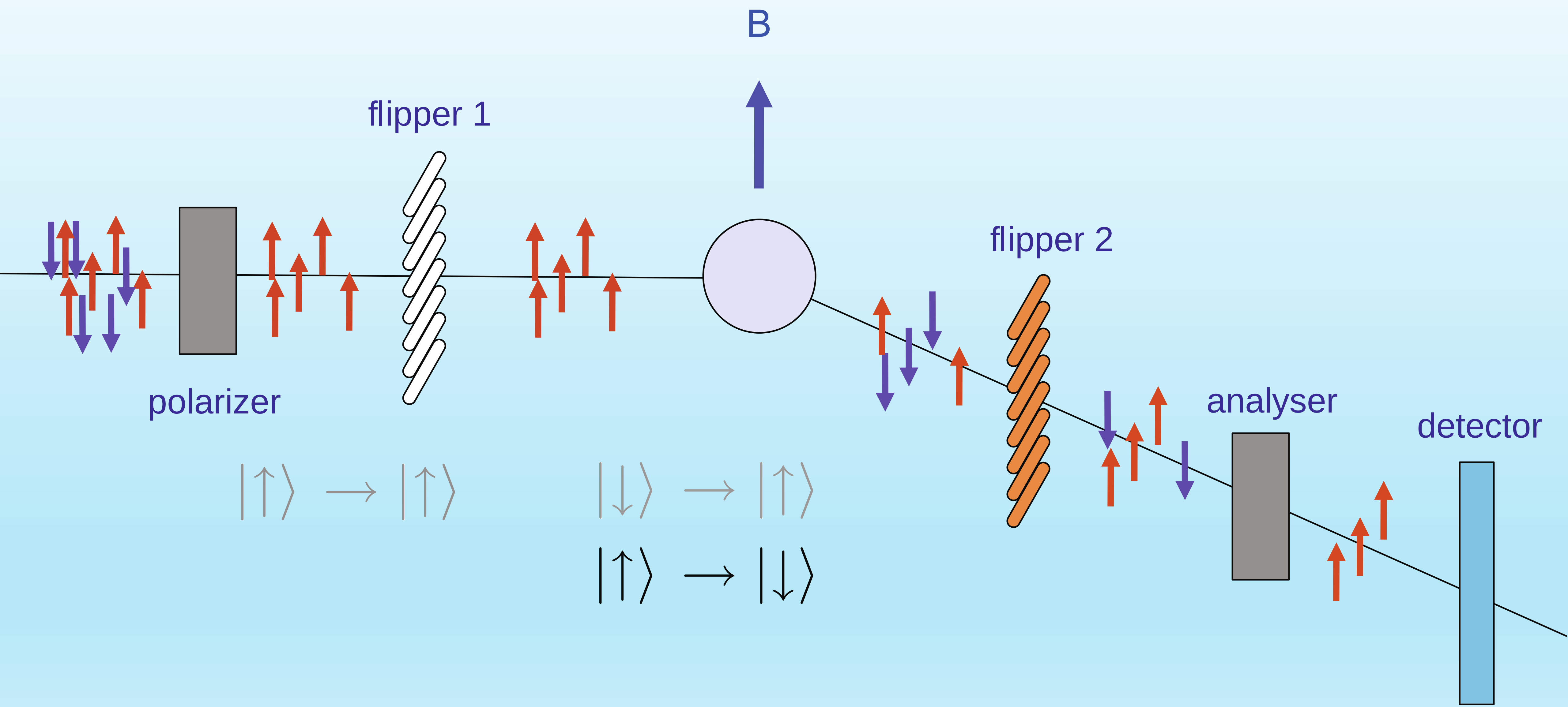


$$|\uparrow\rangle \rightarrow |\uparrow\rangle$$

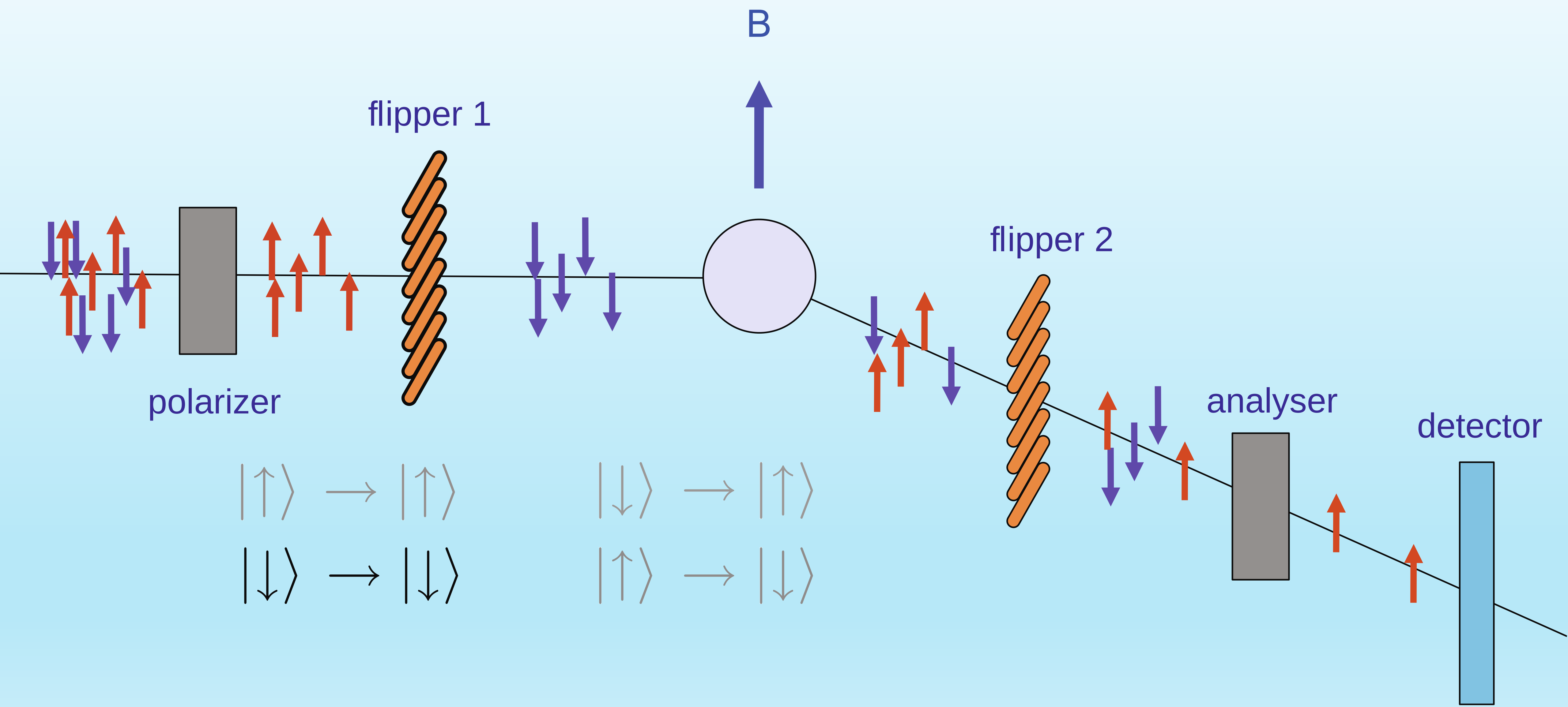
Uniaxial Polarization analysis experiment



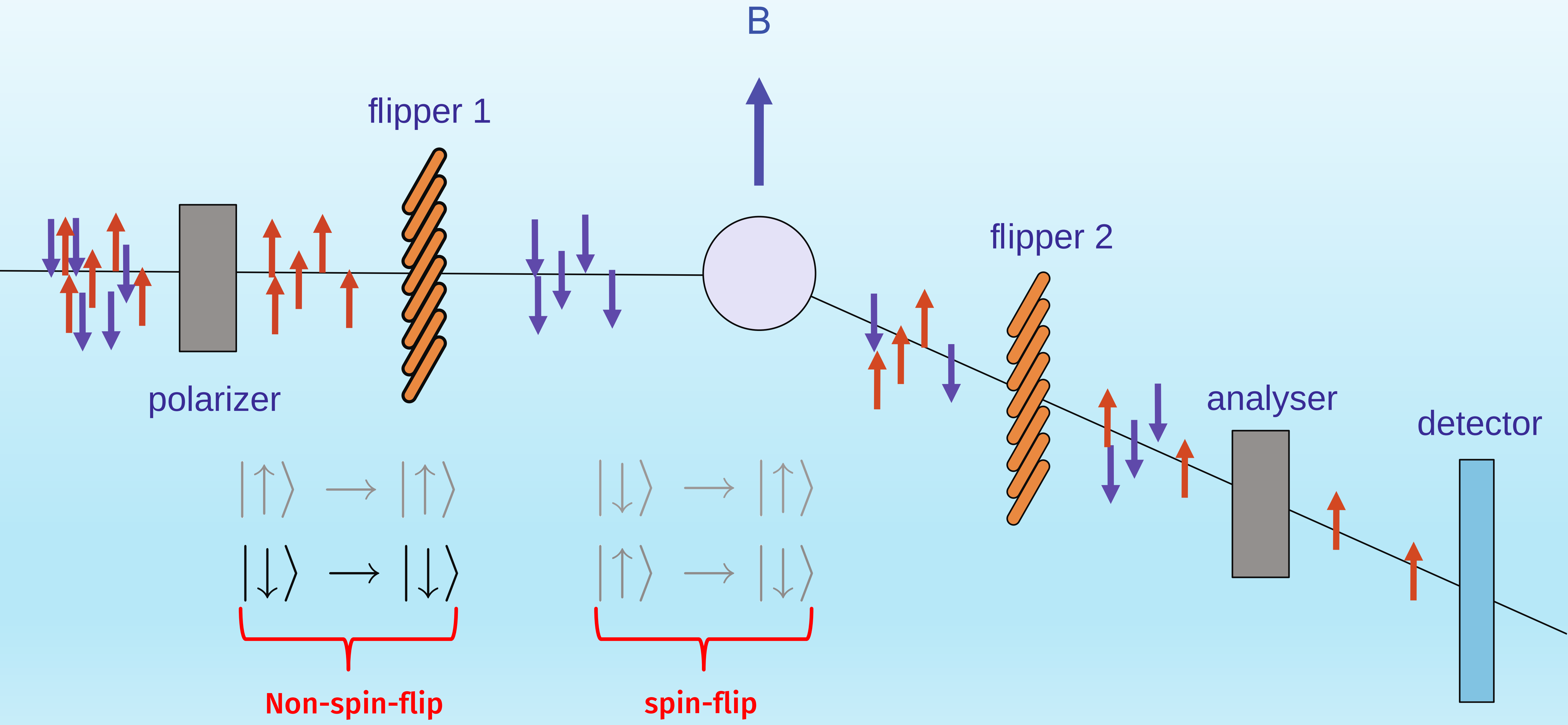
Uniaxial Polarization analysis experiment



Uniaxial Polarization analysis experiment

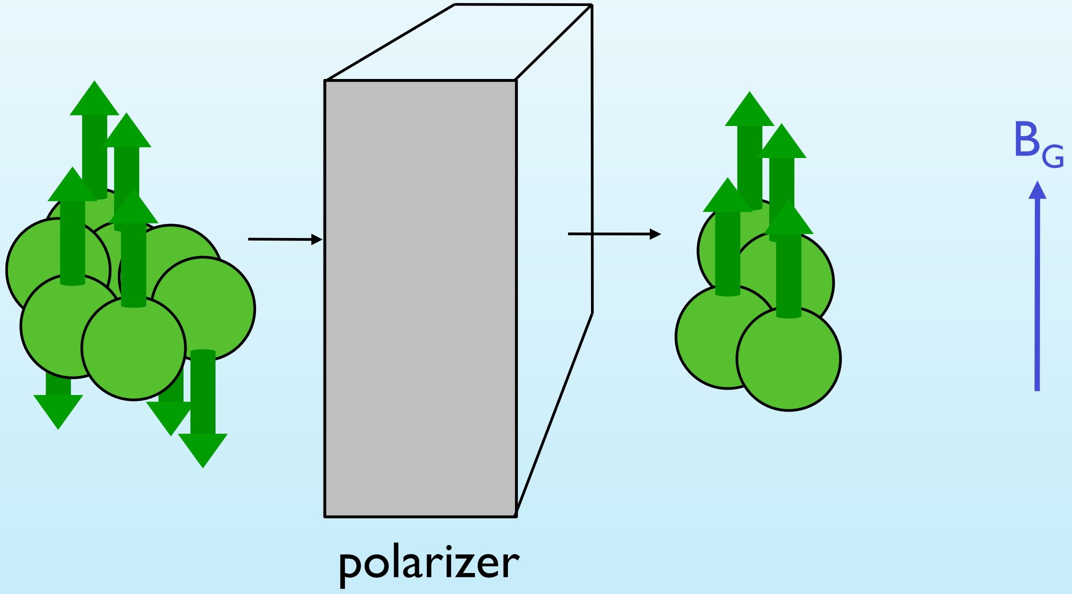


Uniaxial Polarization analysis experiment



IV. Producing a polarized neutron beam

How to polarize neutrons?



Generally, three ways of producing a polarized neutron beam are in use:

- polarizing filters (e.g. preferential absorption by polarized ^3He nuclei)
- polarizing mirrors and supermirrors (using preferential reflection)
- polarizing crystals (e.g. $Co_{92}Fe_8$, Heusler crystals Cu_2MnAl) using preferential Bragg reflection)

Polarizing filters

The two spin states are transmitted differently. Let's call them T_+ and T_-. The polarizing efficiency of a filter is then:

$$P = \frac{T_+ - T_-}{T_+ + T_-} \qquad \text{with total transmission equal:} \qquad T = \frac{T_+ + T_-}{2}$$

The thicker the filter, the higher the efficiency P, at the expense of decreasing T. The quantity being optimized is then: $P\sqrt{T}$.

Let a generalized filter have:

- a total, spin-inependent absorption cross section: σ_0
- and spin-dependent absorption cross section: σ_p

then: $$\sigma_\pm = \sigma_0 \pm \sigma_p$$

Assuming $T = \exp(-N\sigma t)$ where N is the number density of atoms/nuclei responsible for spin selection and t is the filter thickness,

It can be proved, that:

$$P = -\tanh\left(N\sigma_p t\right) \qquad T = \exp(-N\sigma_0 t)\cosh\left(N\sigma_p t\right)$$

^{3}He spin filters

Close to the resonance energy,
the absorption cross sections of nuclei are dependent upon their polarization and the neutron spin direction:

$$\sigma_{\pm} = \sigma_a(1 \pm \rho P_N)$$

where:
σ_a is the mean absorption cross section,
P_N is the nuclear polarization,
and: $\rho = \frac{I(1-2\chi)}{I+1}$ $\chi = \frac{\sigma_{I-\frac{1}{2}}}{\sigma_{I+\frac{1}{2}} + \sigma_{I-\frac{1}{2}}}$

For ^{3}He nuclei, all the absorption occurs in the $\sigma_{I-\frac{1}{2}}$ channel, and therefore, $\chi = 1$ and $\rho = -1$ giving:

$$\sigma_{\pm} = \sigma_a(1 \mp P_N)$$

Therefore, for fully polarized ^{3}He $(P_{He} = 1)$, one spin state passes through the filter with zero absorption. The other spin state is almost fully absorbed since $\sigma_a = 5000$ barns.

^{3}He spin filters

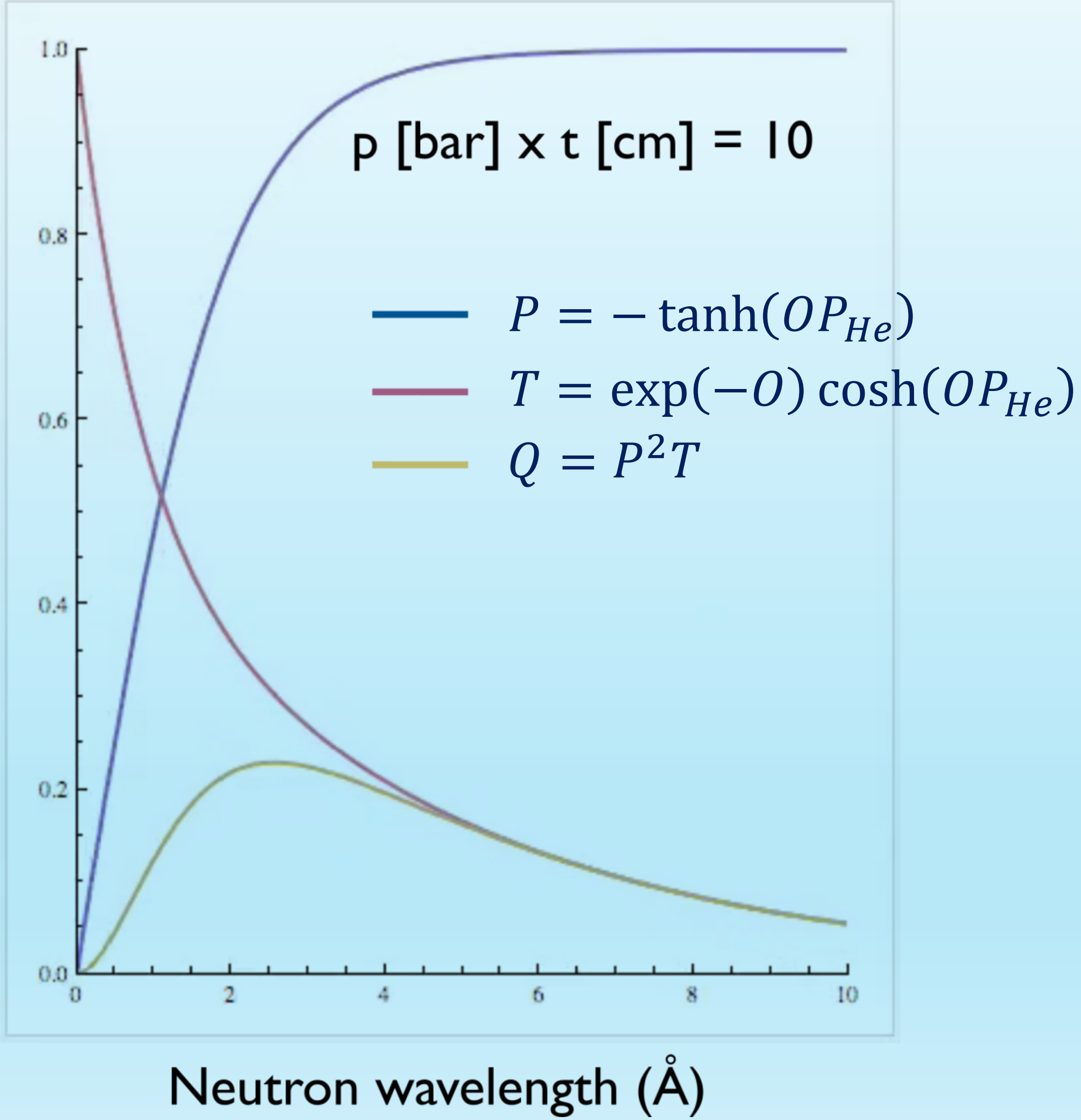
We can now set $\sigma_0 = \sigma_a$ and $\sigma_p = -\sigma_a P_N$
which leads to the expressions:

$$P = -\tanh(OP_{He}) \qquad T = \exp(-O)\cosh(OP_{He})$$

where: O is the opacity of the spin filter:

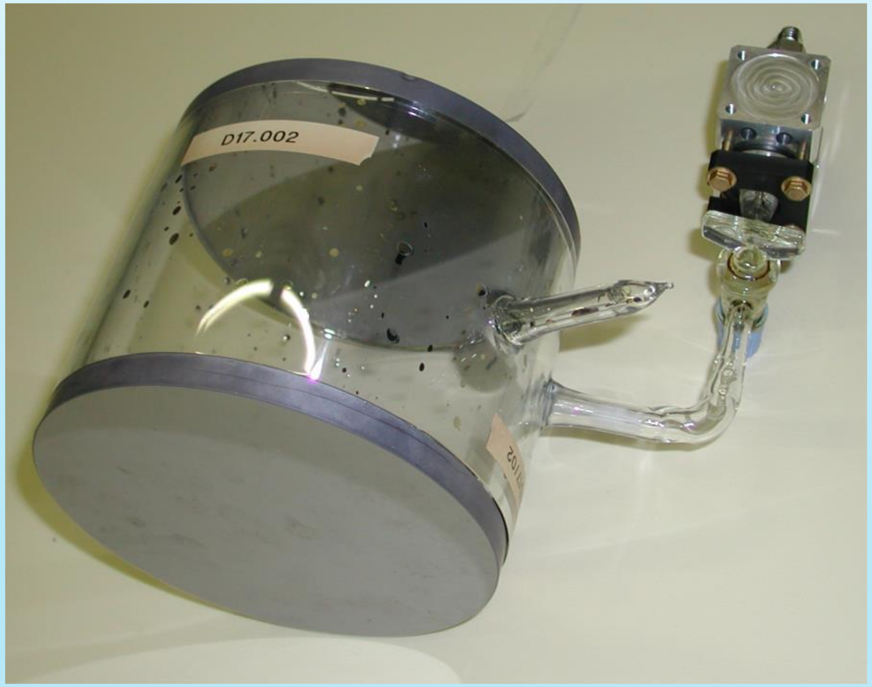
$$O = N\sigma_a t \cong 0.0732 \times \lambda[\text{Å}] \times p[\text{bar}] \times t[\text{cm}]$$

^{3}He polarization produced
via optical pumping methods.

