Polarization elements

by Otto Schärpf

First Summer School on Polarized Neutron Scattering

I. Two sorts of topics

1. *Polarizations*
   - *direct beam*
   - *scattered beam*
2. *Cross sections*
   - *elastic*
   - *inelastic*

} Question: is multi-detector possible?

I. Polarizations

1. *usual definition:* $\uparrow\downarrow$, $\vec{P} \| \vec{B}$
2. *precessing spin polarization* $\angle(\vec{P}, \vec{B}) \neq 0$
   - **most** *authors* **believe:** $P_{\perp \vec{B}}$ *lost*
     only Cryopad or mu-metal shield avoids it: zero field
   - **but:** *spin echo uses it, even broad band* λ
   - **we will see:** *completely measurable with classical PA instruments with small modification (SSPAD)*

I. *Cross sections*

1. *Transition probability method*
   special problems treated:
   - *quantization axis in x,y,z and Pauli spin matrices (always in z)?*
   - *for every combination of spin in and out, direction and flip, special cross section i.e. transition probability to calculate.*
2. *Density matrix method (representation independend, much simpler)*

II. Our method of presentation:

1. *not systematically*
2. *but by experimenting with the spin of the neutrons*
   - *describing the tools when needed*
   - *immediately use the tools*

Such tools are

1. *mathematically:*
   - *spinor*
   - *rotation operator in spinor space*
   - *time dependent Schrödinger equation*
   - *density matrix*

2. *experimentally*
   - *using spinor: tool and application*
     - *precession coil: preparation of spin in* ϑ, φ
     - π*-flipper: polarization measurement for* $\vec{P} \| \vec{B}$
     - $\pi/2$*-flipper: polarization measurement for precessing spin*
     - *adiabatic spin rotator*
   - *using density matrix*

     1. *Description of the tool*
        - *why density matrix formalism describes physics*

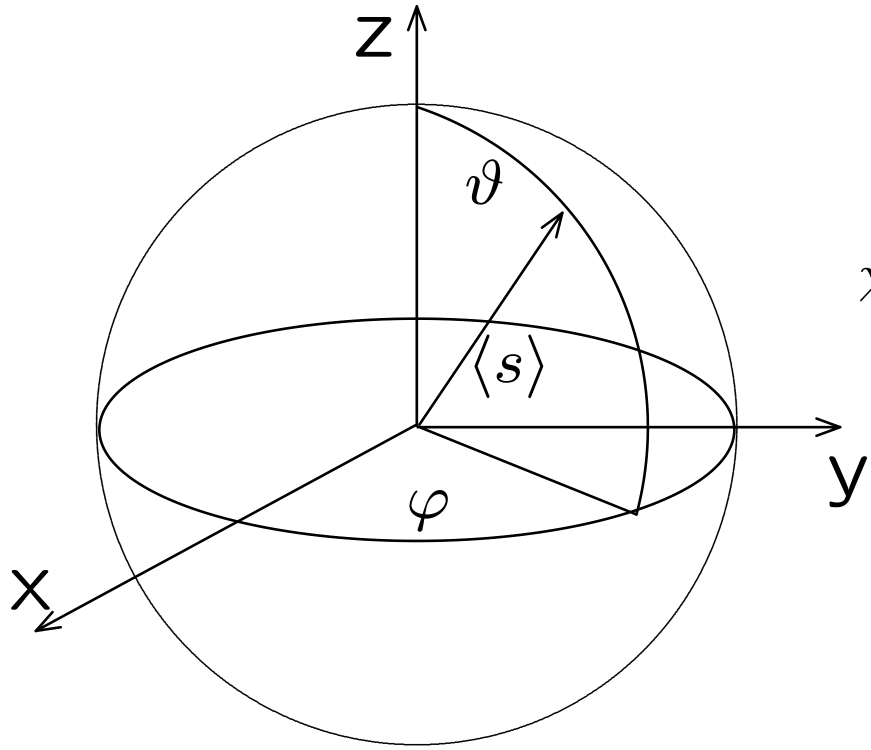
        - *why it is useful*
          - *it is simple (compared with transition probability method*

          - *it is powerful (some formal rules deliver* $d\sigma/d\Omega$ *and* P_{ij}*)*

2. *Applications of this tool:*
   - *spinless target (used for: flipping ratio correction)*
   - *nuclear spin incoherence (used for: calibration (absolute cross sections))*
   - *magnetic scattering*
     * *paramagnetic scattering*
     * *general formulae (magnetic only)*
     * *interference terms*
     * *multidetector application*

Lots of problems are left: to solve by applying the given tools creatively (not just repeating what others wrongly said.)

Polarization and Spinor



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

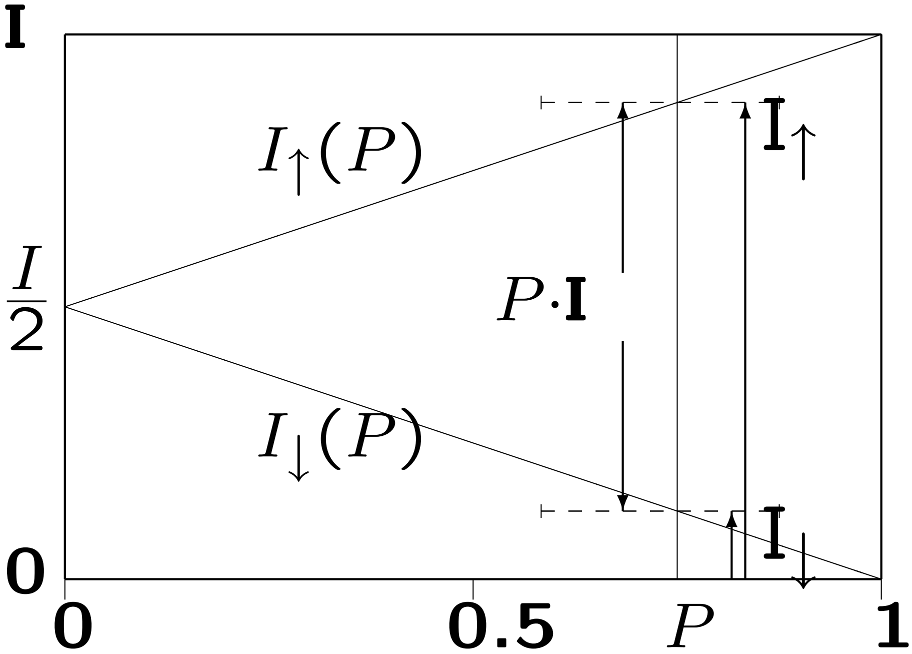
$$\begin{aligned} (\langle s_x\rangle, \langle s_y\rangle, \langle s_z\rangle) &= \frac{\hbar}{2}(\chi^\dagger\sigma_x\chi, \chi^\dagger\sigma_y\chi, \chi^\dagger\sigma_z\chi) \\ &= \frac{\hbar}{2}(\cos\varphi\sin\vartheta, \sin\varphi\sin\vartheta, \cos\vartheta) \end{aligned}$$

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

etc.

Degree of polarization?

Polarization and density matrix



$$P = \frac{I_\uparrow - I_\downarrow}{I_\uparrow + I_\downarrow}$$

Ensemble of pure and mixed states: $\rho = \chi\chi^\dagger$ dyadic product of $\chi = \binom{c_1}{c_2}$ and $\chi^\dagger = (c_1^*, c_2^*)$ or $\sum_m |m\rangle\langle m|$:

$$\begin{aligned}\rho &= \begin{pmatrix} c_1 \\ c_2 \end{pmatrix}(c_1^*, c_2^*) = \begin{pmatrix} |c_1|^2 & c_2^* c_1 \\ c_1^* c_2 & |c_2|^2 \end{pmatrix} = \frac{1}{2}\left(\underline{1} + \vec{P}\cdot\underline{\vec{\sigma}}\right) \\ &= \frac{1}{2}\begin{pmatrix} 1+P_z & P_x - iP_y \\ P_x + iP_y & 1 - P_z \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1+\cos\vartheta & \sin\vartheta e^{-i\varphi} \\ \sin\vartheta e^{i\varphi} & 1-\cos\vartheta \end{pmatrix}\end{aligned}$$

properties: $\mathrm{Tr}\rho = \sum_{i=1}^2 \rho_{ii} = |c_1|^2 + |c_2|^2 = 1$

$\rho^\dagger = \rho$ i.e. ρ is Hermitian.

$|c_1|^2 = \frac{1}{2}(1+P_z) \quad |c_2|^2 = \frac{1}{2}(1-P_z)$

$P_z = |c_1|^2 - |c_2|^2$

$P_x = c_1^* c_2 + c_2^* c_1 = 2\Re\left(c_1^* c_2\right) = 2\Re\left(c_2^* c1\right)$

$P_y = c_1^* c_2 - c_2^* c1 = 2\Im\left(c_1^* c_2\right) = 2\Im\left(c_2^* c1\right)$

The ensemble average of an operator A (also called expectation value, but not to be mixed up with the quantum mechanical expectation value) is $\langle A \rangle$.

$$\begin{aligned}
\langle A \rangle &= (c_1^*, c_2^*) \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} \\
&= (c_1^*, c_2^*) \begin{pmatrix} A_{11}c_1 + A_{12}c_2 \\ A_{21}c_1 + A22c_2 \end{pmatrix} \\
&= A_{11}c_1^*c_1 + A_{12}c_1^*c_2 + A_{21}c_1c_2^* + A_{22}c_2c_2^* \\
&= \text{Tr} \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} \begin{pmatrix} c_1c_1^* & c_1c_2^* \\ c_1^*c_2 & c_2c_2^* \end{pmatrix} \\
&= \text{Tr} \begin{pmatrix} A_{11}c_1c_1^* + A_{12}c_1^*c_2 & A_{11}c_1c_2^* + A_{12}c_2c_2^* \\ A_{21}c_1c_1^* + A_{22}c_1^*c_2 & A_{21}c_1c_2^* + A_{22}c_2c_2^* \end{pmatrix} \\
&= \text{Tr}(A\rho) = \text{Tr}(\rho A)
\end{aligned}$$

Trace does not depend on the representation. $\text{Tr}(\rho A)$ can be evaluated using any convenient basis.

$$\boxed{\langle A \rangle = \text{Tr}(\rho A) = \text{Tr}(A\rho)}$$

Examples: $\text{Tr}\rho < 1$ then $\rho = \sum_m |m\rangle p_m \langle m|$.

completely polarized $\vec{P} = (0,0,1)$ $\rho = |+\rangle\langle +| = \begin{pmatrix} 1 \\ 0 \end{pmatrix} (1,0) = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$

completely polarized $\vec{P} = (\pm 1, 0, 0)$

$$\rho = \frac{1}{2} \begin{pmatrix} 1+\cos\vartheta & \sin\vartheta e^{-i\varphi} \\ \sin\vartheta e^{i\varphi} & 1-\cos\vartheta \end{pmatrix} = \begin{pmatrix} \frac{1}{2} & \pm\frac{1}{2} \\ \pm\frac{1}{2} & \frac{1}{2} \end{pmatrix}$$

unpolarized $\vec{P} = 0$ $\rho = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix}$

partially polarized consisting of 50% in +x-direction and 50% in +y-direction

$$\rho = 0.5 \cdot \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{pmatrix} + 0.5 \cdot \begin{pmatrix} \frac{1}{2} & -\frac{i}{2} \\ \frac{i}{2} & \frac{1}{2} \end{pmatrix} = \begin{pmatrix} \frac{1}{2} & \frac{1-i}{4} \\ \frac{1+i}{4} & \frac{1}{2} \end{pmatrix}$$

this corresponds to degree of P=$1/\sqrt{2} = 0.70$ direction (1,1,0).