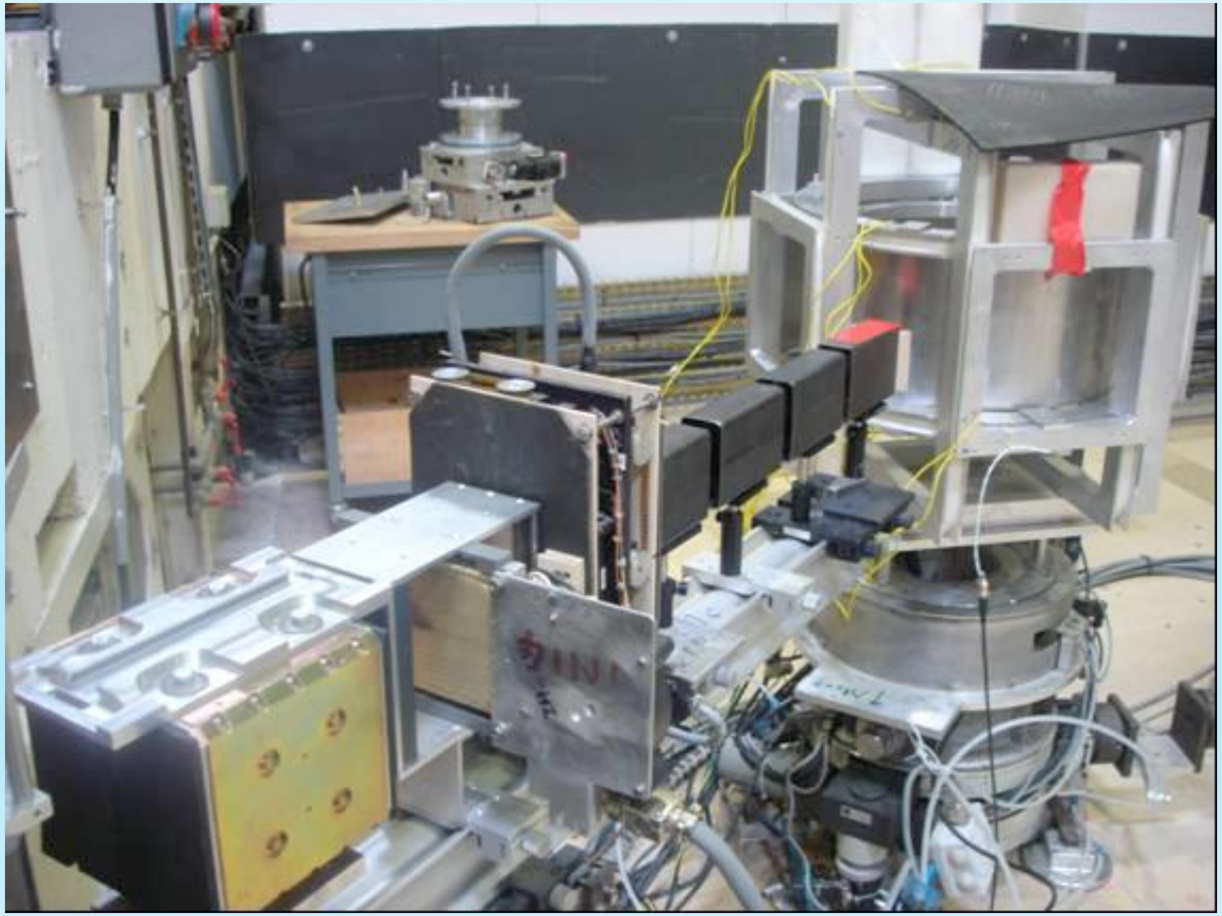


^{3}He spin filters

- Typical values: 75% initial ^{3}He nuclear polarization with a relaxation time of 100 hours.
- Relaxation of the 3He polarization arises from collisions with the container walls, from dipole-dipole interactions, and from stray magnetic fields.

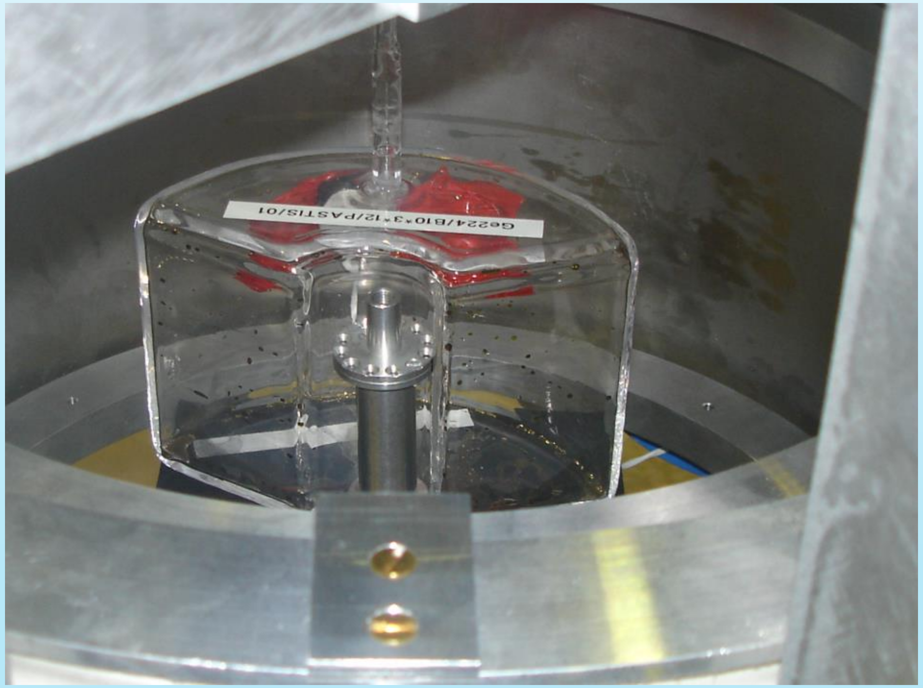


Single crystal Si 3He cell (D17, ILL)

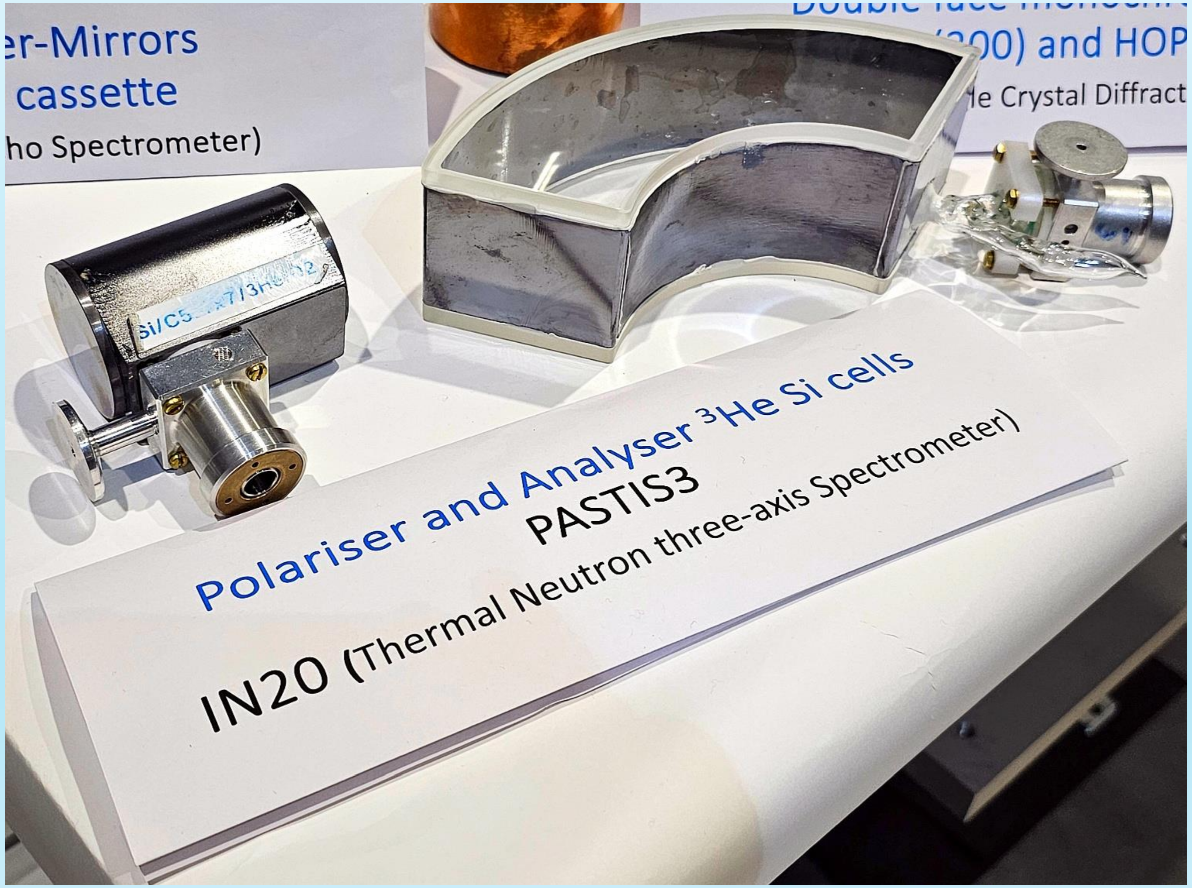


^{3}He spin filters

Time-of-flight spectrometers require a neutron spin-filter that covers a wide solid angle (big detector angles) and is efficient at thermal energies — ^{3}He spin filter is ideal for this.



Single crystal Si 3He cell (D17, ILL)

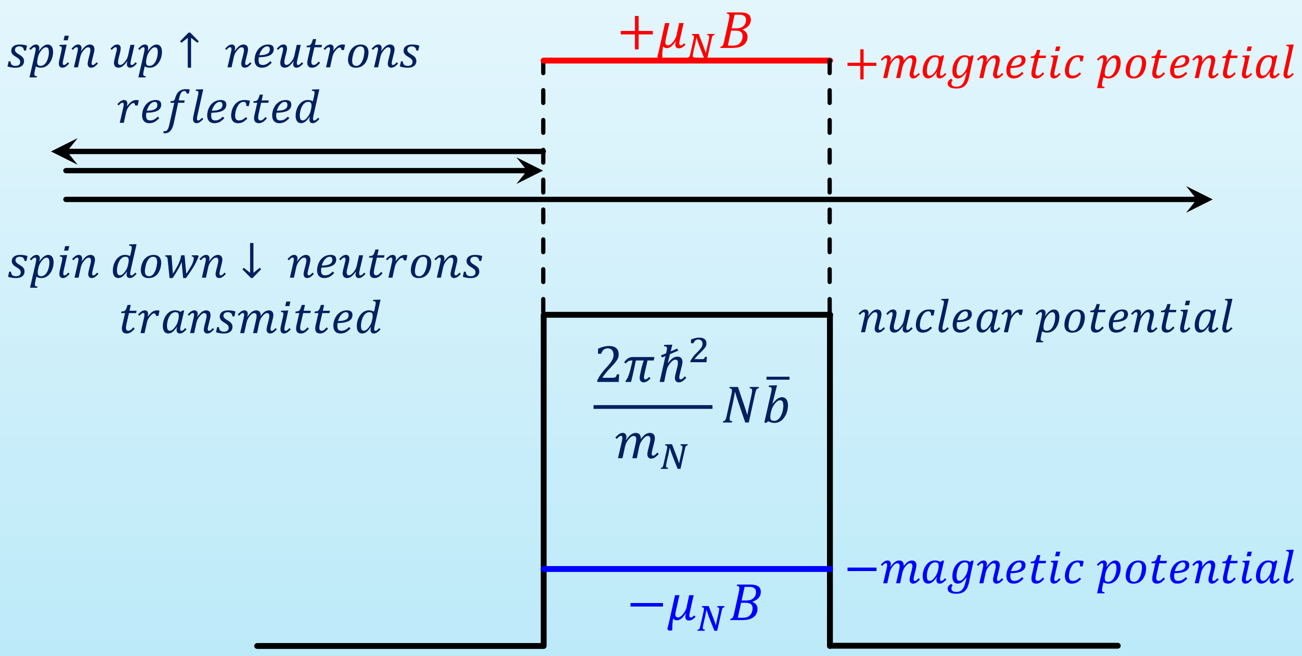


The principle of a mirror polarizer

Inside each material the neutron beam (i.e. the neutrons thereof) have the velocity other than in the free space. This can be described by a potential energy.

For the neutron beam, a layer of material is like a potential well of the depth $\frac{2\pi\hbar^2}{m_N} N\bar{b}$.

If the material is ferromagnetic there is an additional contribution to this potential energy $V_M = \pm\mu N\ B$, the sign depending on the orientation of the neutron magnetic moment with respect to the magnetic induction $\vec{B}$.



N is the number density of scattering nuclei, and $\vec{B}$ is the magnetic induction applied in the plane of the surface.

Mirror polarizer

Whenever speaking about devices designed to transport, collimate, or monochromatize a neutron beam, we referred to the **neutron optics**.

Indeed, nearly all optical phenomena have their neutron counterparts: e.g. refractive index:

optical:

$$n = \frac{c}{v}$$

neutron:

$$n = \frac{\lambda_1}{\lambda_2} = \frac{k_2}{k_1}$$

As said on previous slide, the neutron experiences a change of energy equivalent to $\langle V \rangle$ when it enters medium 2. We can then put:

$$\mathrm{n} = \frac{\mathrm{k}_2}{\mathrm{k}_1} = \left(\frac{\mathrm{E}_1 - \langle \mathrm{V} \rangle}{\mathrm{E}_1}\right)^{\frac{1}{2}} \cong 1 - \frac{\langle \mathrm{V} \rangle}{2\mathrm{E}_1}$$

assuming, that: $\langle \mathrm{V} \rangle \ll E_1$

The potential $\langle \mathrm{V} \rangle$ will in general consist of a nuclear and magnetic part:

$$\langle \mathrm{V} \rangle_n = \frac{2\pi\hbar^2}{m_N} N\bar{b}$$

$$\langle \mathrm{V} \rangle_m = \pm\mu_N B = \frac{2\pi\hbar^2}{m_N} N\bar{p}$$

Mirror polarizer

Therefore, the spin-dependent refractive index of magnetised mirrors for neutrons of wavelength λ is

$$n_{\pm} = 1 - \frac{N\lambda^2}{2\pi}\left(\bar{b} \pm \bar{p}\right)$$

Snell's law for refraction index:

$$n_{1,2} = \frac{\cos\theta_1}{\cos\theta_2}$$

And the critical angle of reflection (defined when $\theta_2 = 0$) is: $$n_{1,2} = \cos\theta_c \cong 1 - \frac{\theta_c}{2}$$

There are therefore two critical glancing angles $\theta_{c\pm}$ for total (external) reflection:

$$\boxed{\theta_{c\pm} = \lambda\left[\frac{N}{\pi}\left(\bar{b} \pm \bar{p}\right)\right]^{\frac{1}{2}}}$$

Mirror polarizer

$$\boxed{\theta_{c\pm} = \lambda \left[\frac{N}{\pi}(\bar{b} \pm \bar{p})\right]^{\frac{1}{2}}}$$

Between these two critical angles the reflected beam is effectively fully polarized, and in some circumstances the critical angle for one spin state can be made zero.

However, the critical angles are very small (typically 10')

In a polarizing neutron mirror, the basic unit is a non-magnetic/magnetic (A/B) bilayer, whose reflectivity is:

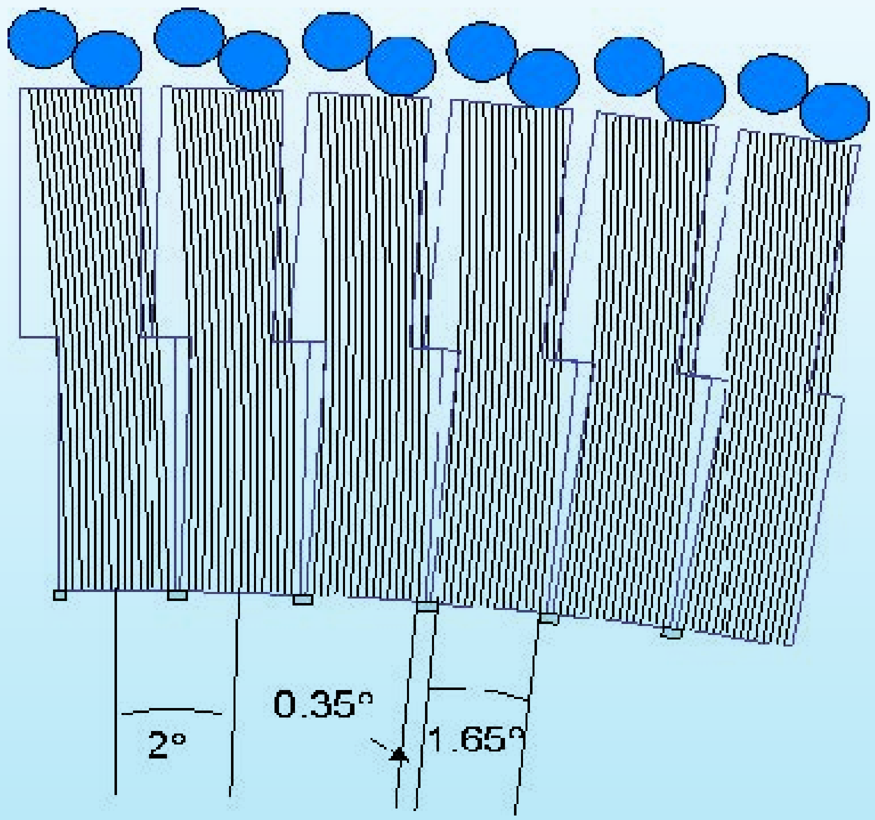
$$R_{\pm} = [N_A b_A - N_B(b_B \pm p_B)]^2$$

Therefore, with a careful choice of N and b, the condition of $R_{-} = 0$ can be achieved, implying perfect beam polarization (but not reflectivity) at all angles of incidence.

In practice this is hardly achievable, since the spin-down neutrons have to go somewhere. They are either transmitted or absorbed in an absorbing layer (often Gd, which has a non-zero reflectivity at very low angles)

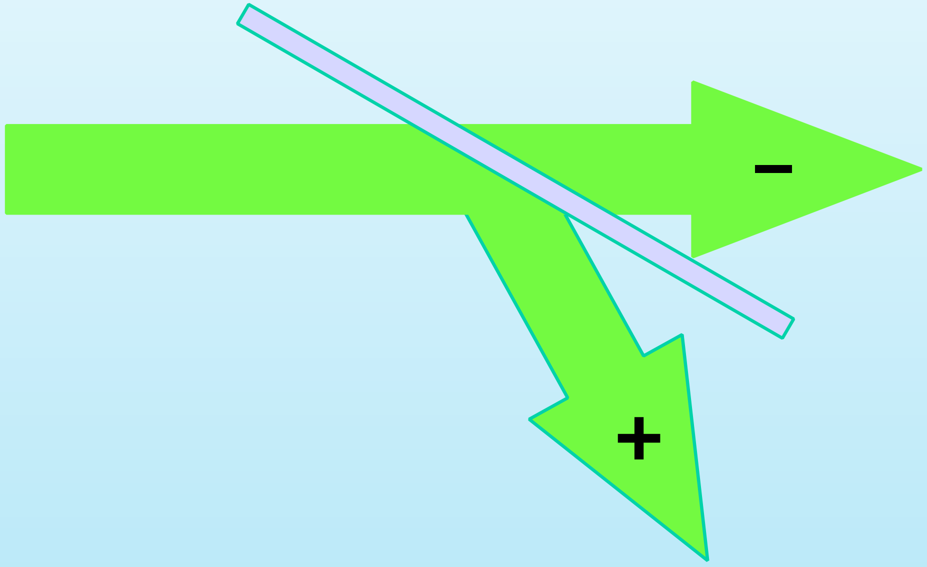
Mirror polarizer

Bender polarizer (O. Schärpf , D7 @ ILL).