<u>Determine the polarization</u> for this mixture using $\mathrm{Tr}(\rho\sigma)$ (example for ensemble average)

$$\langle \sigma_x \rangle = \mathrm{Tr}(\rho\sigma_x) = \mathrm{Tr} \begin{pmatrix} \frac{1}{2} & \frac{1-i}{4} \\ \frac{1+i}{4} & \frac{1}{2} \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$= \mathrm{Tr} \begin{pmatrix} \frac{1-i}{4} & \frac{1}{2} \\ \frac{1}{2} & \frac{1+i}{4} \end{pmatrix} = \frac{1}{2}$ and similarly $\langle \sigma_y \rangle = \frac{1}{2}$ and $\langle \sigma_z \rangle = 0$

$\vec{P} = (\frac{1}{2}, \frac{1}{2}, 0)$ i.e. $|P| = 1/\sqrt{2}$

<u>**Determine ρ for equally distributed P**</u> over range $\Phi = -\pi/10$ to $\Phi = \pi/10$, $\vartheta = \pi/2$

$$2\rho = \begin{pmatrix} 1 & \langle e^{-i\phi} \rangle \\ \langle e^{i\phi} \rangle & 1 \end{pmatrix} \approx \begin{pmatrix} 1 & e^{\frac{-\langle \phi^2 \rangle}{2}} \\ e^{\frac{-\langle \phi^2 \rangle}{2}} & 1 \end{pmatrix} = \begin{pmatrix} 1 & 0.98 \\ 0.98 & 1 \end{pmatrix}$$

$$\langle e^{i\phi} \rangle = \langle \cos\phi \rangle + i \langle \sin\phi \rangle = \langle \cos\phi \rangle + 0$$
$$= 1 - \frac{1}{2}\langle \phi^2 \rangle + \frac{1}{4!}\langle \phi^4 \rangle \dots$$

$$e^{-\frac{\langle \phi^2 \rangle}{2}} = 1 - \frac{1}{2}\langle \phi^2 \rangle + \frac{1}{8}\langle \phi^2 \rangle^2 \dots$$

$$\langle \phi^2 \rangle = \frac{5}{\pi} \int_{-\pi/10}^{\pi/10} \phi^2 d\phi = \frac{5}{\pi} \cdot \frac{2}{3} \left(\frac{\pi}{10}\right)^3 \approx 0.032898$$

Other useful relations: $\rho|\phi\rangle = |\chi\rangle\langle\chi|\phi\rangle = \langle\chi|\phi\rangle|\chi\rangle$

$\rho^2 = \rho \quad$ if ρ is a pure state; $\vec{P}\underline{\sigma}\chi = (2\rho - 1)\chi = 2\rho\chi - \chi = 2\chi\chi^\dagger\chi - \chi = 2\chi - \chi = \chi$ i.e. $\vec{P} \| \vec{S}$

1. Time dependence of ρ

$$
\begin{aligned}
i\hbar\frac{\partial\chi}{\partial t} &= H\chi \\
\frac{\partial\rho}{\partial t} &= \frac{\partial\chi}{\partial t}\chi^\dagger + \chi\frac{\partial\chi^\dagger}{\partial t} = \frac{1}{i\hbar}(H\chi\chi^\dagger - \chi\chi^\dagger H \\
i\hbar\frac{\partial\rho}{\partial t} &= H\rho - \rho H = [H,\rho]
\end{aligned}
$$

2. Time dependence of $\vec{P}$ in field $\vec{B}$

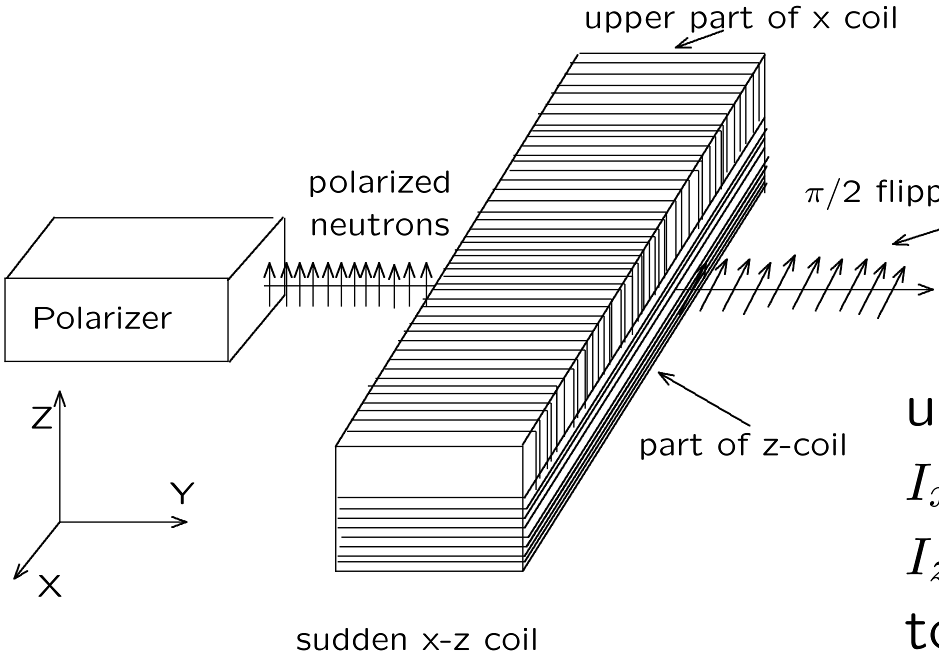
$$
\begin{aligned}
H &= \frac{1}{2}(B_0\binom{10}{01} + \vec{B}\cdot\vec{\sigma}) \\
\frac{\partial\vec{P}}{\partial t} &= \frac{\partial\langle\vec{\sigma}\rangle}{\partial t} = \frac{1}{2i\hbar}\langle\vec{\sigma}H - H\vec{\sigma}\rangle = \frac{1}{2i\hbar}\langle\vec{\sigma}(\vec{B}\cdot\vec{\sigma}) - (\vec{B}\cdot\vec{\sigma})\vec{\sigma}\rangle \\
&= \frac{1}{2i\hbar}\langle\vec{B}\times(\vec{\sigma}\times\vec{\sigma})\rangle = \frac{1}{\hbar}\vec{B}\times\langle\vec{\sigma}\rangle \text{ with } \sigma\times\sigma = 2i\sigma \\
\hbar\frac{\partial\vec{P}}{\partial t} &= \vec{B}\times\vec{P} \text{ equation of the precession of } \vec{P} \text{ in field } \vec{B}
\end{aligned}
$$

3. Polarization of a statistical ensemble of N systems

each system has its own spinor χ_ν and its own density matrix ρ_ν

$$
\begin{aligned}
\overline{\rho} &= \frac{1}{N}\sum_{\nu=1}^{N}\rho_\nu = \frac{1}{2}[(\underline{1} + ((\frac{1}{N}\sum_\nu P_\nu)\cdot\sigma))] = \frac{1}{2}(\underline{1} + (\overline{P}\cdot\sigma)) \\
\overline{\langle A\rangle} &= \frac{1}{N}\sum_{\nu=1}^{N}\langle A\rangle_\nu = \frac{1}{N}\sum_{\nu=1}^{N}\mathrm{Tr}_\sigma(\rho_\nu A) = \mathrm{Tr}(\overline{\rho}A) \\
\overline{P} &= \overline{\langle\sigma\rangle} = \frac{1}{N}\sum_{\nu=1}^{N}\langle\vec{\sigma}\rangle_\nu = \frac{1}{N}\sum \mathrm{Tr}(\rho_\nu\sigma) = \frac{1}{2}\mathrm{Tr}_\sigma[(\underline{1} + \overline{P}\cdot\sigma)\sigma]
\end{aligned}
$$