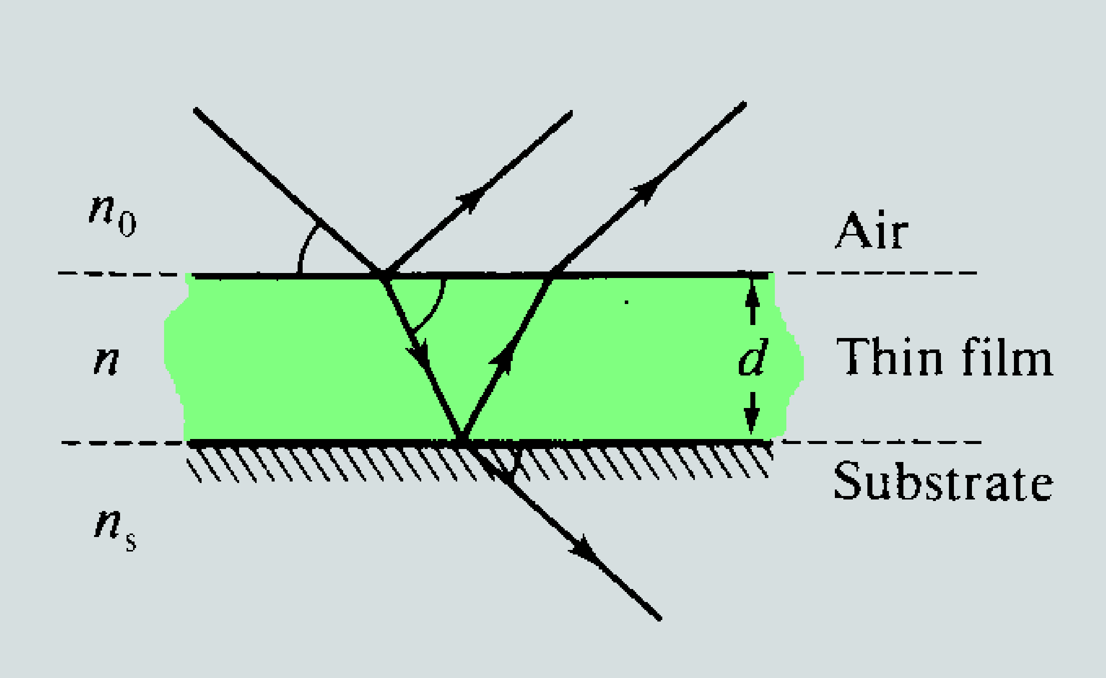
Mirrors are bent to ensure at least one reflection of the neutrons. Polarization less good due to finite reflectivity of absorbing layer. But able to accept large divergence of angles (stacked device).

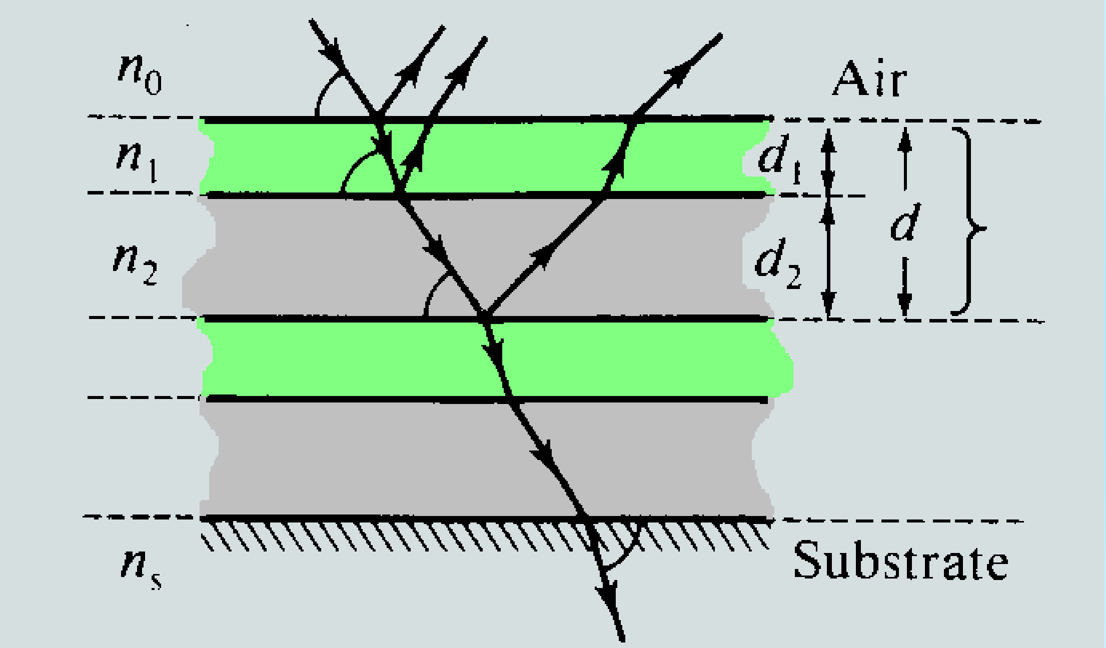
Transmission polarizer

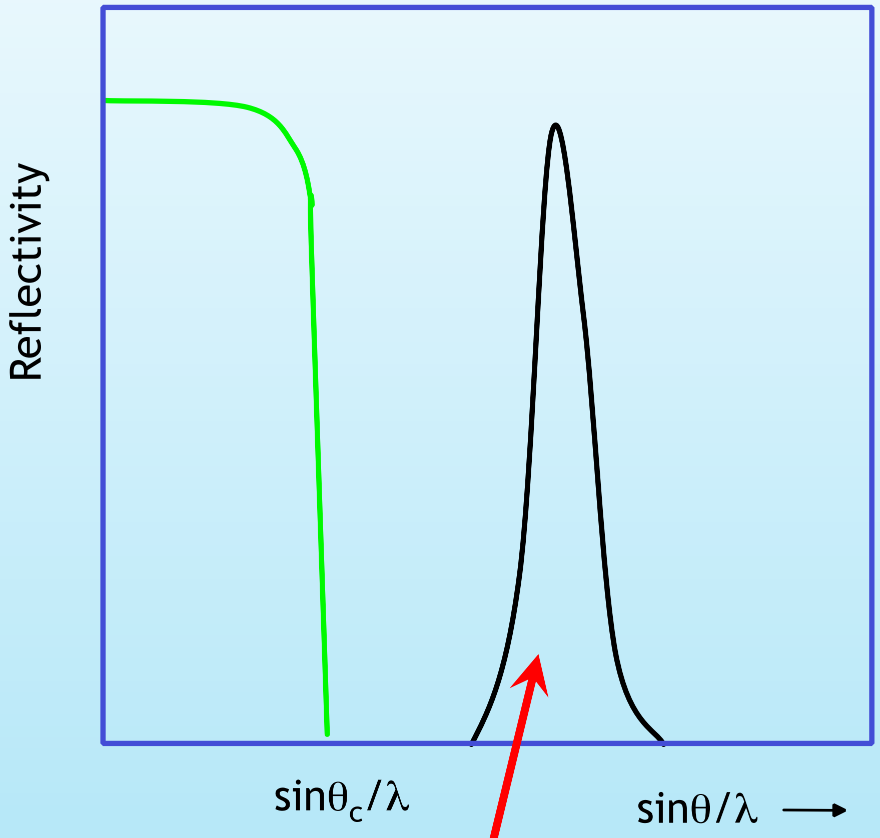


Very good polarization, since clean separation of polarization states is achieved.
Can only accept limited divergence and one wavelength.

Neutron supermirrors

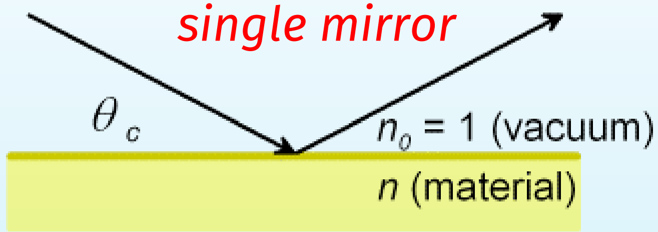


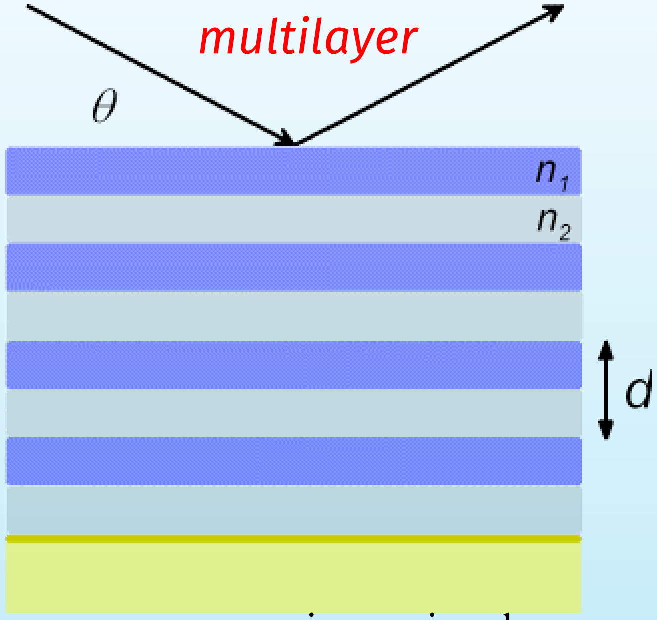


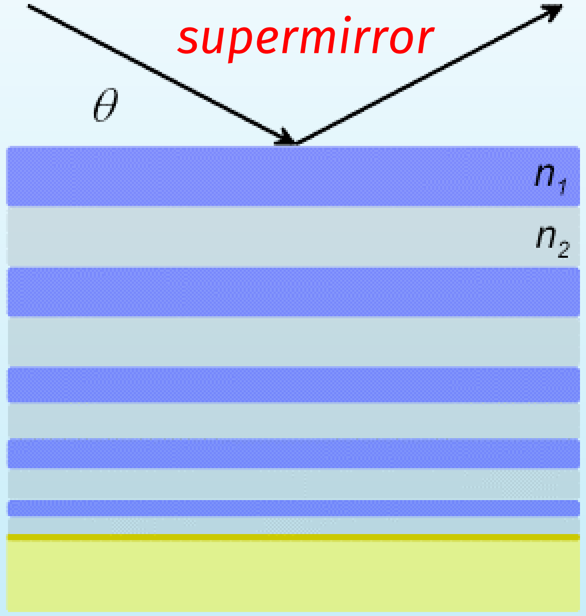


The multi-bilayer system introduces an additional Bragg peak at $\sin\frac{\theta}{\lambda} = \frac{1}{2}d$.

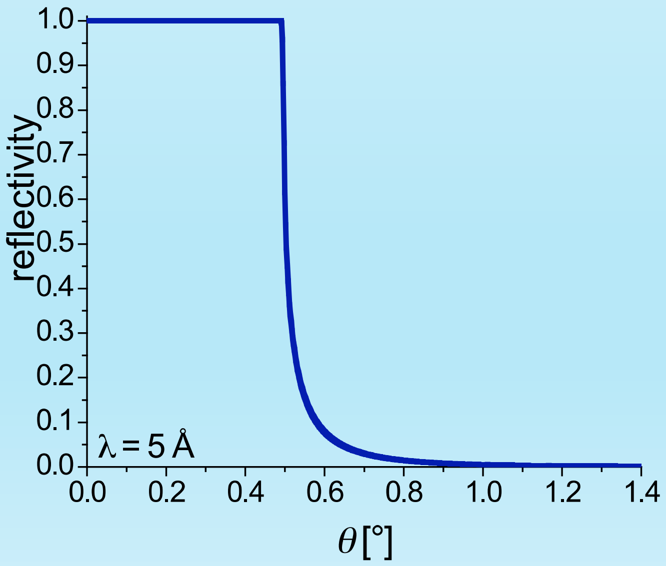
Neutron supermirrors

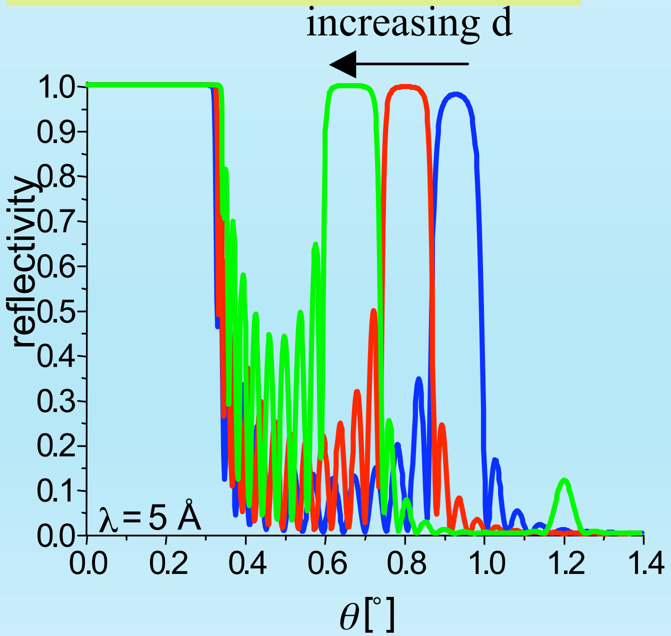


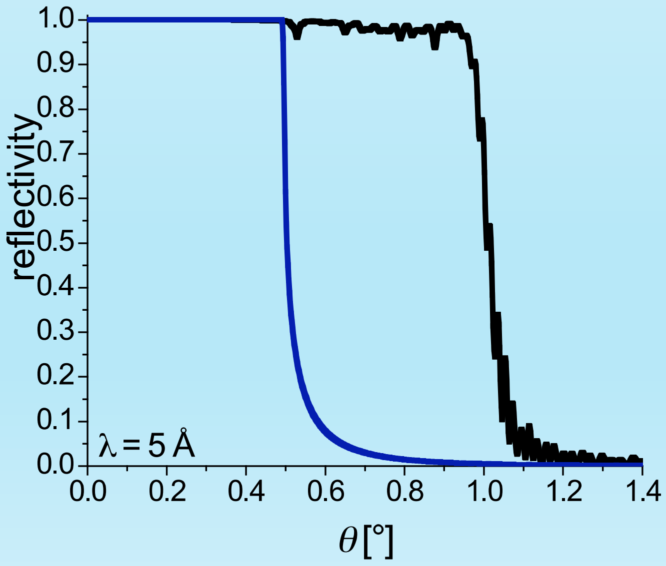




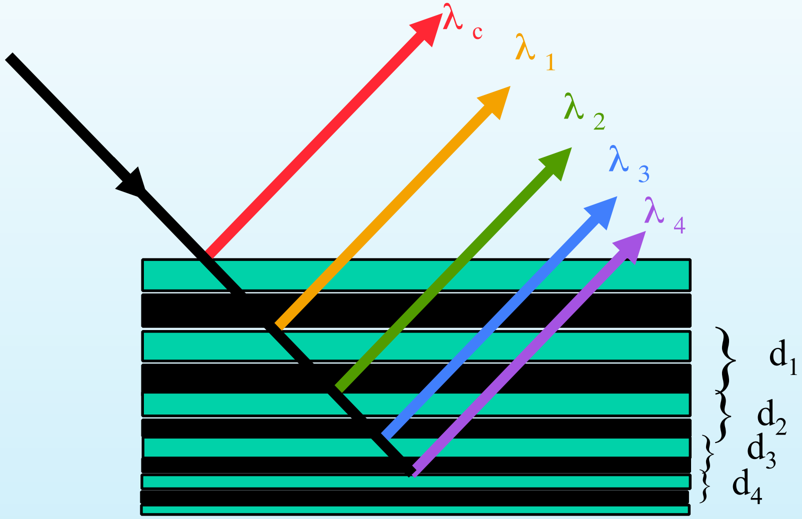
- *refractive index* $n < 1$
- *total external reflection*
  e.g. $Ni\ \theta_c = 0.1\ °/\text{Å}$



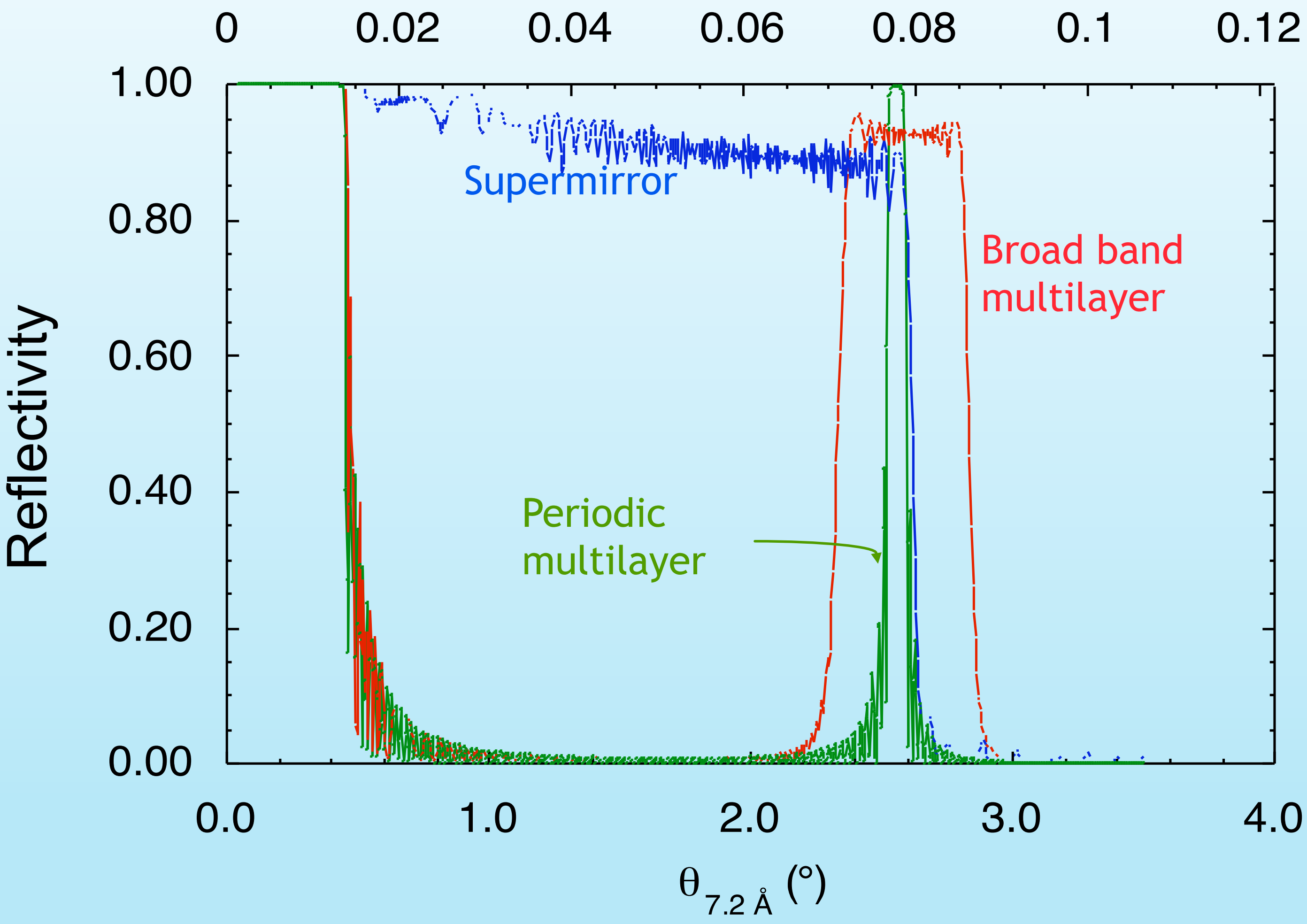




Neutron supermirrors



Supermirror systems
(eg Co/Ti, Fe/Si etc)

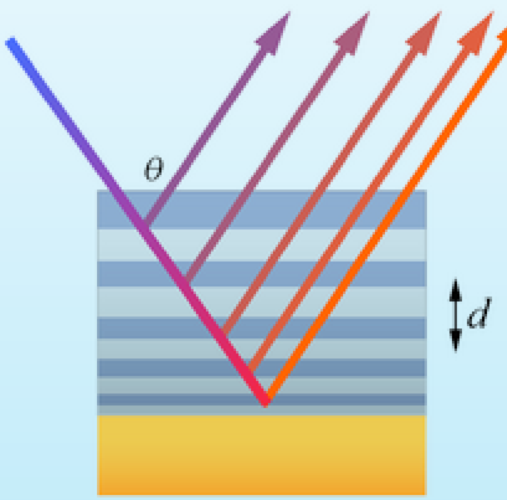


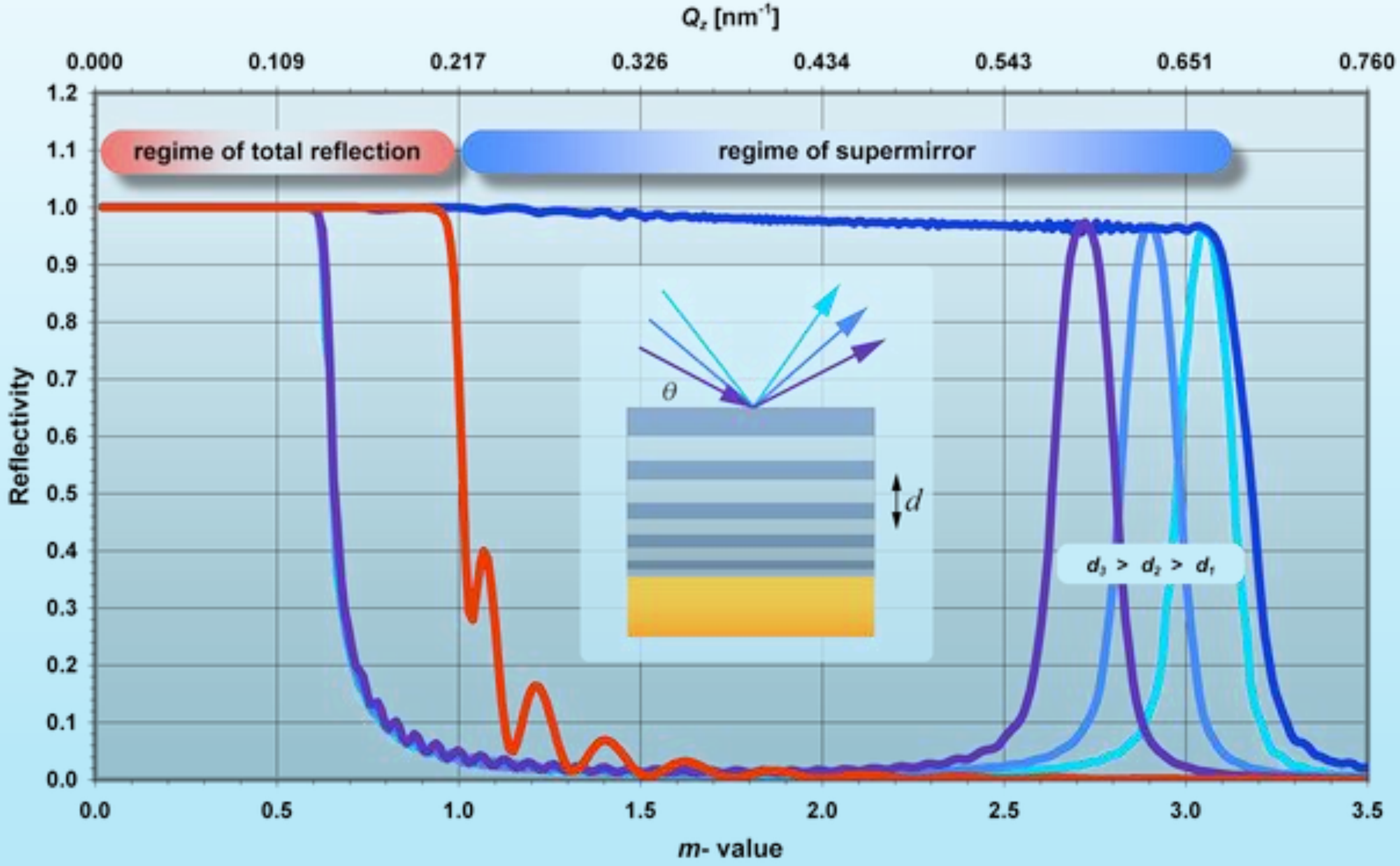
A gradient in the spacing of the bilayers results in a range of effective Bragg angles, and therefore a reflectivity which extends beyond values expected for normal mirror reflections.

Supermirror *m*-number indicates the range of angles for good reflectivity

For a single (thick) layer of Ni, $m = 1 = 0.1°/\text{Å}$.

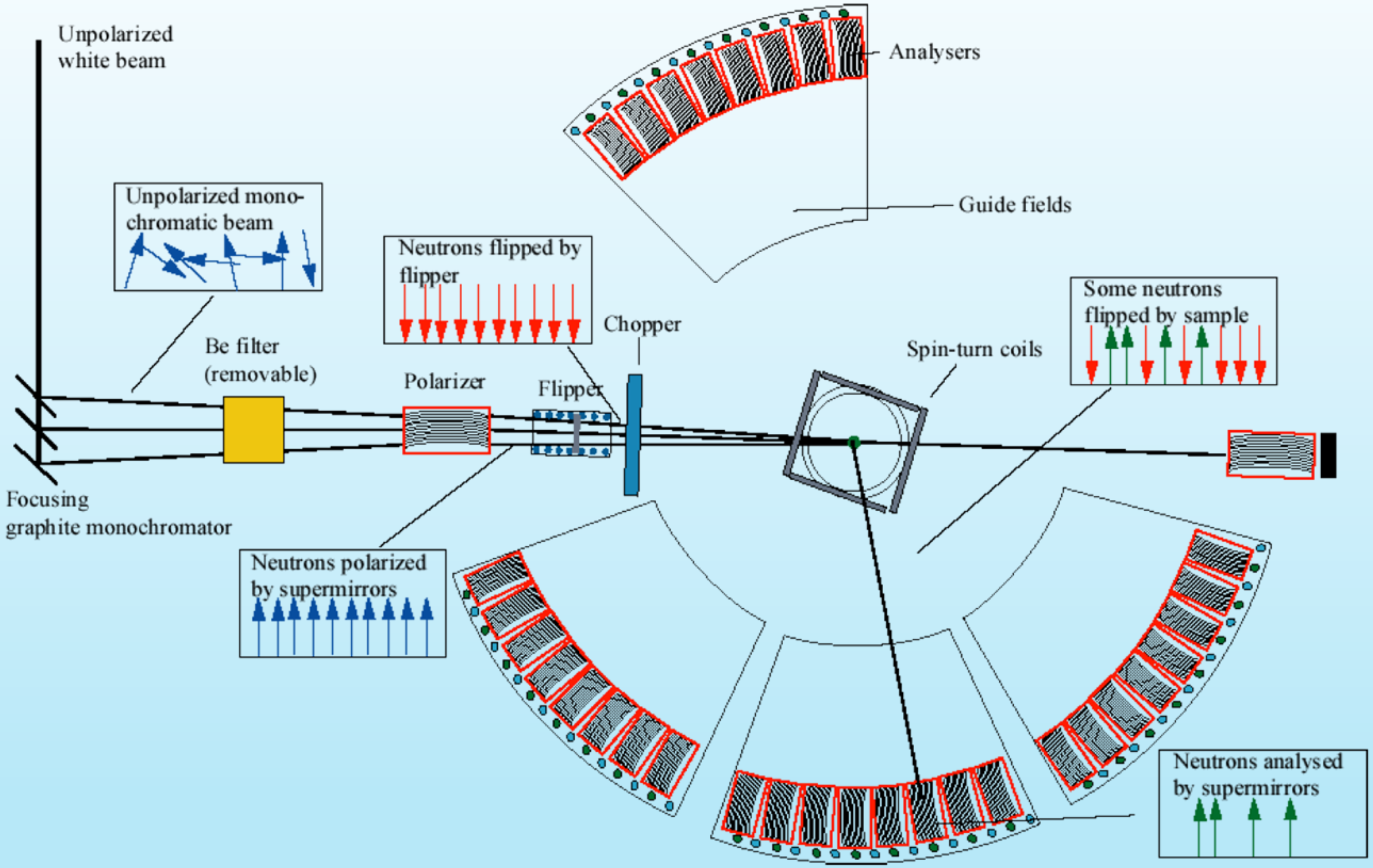
Neutron supermirrors





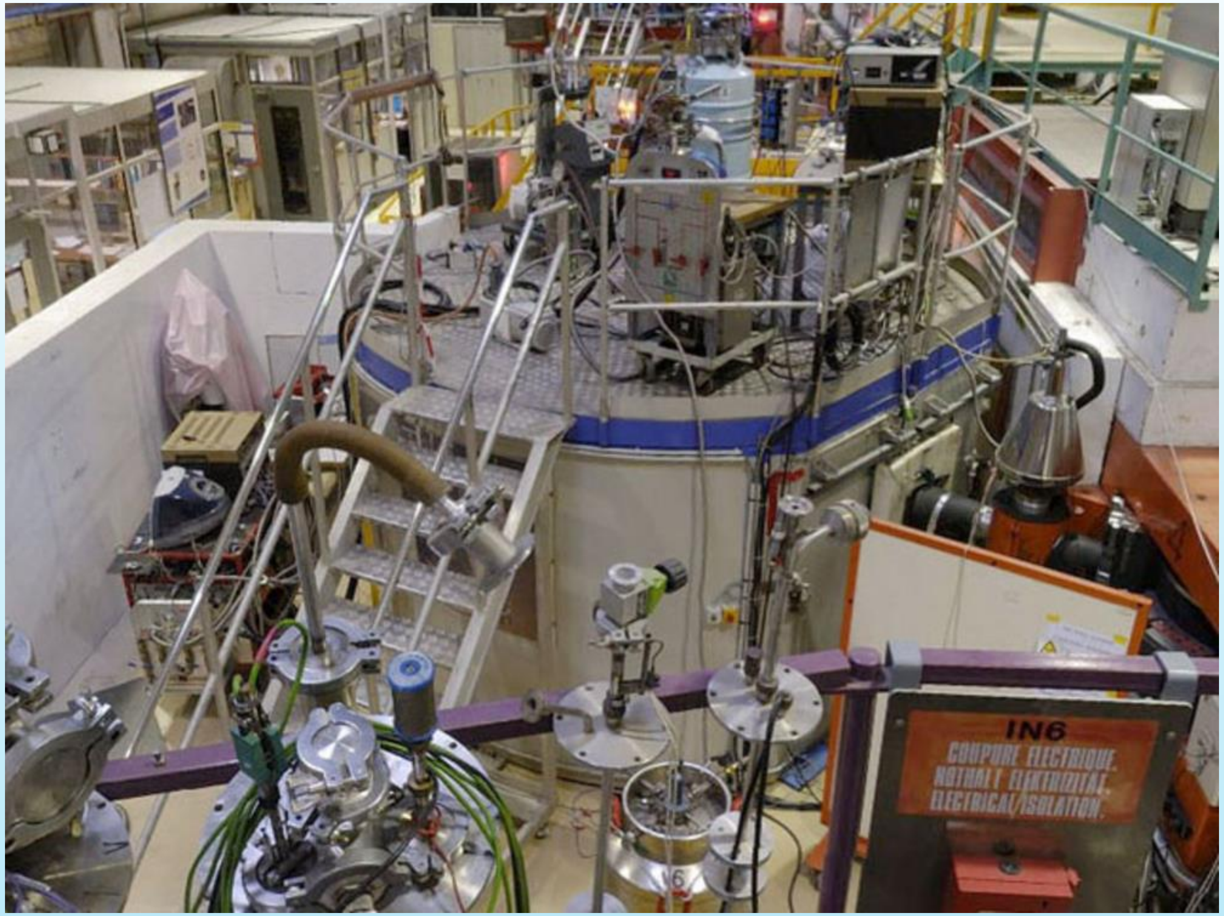
Now commercially available from Swiss Neutronics

D7 @ ILL

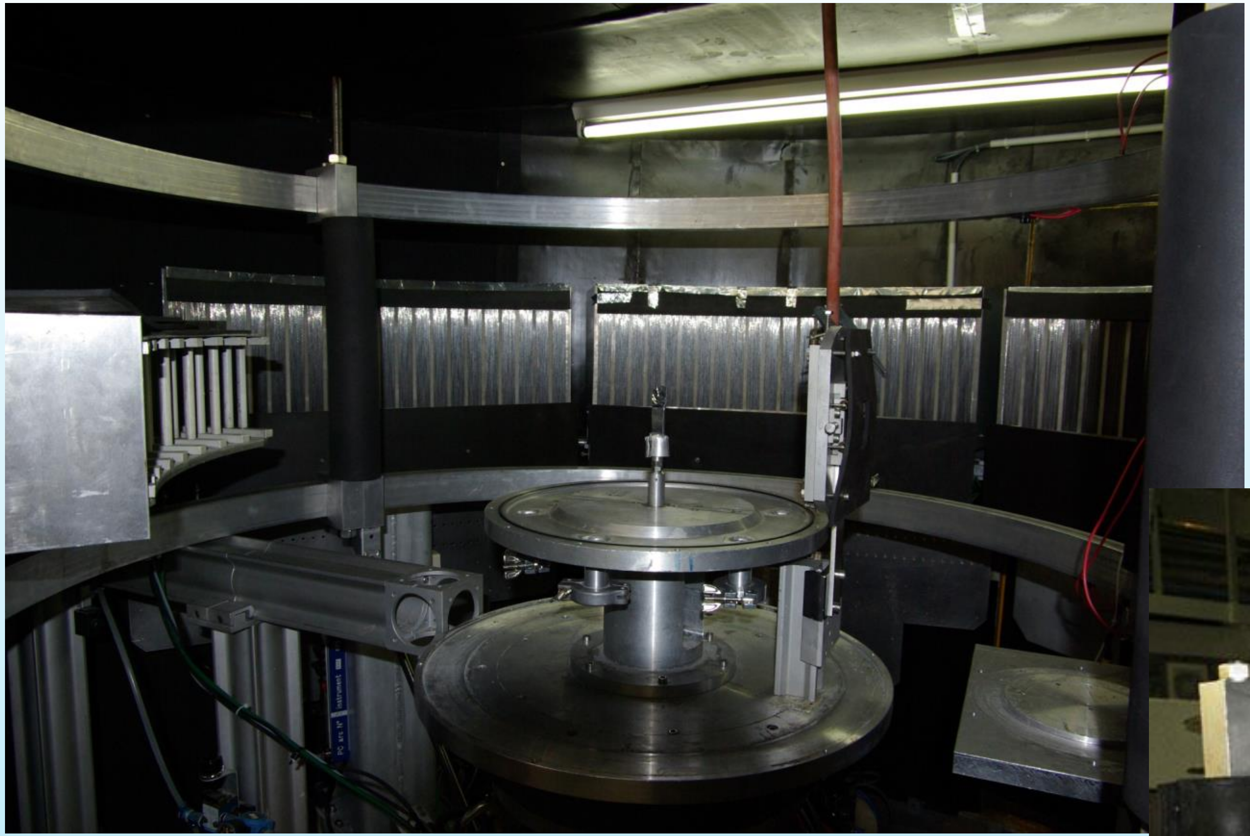


D7 has been dismantled to be replaced with a new instrument called D007. D007 will soon be commissioned.