Precession coil to rotate spinor into any direction Θ,Φ

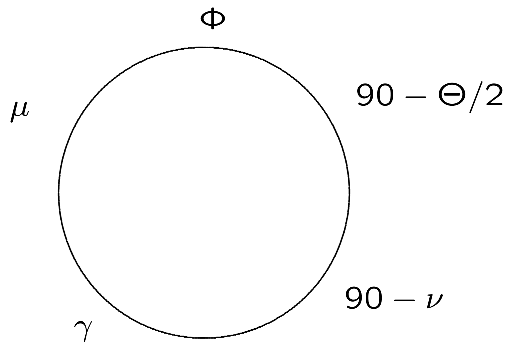


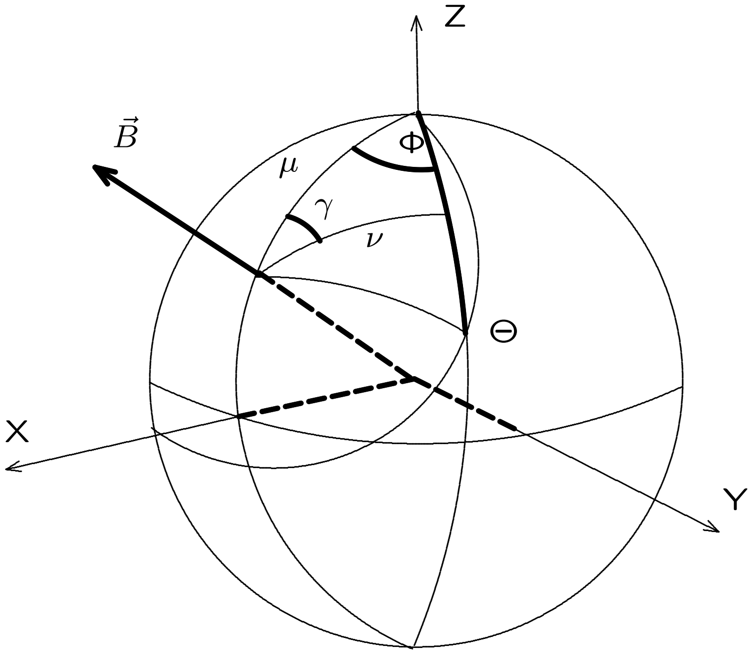
use $I = I_\pi * \frac{2\gamma}{\pi}$

$I_x = I \sin \mu$

$I_z = (I - I_c) \cos \mu$

to get spin in Θ,Φ





Nepers rule gives

$\cos \Phi = \cot \mu \cdot \cot(90 - \frac{\Theta}{2})$

$= \frac{\tan \frac{\Theta}{2}}{\tan \mu}$

$\tan \mu = \frac{\tan \frac{\Theta}{2}}{\cos \Phi}$

$\cos \gamma = \sin \Phi \cdot \cos \frac{\Theta}{2}$

Adjust the coil as π-flipper gives $I_{c(ompensation)}$, I_π

Rotation in spinor space.

Rotation around the z-axis by an angle φ

$$e^{i\frac{\varphi}{2}\sigma_z} \equiv \begin{pmatrix} e^{i\frac{\varphi}{2}} & 0 \\ 0 & e^{-i\frac{\varphi}{2}} \end{pmatrix}$$

this identity is valid

$$e^{i\frac{\varphi}{2}\sigma_z} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + i\frac{\varphi}{2}\sigma_z + i^2\frac{\varphi^2}{4}\cdot\frac{1}{2!}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \frac{i^3\varphi^3}{2^3\cdot 3!}\sigma_z + \frac{i^4\varphi^4}{2^4\cdot 4!}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} =$$
$$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\cos\frac{\varphi}{2} + i\sigma_z\sin\frac{\varphi}{2} = \begin{pmatrix} \cos\frac{\varphi}{2} + i\sin\frac{\varphi}{2} & 0 \\ 0 & \cos\frac{\varphi}{2} - i\sin\frac{\varphi}{2} \end{pmatrix} =$$
$$\begin{pmatrix} e^{i\frac{\varphi}{2}} & 0 \\ 0 & e^{-i\frac{\varphi}{2}} \end{pmatrix}$$