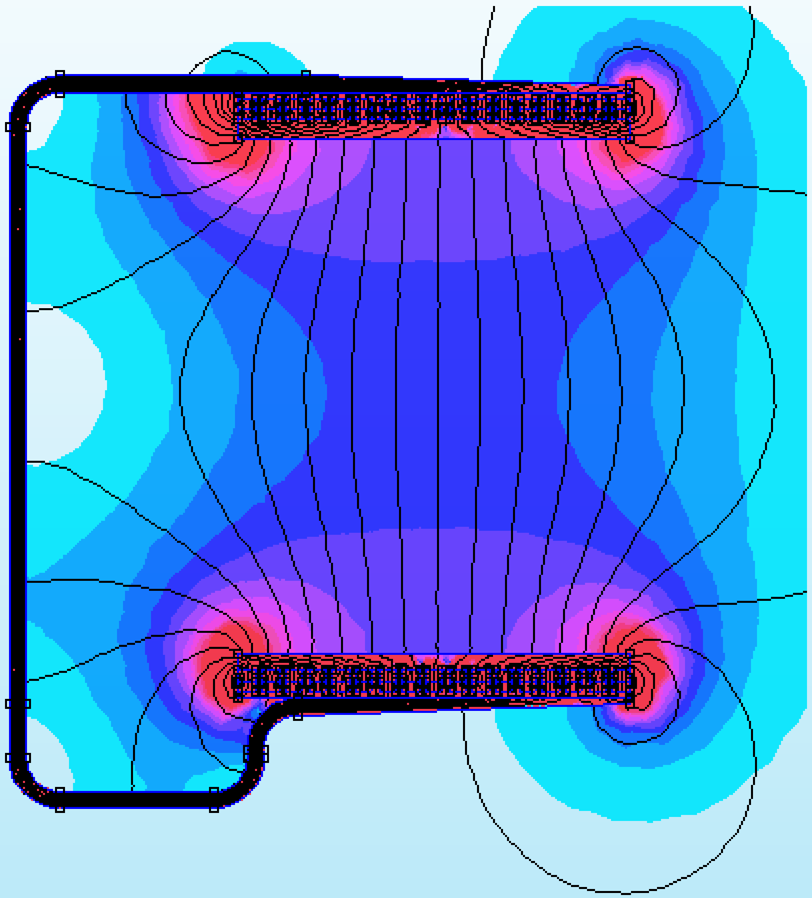
D7 @ ILL

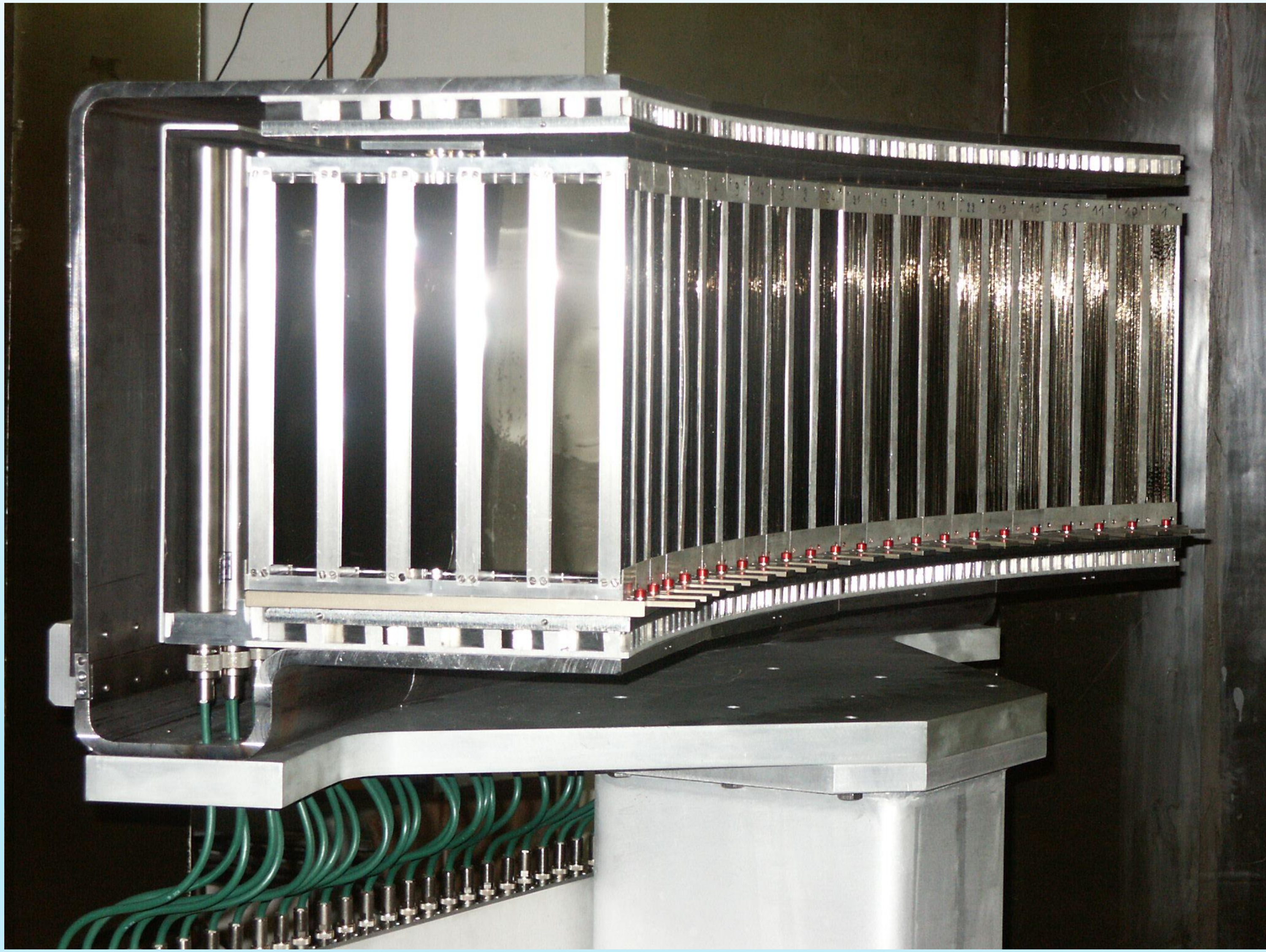


D7 @ ILL



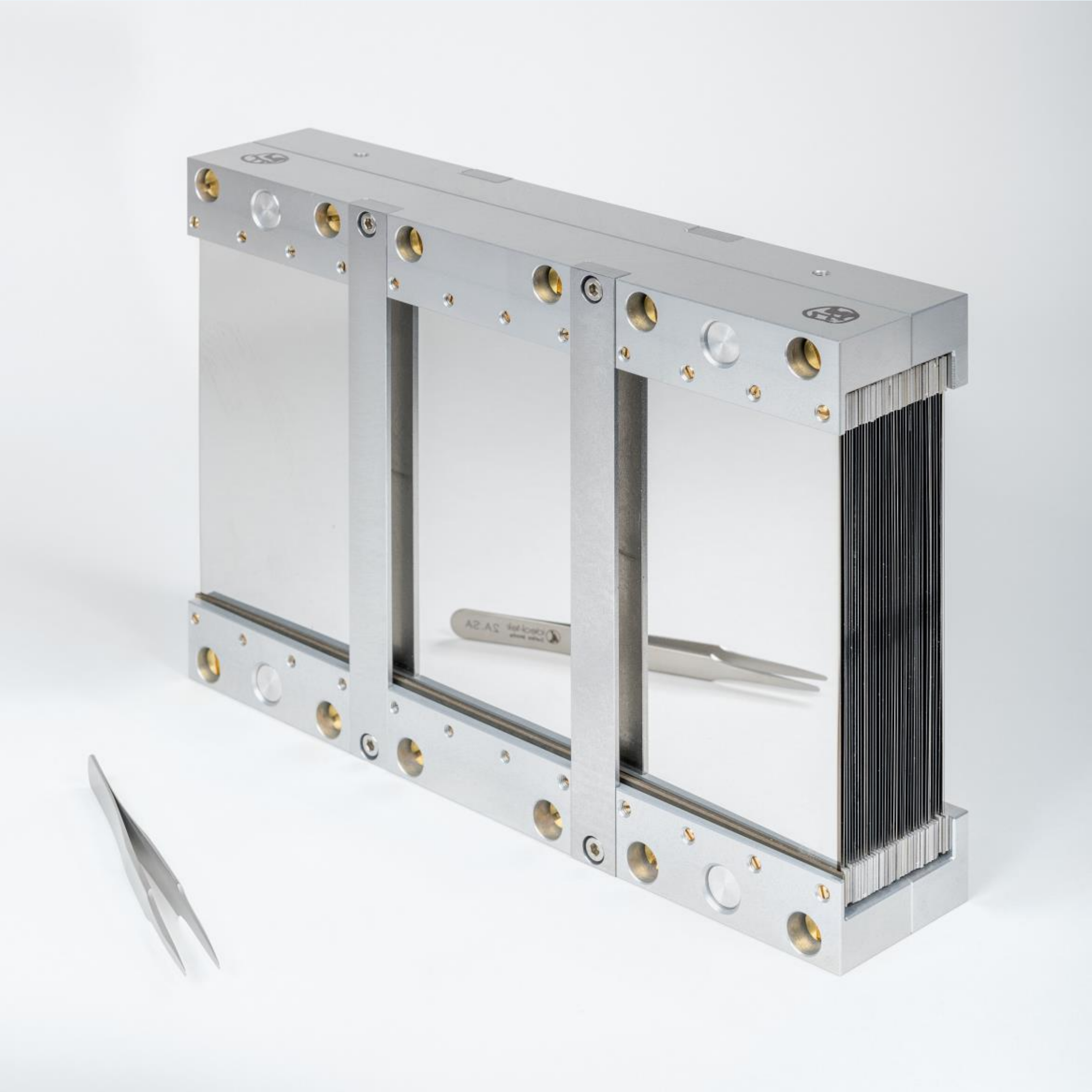
Neutron supermirrors





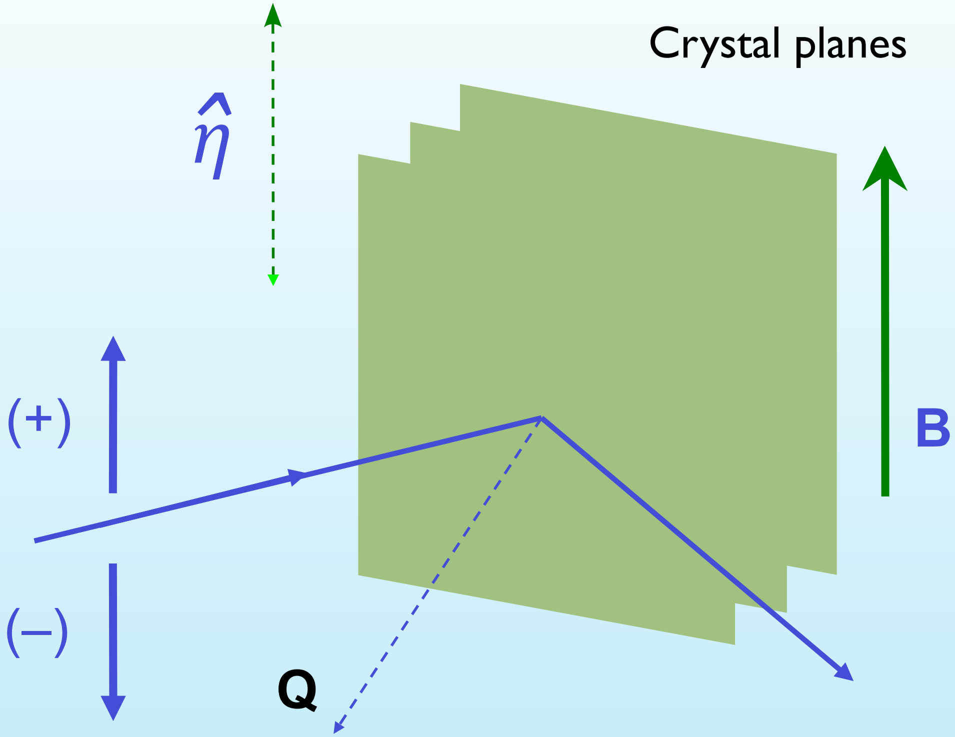
Supermirror “bender” analyser array on D7, ILL. There is over 250 m^2 of supermirror in the full analyser array.

Neutron supermirrors



New "Schärpf-type" bender supermirrors now produced at the ILL.

Polarizing crystals



Cu_2MnAl (Heusler) crystal grown at ILL

If the incident beam is considered as a superposition of $P = 1$ and $P = -1$ states, then the cross section for Bragg reflection is:

$$\frac{d\sigma}{d\Omega} = F_N^2(\mathbf{Q}) + 2F_N(\mathbf{Q})F_M(\mathbf{Q})(\mathbf{P}\cdot\hat{\boldsymbol{\eta}}) + F_M^2(\mathbf{Q})$$

For $\mathbf{P}\cdot\hat{\boldsymbol{\eta}} = +1$ $\quad \frac{d\sigma}{d\Omega} = \left(F_N(\mathbf{Q}) + F_M(\mathbf{Q})\right)^2$

For $\mathbf{P}\cdot\hat{\boldsymbol{\eta}} = -1$ $\quad \frac{d\sigma}{d\Omega} = \left(F_N(\mathbf{Q}) - F_M(\mathbf{Q})\right)^2$

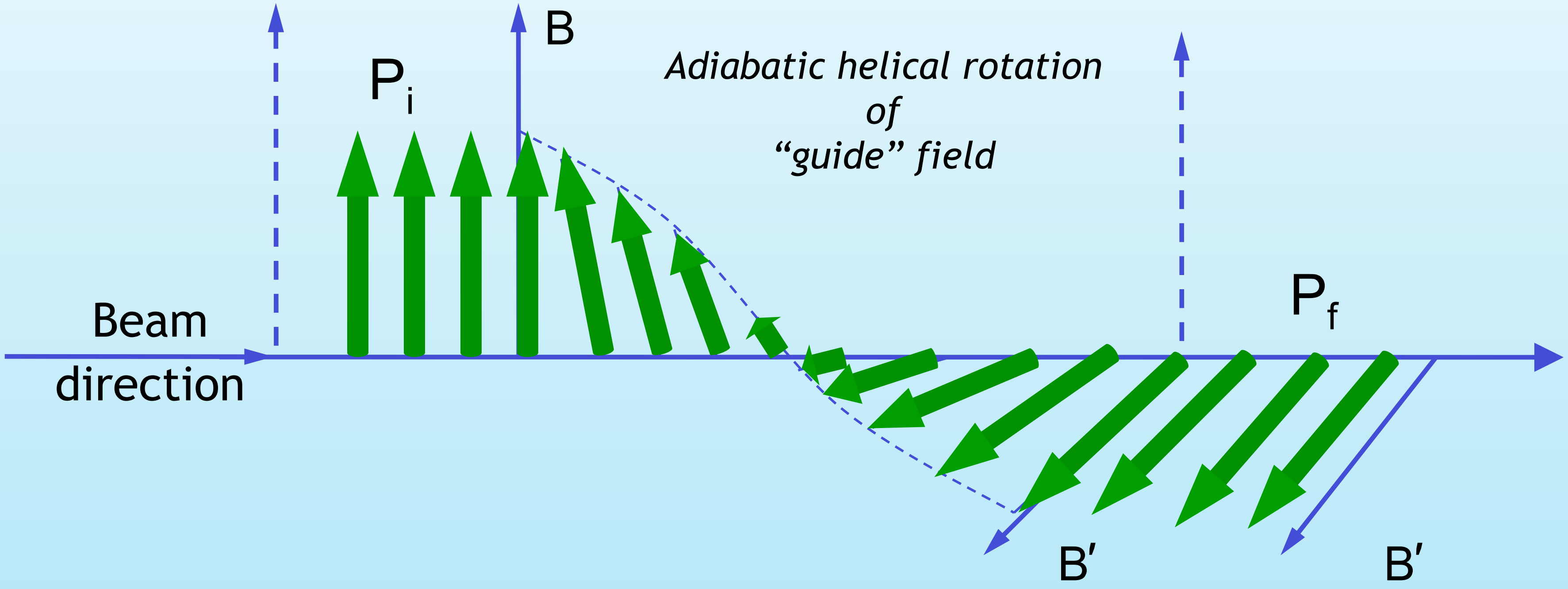
For $|F_N(\mathbf{Q})| = |F_M(\mathbf{Q})|$ the reflected beam will be polarized

Polarizing efficiency $\quad P_f = \dfrac{2F_N(\mathbf{Q})F_M(\mathbf{Q})}{[F_N^2(\mathbf{Q}) + F_M^2(\mathbf{Q})]}$

V. Guiding and flipping

Guiding the polarization

If the direction of the magnetic field (quantisation axis) remains constant in the rest frame of the neutrons then the direction of the polarization of the neutron beam will be preserved.

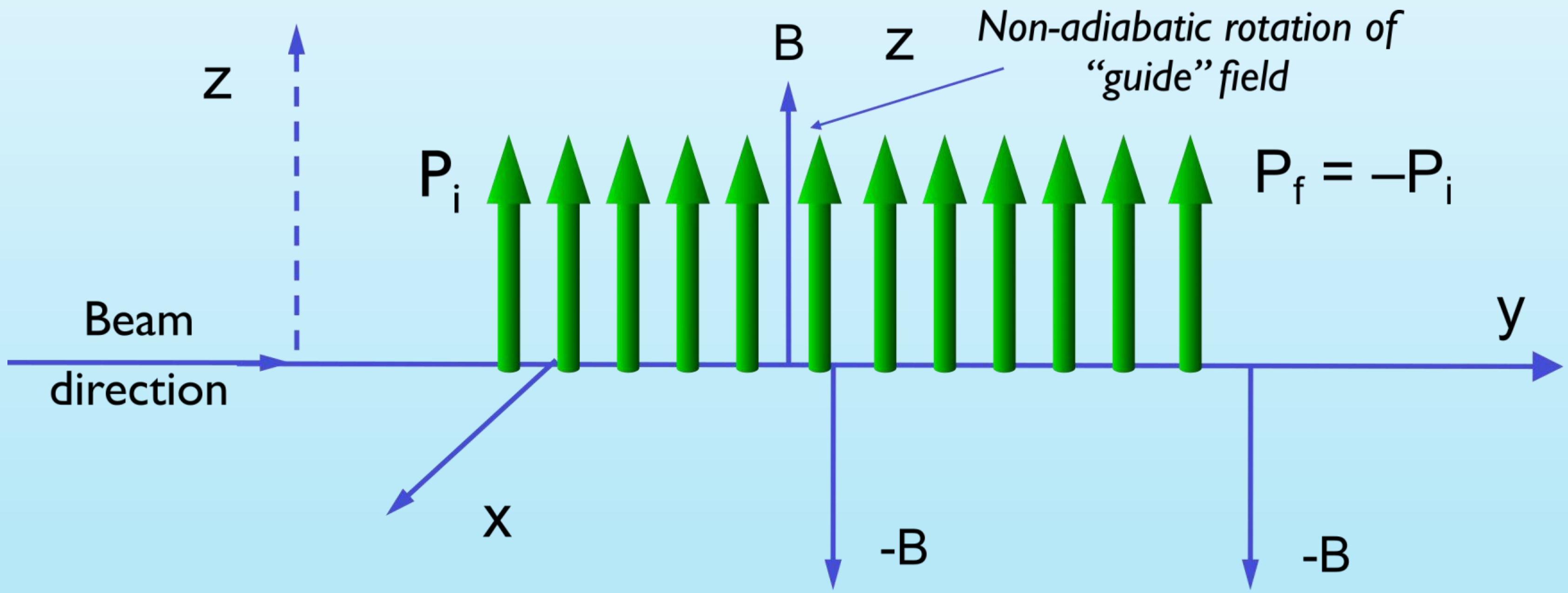


If the direction of the field **B** changes sufficiently slowly in the rest frame of the neutrons, then an adiabatic (or reversible) rotation of the polarization occurs.

In an adiabatic process, the system is always "infinitesimally close" to equilibrium.

Non-adiabatic field change

For a non-adiabatic reorientation of the guide field the polarization will not re-orient. Instead, the beam will preserve its initial direction, and begin to precess about the new field direction.



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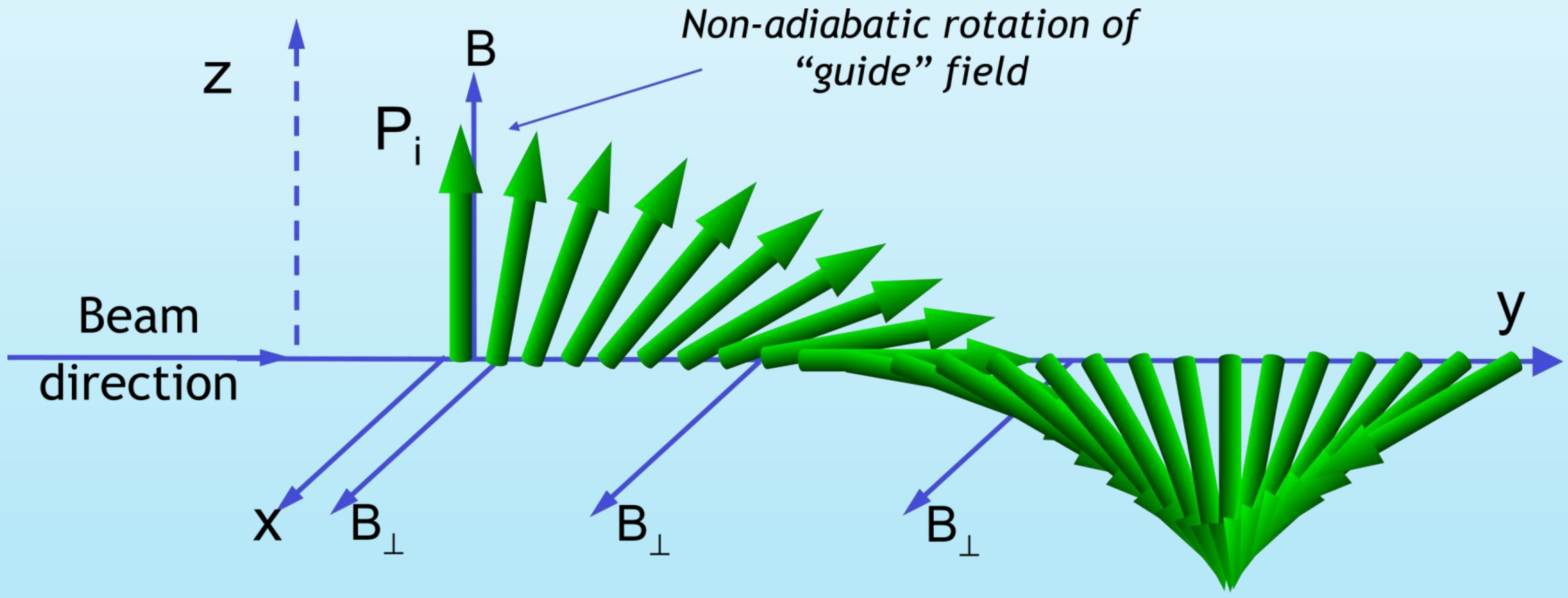
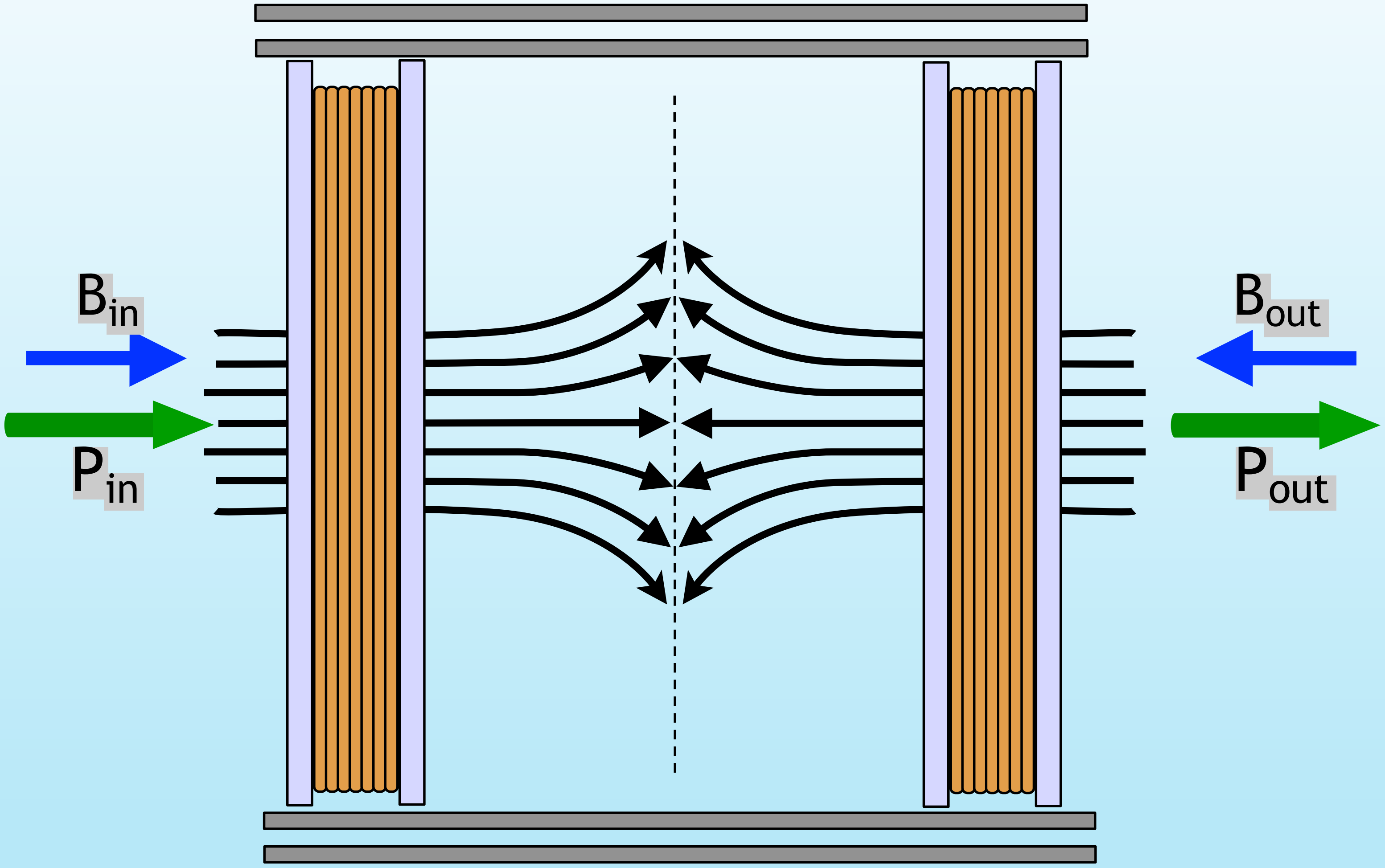


Non-adiabatic rotations enable the beam polarization to be effectively "flipped" with respect to the guide field.

Drabkin π-flipper



Drabkin flipper: useful for white beams of limited size

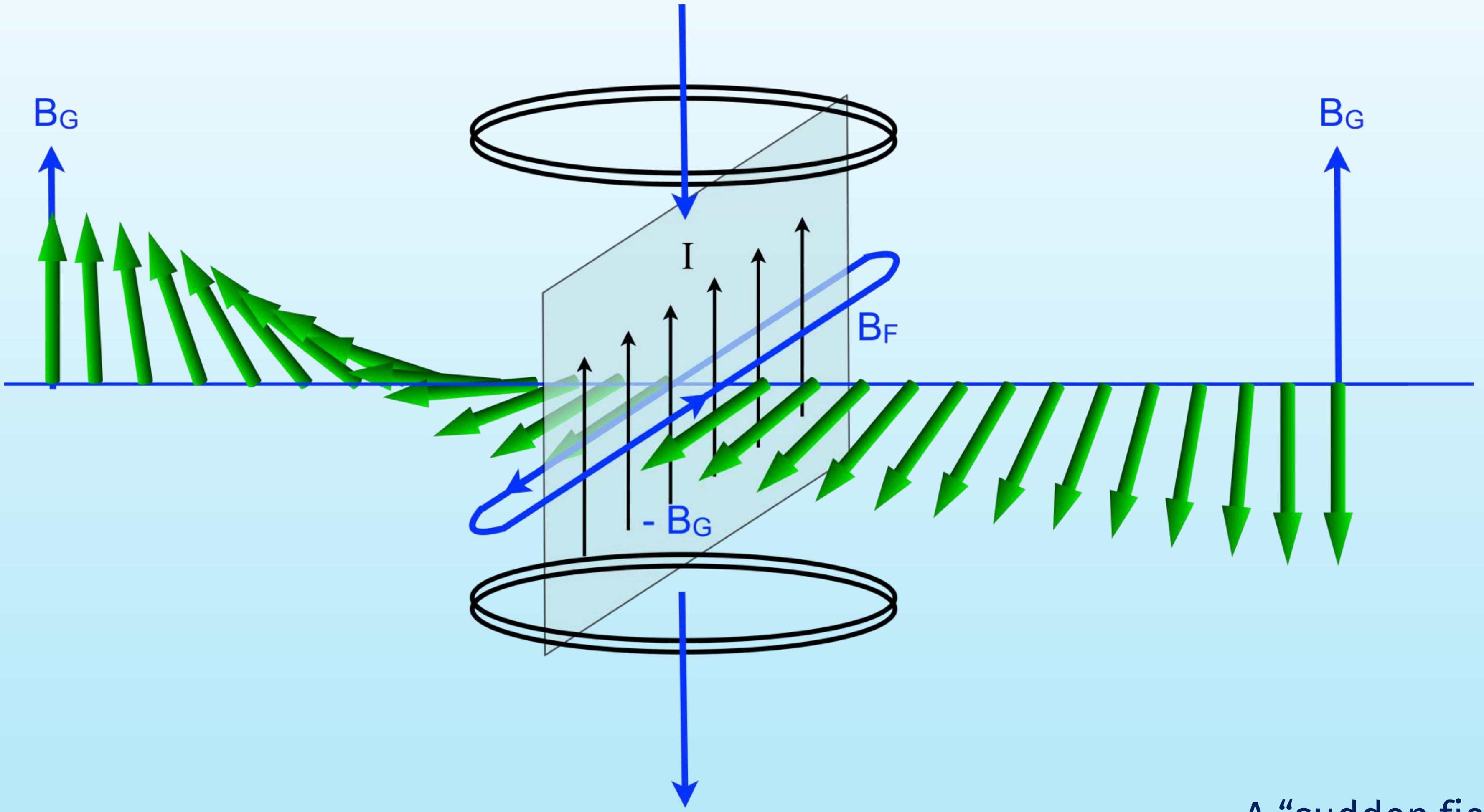
— used on the reflectometers CRISP and SURF at ISIS

Radial magnetic field off-axis results in low flipping ratios.

Useful for thin beams only

BUT: No material in beam.

Current Sheet (Dabbs Foil)

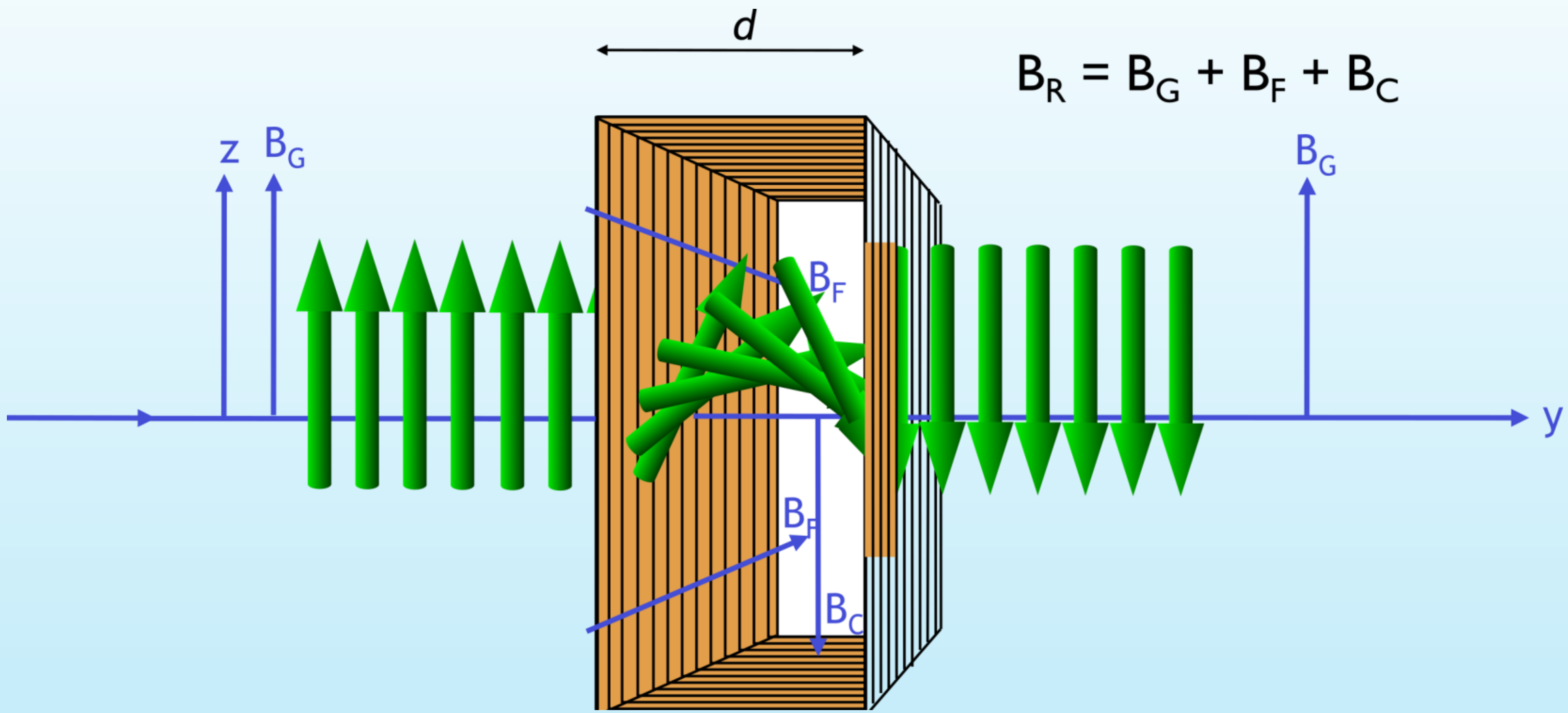


A "sudden field-reversal" π-flipper.

Works for wide wavelength band

(for wavelengths which adiabatically follow the field).

Mezei flipper



The **Mezei flipper** uses a non-adiabatic 90° field change to project the polarization direction of the beam onto any arbitrary field axis.

A flip of φ radians with respect to the guide field can be achieved if the resultant field within the coil, $\mathbf{B}_R$, is perpendicular to $\mathbf{B}_G$ and:

$$d = \frac{\varphi v}{\gamma_n B_R}$$

For example: a 1 Å neutron will be spin-flipped by π in a distance of 1cm if $B_R = 1\ \mathrm{mT}$.

VI. XYZ Polarization analysis

Magnetic scattering

A complete, in-depth desciption of the magnetic neutron scattering (magnetic dipole interactions, as opposed to strong nuclear interactions) requires a state-of-the-art density matrix formalism, and is far beyond the scope of this lecture. An extensive treatment of this subject can be found in Otto Schärpf's report: *The spin of the neutron as a measuring probe. Application of spin polarized neutrons to measure electronic (including magnetic) properties of metals, semiconductors, superconductors**.

The magnetic neutron scattering formalism is laid out in the Squires book ***Introduction to the Theory of Thermal Neutron Scattering***.

Here we confine ourselves to merely touching upon the main issues, reproducing largely from Gøran Nilsen's OSNS'17 talk.

The scattered polarization and cross section (translating into the intensity) depends on the relative orientation of the beam polarization and the magnetic moments in the sample, making the experiment itself, and subsequent data analysis by no means a trivial task.

*used to be available on the web, now I can give it to anybody interested.

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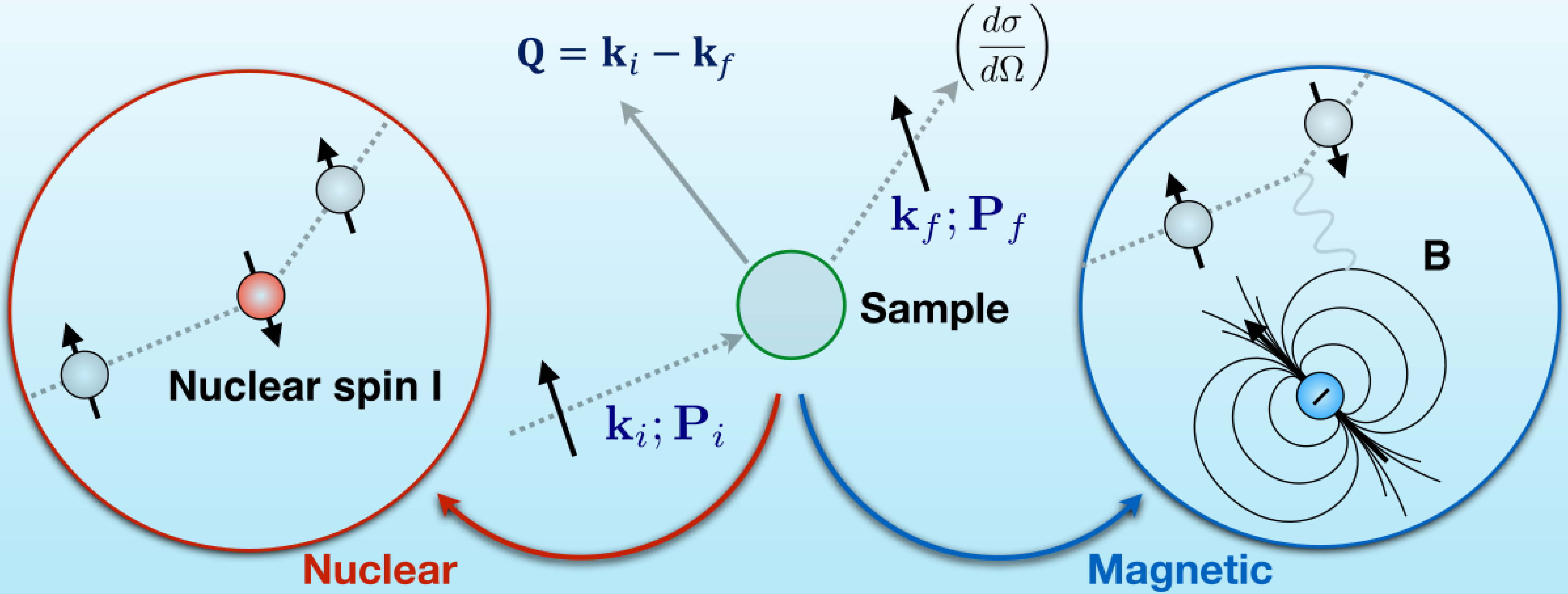
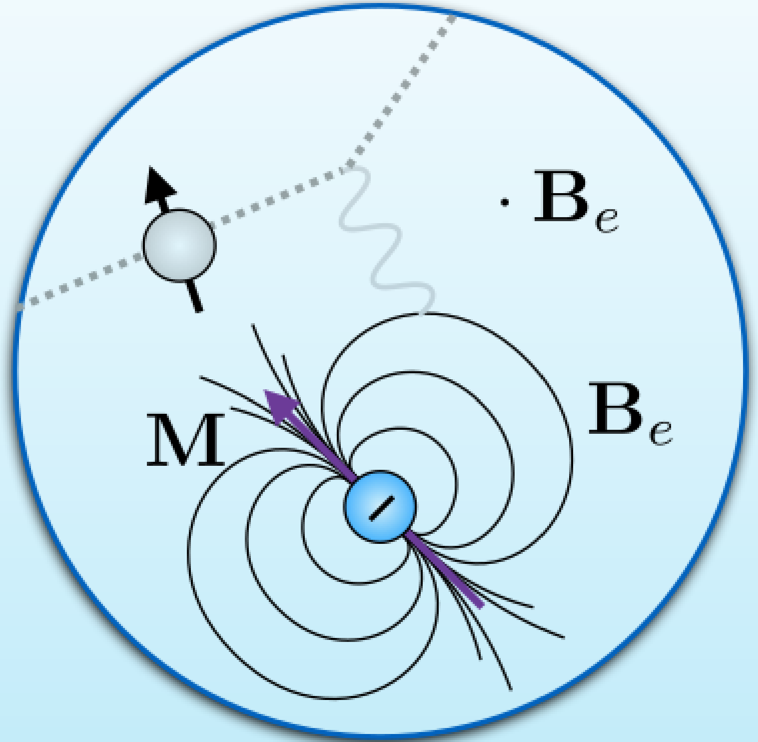
Magnetic scattering



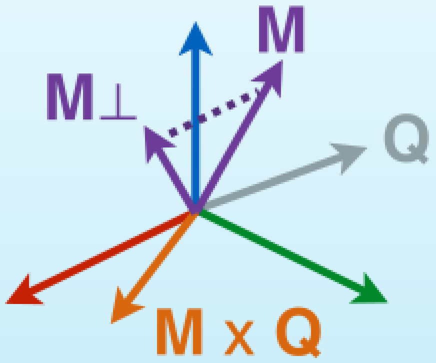
Most samples also contain magnetic moments, originating either from nuclei or the electrons — they exhibit magnetic properties.

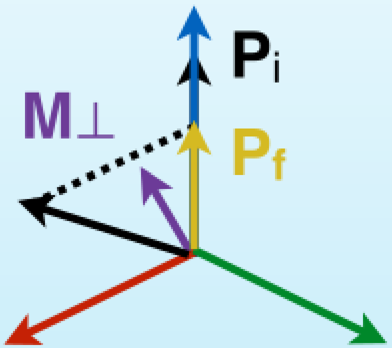
(after Gøran Nilsen, OSNS'17)

Magnetic scattering



Magnetic





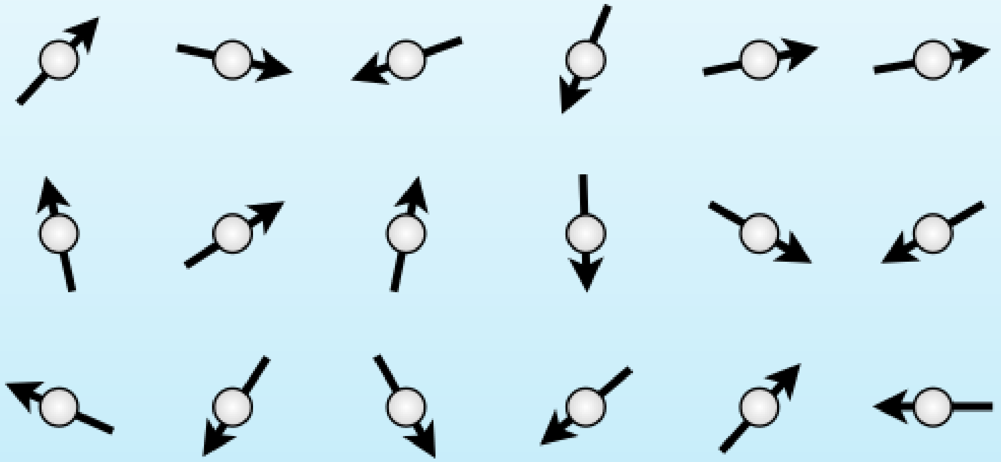
$$\mathbf{M}_\perp = \mathbf{Q} \times \mathbf{M}(\mathbf{Q}) \times \mathbf{Q}$$

(after Gøran Nilsen, OSNS'17)

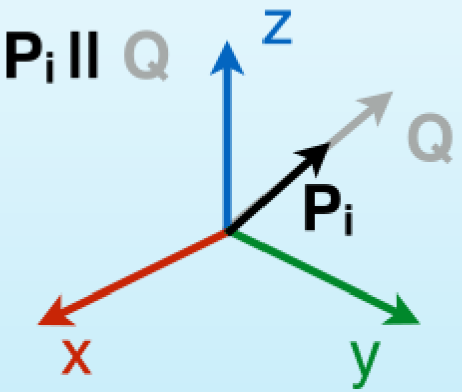
1. One can only measure the components $\mathbf{M} \perp \mathbf{Q}$
2. If $\mathbf{M}_\perp \perp \mathbf{P}_i$ – scattering with neutron spin flip (SF)
3. If $\mathbf{M}_\perp \parallel \mathbf{P}_i$ – scattering with no neutron spin flip (NSF)

Study case I.

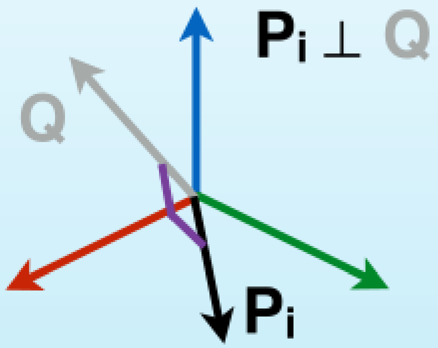
Disordered electronic magnetic moments of the sample.



<M> = 0



$$\frac{\mathrm{NSF}}{\mathrm{SF}} = \frac{0}{1}$$



$$\frac{\mathrm{NSF}}{\mathrm{SF}} = \frac{1/2}{1/2}$$

$$\left(\frac{d\sigma}{d\Omega}\right)_{\uparrow\uparrow} = \left(\frac{d\sigma}{d\Omega}\right)_{\downarrow\downarrow} \propto 1 - \left(\widehat{\mathbf{Q}} \cdot \widehat{\mathbf{P}}_i\right)^2$$

$$\left(\frac{d\sigma}{d\Omega}\right)_{\uparrow\downarrow} = \left(\frac{d\sigma}{d\Omega}\right)_{\downarrow\uparrow} \propto 1 + \left(\widehat{\mathbf{Q}} \cdot \widehat{\mathbf{P}}_i\right)^2$$

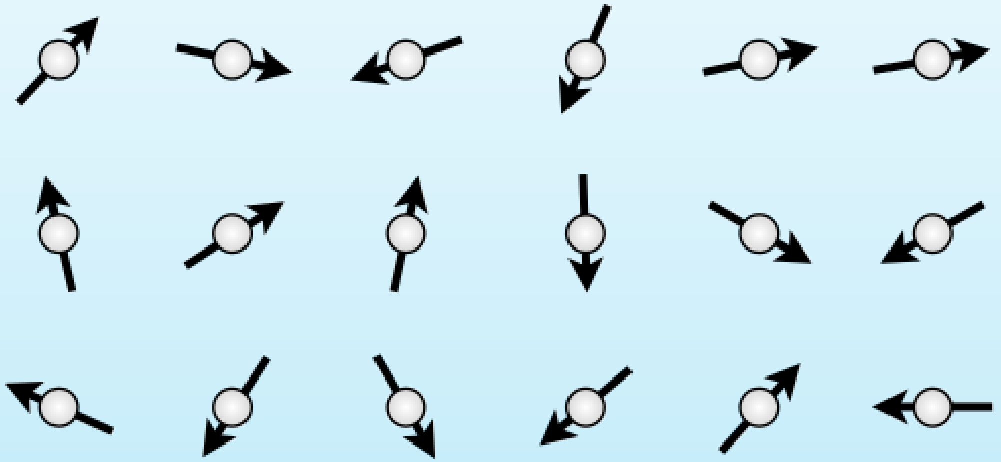
After averaging over the random direction of $\mathbf{M}$, the magnetic elastic scattering cross section only depends on angle between the incident polarization $\mathbf{P}_i$ and $\mathbf{Q}$.

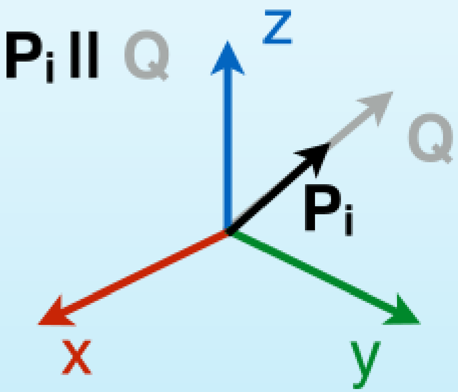
(after Gøran Nilsen, OSNS'17)

Magnetic scattering

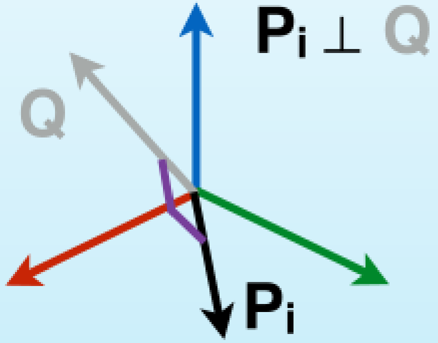
Study case I.

Disordered electronic magnetic moments of the sample.





$$\frac{NSF}{SF} = \frac{0}{1}$$



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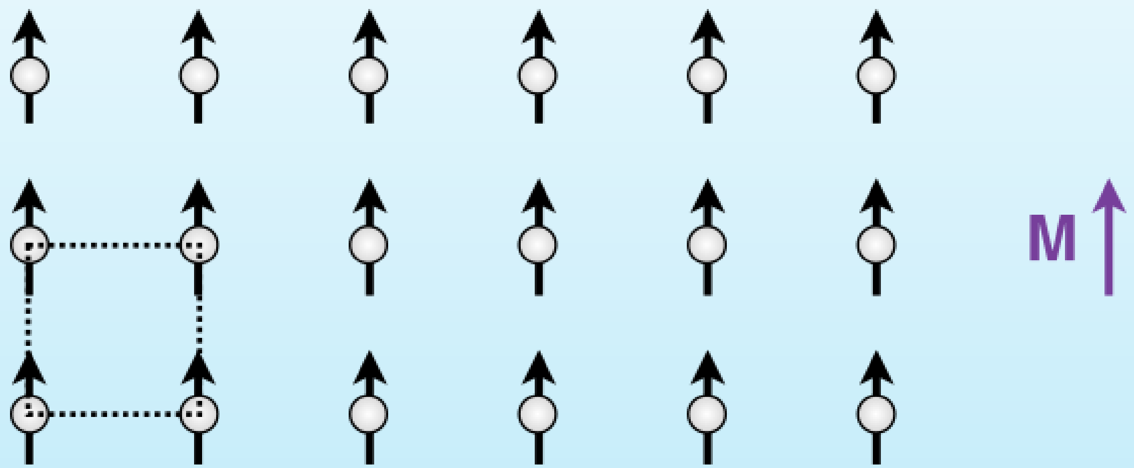
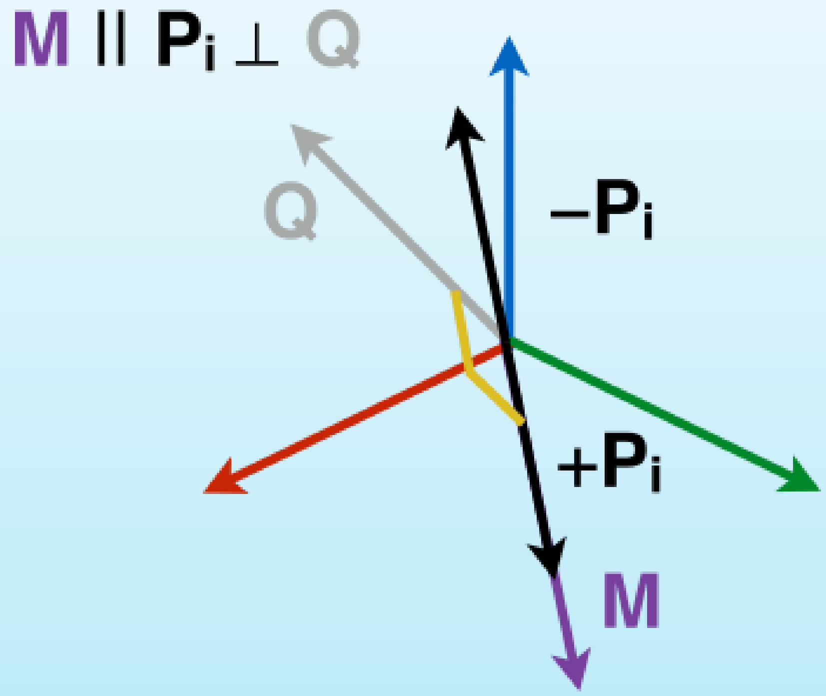
After averaging over the random direction of $\mathbf{M}$, the magnetic elastic scattering cross section only depends on angle between the incident polarization $\mathbf{P}_i$ and $\mathbf{Q}$.

(after Gøran Nilsen, OSNS'17)

Study case II.

Electronic magnetic moments of the sample all aligned.





1. $\mathbf{M} \perp \mathbf{Q}$ – all of $\mathbf{M}$ measured.
2. $\mathbf{P}_i \parallel \mathbf{M} \perp \mathbf{Q}$ – all scattering with spin flip

- $+\mathbf{P}_i \parallel \mathbf{M}$: $\left(\frac{d\sigma}{d\Omega}\right)_{\uparrow\uparrow} \propto |b_N + b_M|^2$
- $-\mathbf{P}_i \parallel \mathbf{M}$: $\left(\frac{d\sigma}{d\Omega}\right)_{\downarrow\downarrow} \propto |b_N - b_M|^2$

Different!

(the indices N and M refer to „nuclear” and „magnetic”, resp.)

(after Gøran Nilsen, OSNS’17)

Magnetic scattering

Problem:

Can an XYZ-difference experiment be performed on a multidetector instrument?

phys. stat. sol. (a) **135**, 359 (1993)

Subject classification: 61.12 and 75.25; 85

Institut Laue-Langevin, Grenoble[1]) *(a) and*
Institut für theoretische Physik der Rheinisch-Westfälischen Technischen Hochschule Aachen[2]) *(b)*

The *XYZ*-Difference Method with Polarized Neutrons and the Separation of Coherent, Spin Incoherent, and Magnetic Scattering Cross Sections in a Multidetector

By

O. SCHÄRPF (a) and H. CAPELLMANN (b)

Dedicated to Professor Dr. CHRISTOPH SCHWINK on the occasion of his 65th birthday

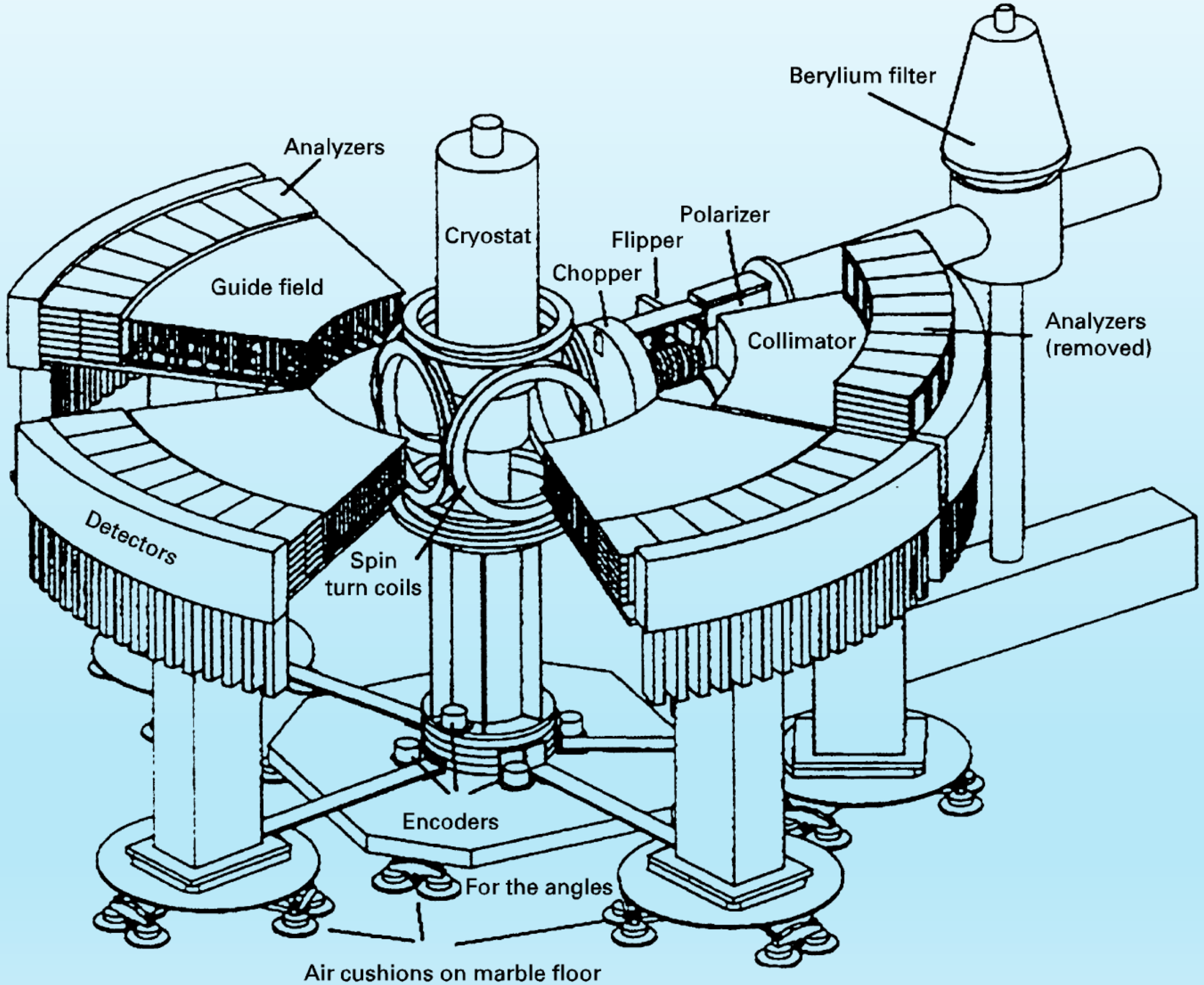
Equations are derived for the polarization analysis in a multidetector to separate coherent, spin incoherent, and magnetic scattering using three-dimensional analysis or the *xyz*-difference method. Then the conditions for the magnetic guide fields to rotate the polarization into the three directions *x*, *y*, and *z* are discussed on the basis of the existing instrument D7 at the ILL in Grenoble.

Magnetic scattering

This means that, the polarized neutron scattering experiment on a magnetically ordered sample requires:

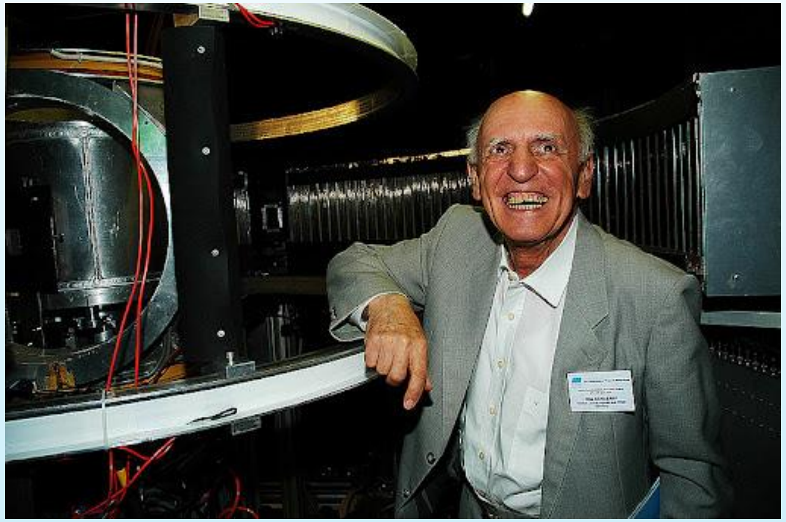
1. the π (180°) rotation of $\mathbf{P}_i$ about $\mathbf{M}$
2. projection of $\mathbf{M}$ onto $\mathbf{P}_i$
3. the measuring of the $\frac{\mathrm{NSF}}{\mathrm{SF}}$ ratio

On D7 we carried out this rotation by means of three pairs of mutually perpendicular Helmholtz coils.



Diffuse scattering instrument D7 with full 3D polarization analysis. The sample in the cryostat positioned in the centre of three Helmholtz coils.

The Schärpf Equations



$$\left(\frac{d\sigma}{d\Omega}\right)_x^{NSF} = \left(\frac{d\sigma}{d\Omega}\right)_{coh+II} + \frac{1}{3}\left(\frac{d\sigma}{d\Omega}\right)_{SI} + \frac{\sin^2\alpha}{2}\left(\frac{d\sigma}{d\Omega}\right)_{mag}$$

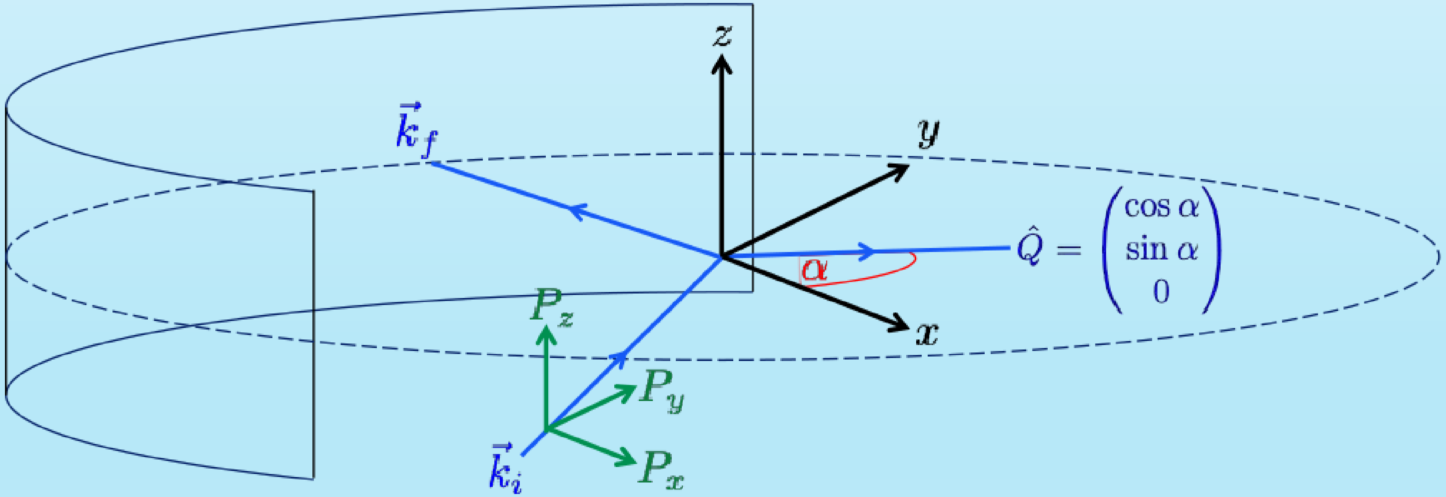
$$\left(\frac{d\sigma}{d\Omega}\right)_y^{NSF} = \left(\frac{d\sigma}{d\Omega}\right)_{coh+II} + \frac{1}{3}\left(\frac{d\sigma}{d\Omega}\right)_{SI} + \frac{\cos^2\alpha}{2}\left(\frac{d\sigma}{d\Omega}\right)_{mag}$$

$$\left(\frac{d\sigma}{d\Omega}\right)_z^{NSF} = \left(\frac{d\sigma}{d\Omega}\right)_{coh+II} + \frac{1}{3}\left(\frac{d\sigma}{d\Omega}\right)_{SI} + \frac{1}{2}\left(\frac{d\sigma}{d\Omega}\right)_{mag}$$

$$\left(\frac{d\sigma}{d\Omega}\right)_x^{SF} = \frac{2}{3}\left(\frac{d\sigma}{d\Omega}\right)_{SI} + \frac{1+\cos^2\alpha}{2}\left(\frac{d\sigma}{d\Omega}\right)_{mag}$$

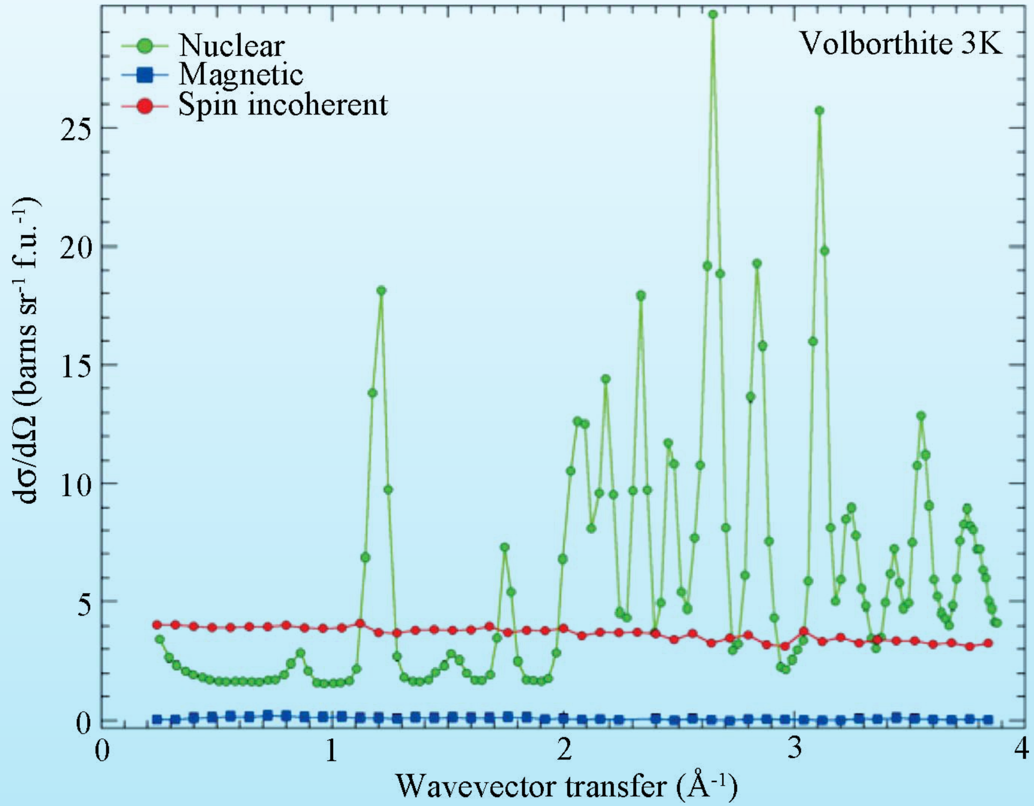
$$\left(\frac{d\sigma}{d\Omega}\right)_y^{SF} = \frac{2}{3}\left(\frac{d\sigma}{d\Omega}\right)_{SI} + \frac{1+\sin^2\alpha}{2}\left(\frac{d\sigma}{d\Omega}\right)_{mag}$$

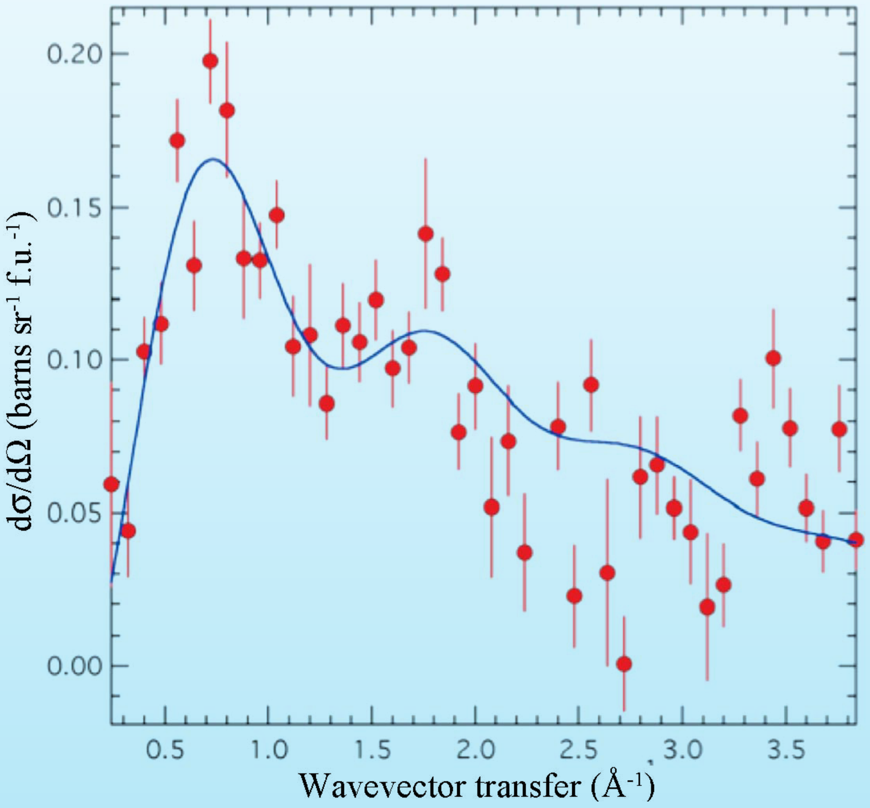
$$\left(\frac{d\sigma}{d\Omega}\right)_z^{SF} = \frac{2}{3}\left(\frac{d\sigma}{d\Omega}\right)_{SI} + \frac{1}{2}\left(\frac{d\sigma}{d\Omega}\right)_{mag}$$



α known as the Schärpf angle

Example: Volborthite





Volborthite measuredon D7 with an incident wavelength of 3.1Å.

The magnetic scattering is dwarfed by the enormous nuclear Bragg scattering for Q > 2 Å^{-1} and also by the nuclear spin-incoherent scattering due to hydrogen, and, to a lesser extent, vanadium, in the sample. (J. R. Stewart et al. J. Appl. Cryst. (2009) ***42****, 69–84)*

VII. Separation of coherent and incoherent scattering in uniaxial experiment

coh/incoh separation

Let I be the non-zero nuclear spin and let b_+ and b_- denote scattering lengths associated with the $I+\frac{1}{2}$ and $I-\frac{1}{2}$ compound states of the nucleus-neutron system. Let $\hat{B}$ denote the scattering length operator. Then let b_+ and b_- are its eigenvalues. It can be shown that:

$$\hat{B} = \bar{b} + \frac{1}{2} b_N \hat{\sigma} \cdot \hat{I}$$

Here $\hat{\sigma}$ is the Pauli spin operator and $\hat{I}$ is the nuclear spin operator. $\bar{b}$ and b_N are expressed in terms of b_+ and b_- through:

$$\bar{b} = \frac{(I+1)b_+ + I b_-}{2I+1} \qquad b_N = \frac{2(b_+ - b_-)}{2I+1}$$

Further calculations are carried out by means of the density matrix formalism, and lead to the expression for the differential nuclear scattering cross-section:

coh/incoh separation

$$\frac{d\sigma}{d\Omega} = Tr\left[\rho \hat{B}^{\dagger}\left(\hat{\sigma} \cdot \hat{I}^{\dagger}\right)\hat{B}\left(\hat{\sigma} \cdot \hat{I}\right)\right]$$

Let $\mathbf{s}_n$ denote the spin of an individual ("*n*-th") neutron in the ensemble $\left(|\mathbf{s}_n| = \frac{1}{2}\right)$, and let's define the beam polarization **P** as the ensemble average over all the neutron spin vectors, normalised to their modulus:

$$\mathbf{P} = \frac{\langle \mathbf{s}_n \rangle}{\frac{1}{2}} = 2\langle \mathbf{s}_n \rangle$$

In the presence of an external field, providing a natural quantization axis, the beam polarization becomes a scalar value:

$$P = \frac{N_+ - N_-}{N_+ + N_-}$$

where N_+ and N_- are the number of neutrons with spin-up and spin-down with respect to the field direction. R is the so called flipping, a measurable quantity:

$$R = \frac{N_+}{N_-} \qquad \text{so} \qquad R = \frac{R-1}{R+1}$$

coh/incoh separation

Now the differential cross section (2.21) can also be expressed as a function of incoming beam polarization :

$$\frac{d\sigma}{d\Omega} = \hat{B}^{\dagger}\hat{B}\left[I(I+1) + i\mathbf{P}^{(in)} \cdot \left(\hat{I}^{\dagger} \times \hat{I}\right)\right]$$

If nuclear spins are unpolarized, which is normally the case, averaging over nuclear spin orientations must be performed. Then, after taking into account the properties of the nuclear spin operator and $\hat{I}$, one obtains for the differential cross section :

$$\frac{d\sigma}{d\Omega} = I(I+1)\hat{B}^{\dagger}\hat{B}$$

and for the scattered polarization:

$$P_{\gamma}^{(out)}\frac{d\sigma}{d\Omega} = Tr\left[\rho\hat{B}^{\dagger}\left(\hat{\sigma}\cdot\hat{I}^{\dagger}\right)\gamma\left(\hat{\sigma}\cdot\hat{I}\right)\hat{B}\right]$$

where γ denotes a particular direction in space. Again, evaluation of the right-hand followed by averaging over nuclear spin orientation, gives:

$$P_{\gamma}^{(out)}\frac{d\sigma}{d\Omega} = -\frac{1}{3}P^{(in)}\,I(I+1)\hat{B}^{\dagger}\hat{B}$$

coh/incoh separation

Let us introduce the conventional notation $I^{\uparrow\downarrow}$ and $I^{\uparrow\uparrow}$ for the scattered intensity with and without the spin flip. Then:

$$\frac{d\sigma}{d\Omega} = I^{\uparrow\uparrow} + I^{\uparrow\downarrow} = I_\gamma^{\uparrow\uparrow} + I_\gamma^{\uparrow\downarrow}$$

and:

$$P_\gamma^{(out)} \frac{d\sigma}{d\Omega} = \frac{I^{\uparrow\uparrow} - I^{\uparrow\downarrow}}{I^{\uparrow\uparrow} + I^{\uparrow\downarrow}} \left(I^{\uparrow\uparrow} + I^{\uparrow\downarrow}\right) = I^{\uparrow\uparrow} - I^{\uparrow\downarrow}$$

Rewritting the previous result:

$$\frac{d\sigma}{d\Omega} = I^{\uparrow\uparrow} + I^{\uparrow\downarrow} = I(I+1)\hat{B}^\dagger \hat{B}$$

and:

$$P_\gamma^{(out)} \frac{d\sigma}{d\Omega} = \frac{I^{\uparrow\uparrow} - I^{\uparrow\downarrow}}{I^{\uparrow\uparrow} + I^{\uparrow\downarrow}} \left(I^{\uparrow\uparrow} + I^{\uparrow\downarrow}\right) = I^{\uparrow\uparrow} - I^{\uparrow\downarrow} = -\frac{1}{3}\, I(I+1)\hat{B}^\dagger \hat{B}$$

coh/incoh separation

Finally:

$$I^{\uparrow\uparrow} = \frac{1}{3}|B|^2 I(I+1) \quad \text{and} \quad I^{\uparrow\downarrow} = \frac{2}{3}|B|^2 I(I+1)$$

Thus the outgoing scattering intensity from unpolarized nuclear spins is always one third without, and two thirds with flip of the neutron spin from the polarized beam.

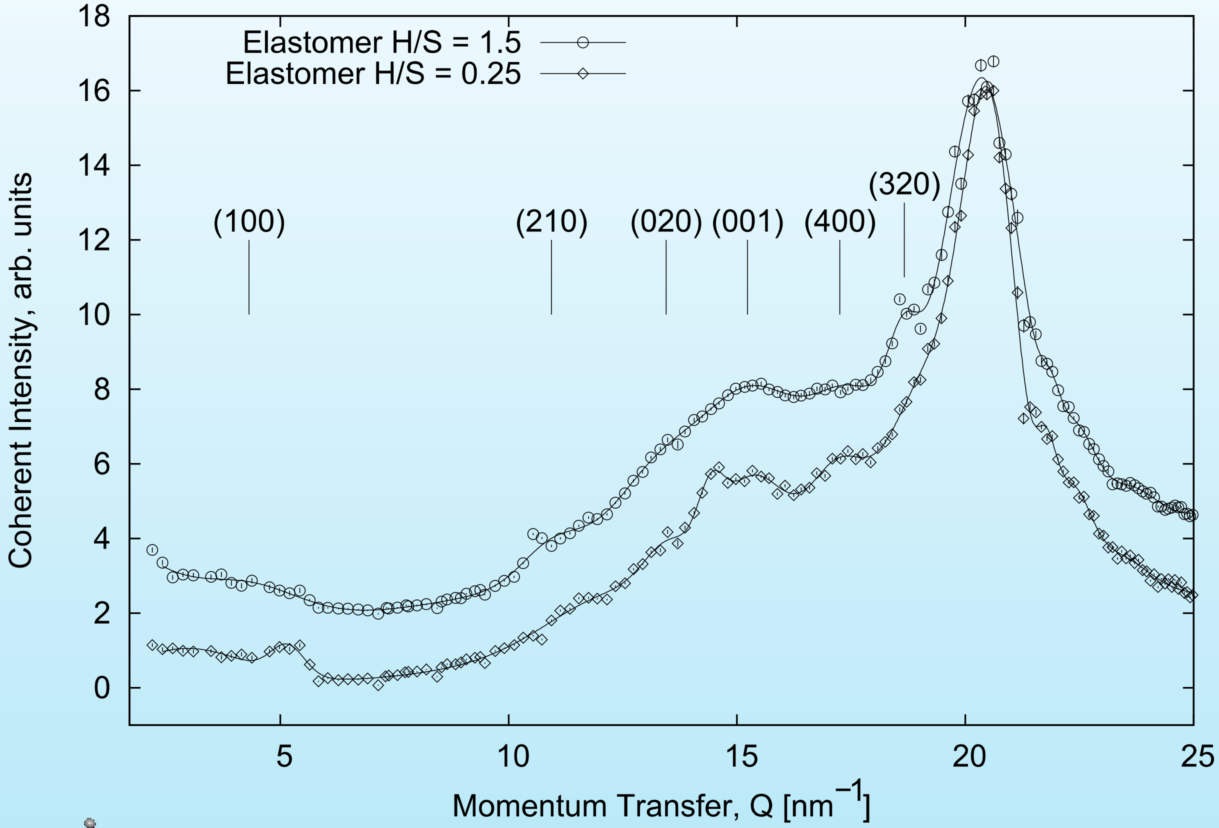
The coherent scattering Icoh and incoherent scattering Iinc are linearly related to the measured spin-flip and non-spin-flip scattering.

$$I_{coh} = I^{\uparrow\uparrow} - \frac{1}{2} I^{\uparrow\downarrow} \quad \text{and} \quad I_{inc} = \frac{3}{2} I^{\uparrow\downarrow}$$

In this way, shining a polarized neutron beam upon the sample and separately recording neutrons scattered with their spin conserved and with spin flipped, the experimenter can separate coherent from incoherent scattering right at the instrument level.

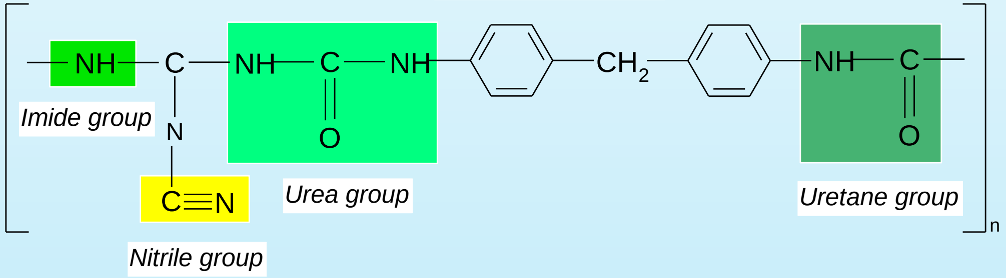
V. Real-life example

Example: residua strain in PU elastomer

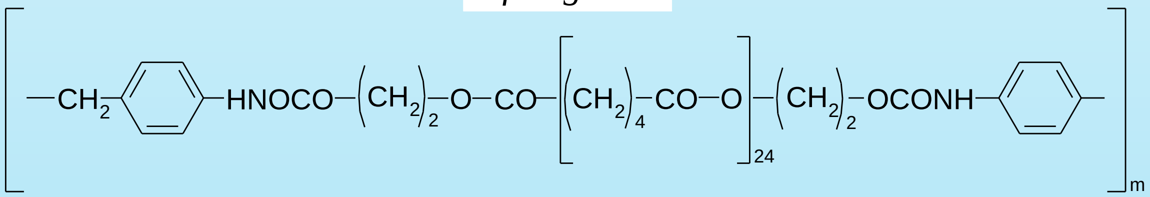


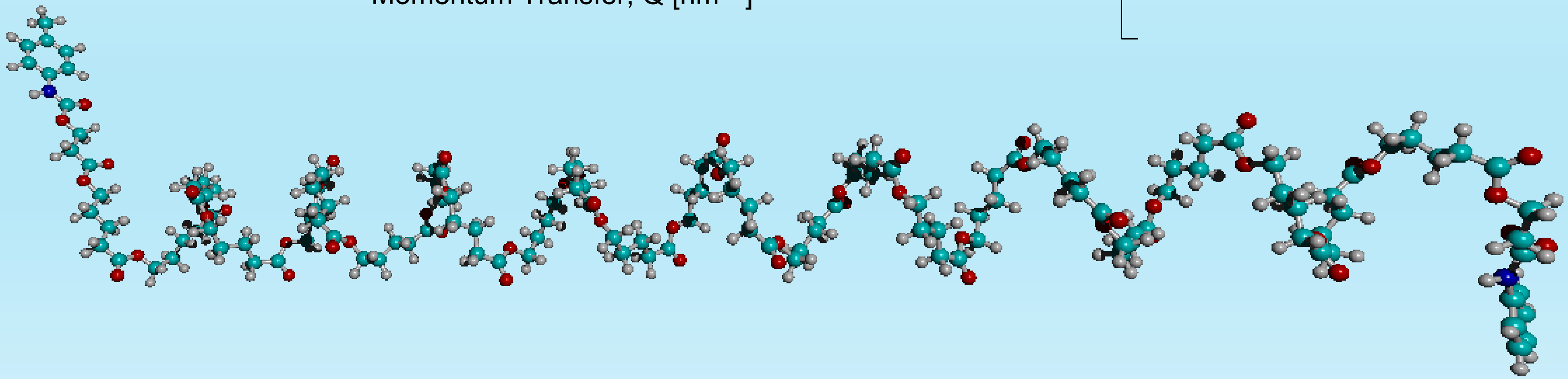
The peak @ $Q = 20.35\ \mathrm{nm}^{-1}$ originates most likely from the short-range arrangement of the soft segments

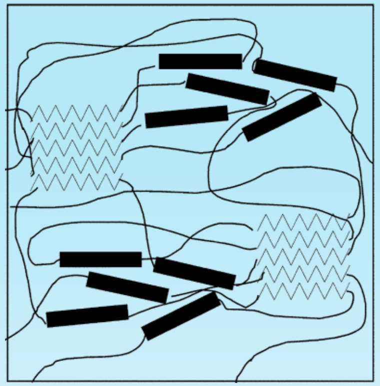
Hard segments



Soft segments







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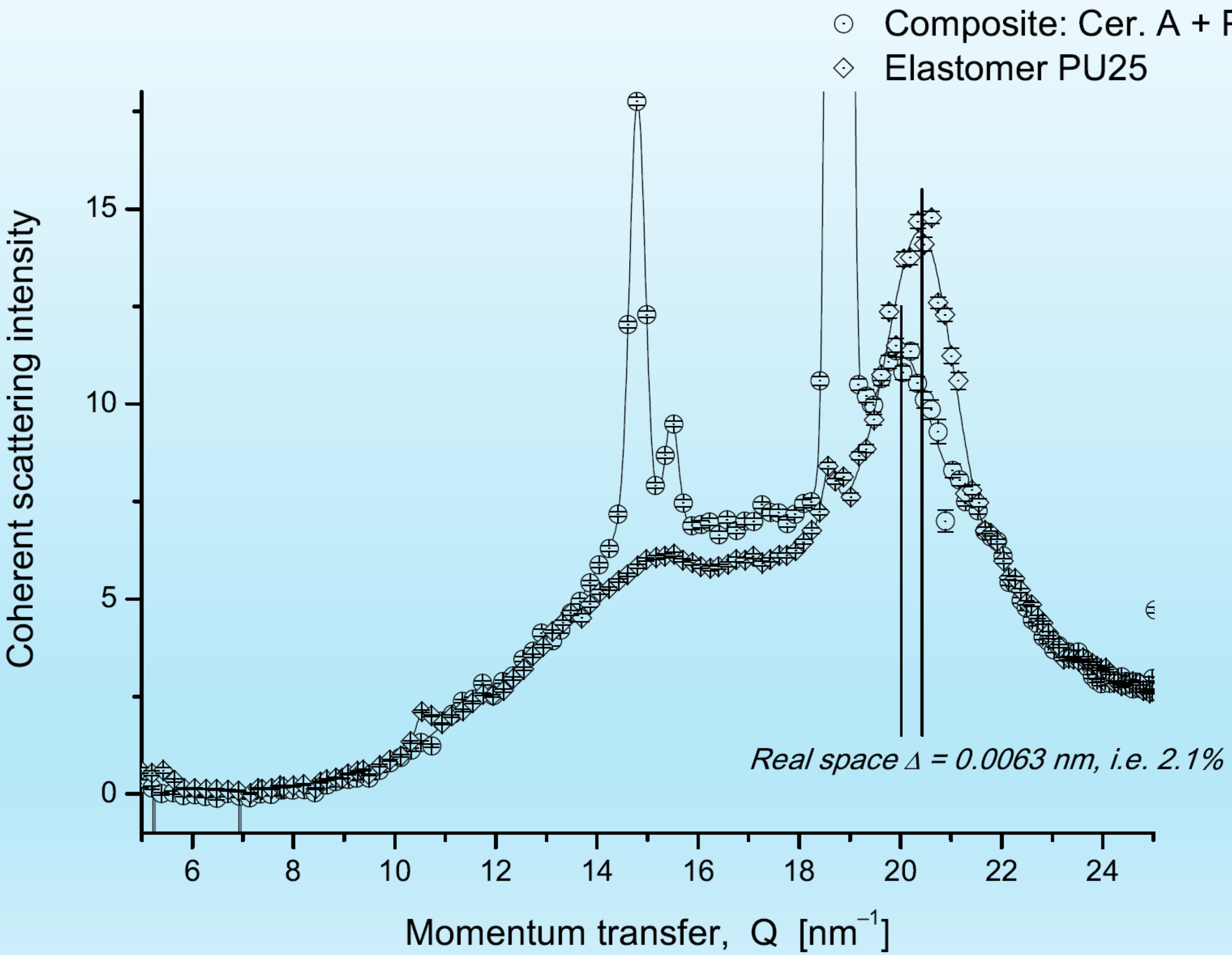

W. Zając, A. Boczkowska, K. Babski, K. Kurzydłowski, P. Deen, *Measurements of residual strains in ceramic–elastomer composites with diffuse scattering of polarized neutrons*, Acta Materialia. 56 (2008) 5964-5971