it represents a rotation

$$e^{i\frac{\gamma}{2}\sigma_z}\begin{pmatrix} \cos\frac{\vartheta}{2}e^{-i\frac{\varphi}{2}} \\ \sin\frac{\vartheta}{2}e^{i\frac{\varphi}{2}} \end{pmatrix} = \begin{pmatrix} e^{i\frac{\gamma}{2}} & 0 \\ 0 & e^{-i\frac{\gamma}{2}} \end{pmatrix}\begin{pmatrix} \cos\frac{\vartheta}{2}e^{-i\frac{\varphi}{2}} \\ \sin\frac{\vartheta}{2}e^{i\frac{\varphi}{2}} \end{pmatrix} = \begin{pmatrix} \cos\frac{\vartheta}{2}e^{-i\frac{(\varphi-\gamma)}{2}} \\ \sin\frac{\vartheta}{2}e^{i\frac{(\varphi-\gamma)}{2}} \end{pmatrix}$$

This shows that application of $e^{i\frac{\gamma}{2}\sigma_z}$ diminishes φ i.e. a rotation around the z axis in the clockwise sense.

Rotation about x axis

$$e^{i\frac{\chi}{2}\sigma_x} = \underline{1}\cos\frac{\chi}{2} + i\sigma_x\sin\frac{\chi}{2} = \begin{pmatrix} \cos\frac{\chi}{2} & i\sin\frac{\chi}{2} \\ i\sin\frac{\chi}{2} & \cos\frac{\chi}{2} \end{pmatrix}$$

rotation about the y axis

$$e^{i\frac{\mu}{2}\sigma_y} = \underline{1}\cos\frac{\mu}{2} + i\sigma_y\sin\frac{\mu}{2} = \begin{pmatrix} \cos\frac{\mu}{2} & \sin\frac{\mu}{2} \\ -\sin\frac{\mu}{2} & \cos\frac{\mu}{2} \end{pmatrix}$$

$$\begin{pmatrix} \cos\frac{\mu}{2} & \sin\frac{\mu}{2} \\ -\sin\frac{\mu}{2} & \cos\frac{\mu}{2} \end{pmatrix}\begin{pmatrix} \cos\frac{\vartheta}{2}e^{-i\frac{\varphi}{2}} \\ \sin\frac{\vartheta}{2}e^{i\frac{\varphi}{2}} \end{pmatrix} = \begin{pmatrix} \cos\frac{\vartheta-\mu}{2}\cos\frac{\phi}{2} + i\cos\frac{\vartheta+\mu}{2}\sin\frac{\phi}{2} \\ \sin\frac{\vartheta-\mu}{2}\cos\frac{\phi}{2} + i\sin\frac{\vartheta+\mu}{2}\sin\frac{\phi}{2} \end{pmatrix}$$

Generally **rotation operator around axis $\vec{n}$ by angle ω**

$$
\begin{aligned}
e^{i\frac{\omega}{2}\vec{n}\cdot\vec{\sigma}} &= \underline{1}\cos\frac{\omega}{2} + i\sin\frac{\omega}{2}\vec{n}\cdot\vec{\sigma} \\
&= \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\cos\frac{\omega}{2} + i\sin\frac{\omega}{2}\begin{pmatrix} \cos\vartheta & \sin\vartheta e^{-i\varphi} \\ \sin\vartheta e^{i\varphi} & -\cos\vartheta \end{pmatrix}
\end{aligned}
$$

with

$$\vec{n} = (\cos\varphi\sin\vartheta, \sin\varphi\sin\vartheta, \cos\vartheta)$$

Spin in homogeneous magnetic field

$\vec{B} = B\vec{n}$ and $\omega_L = 2\mu B/\hbar$

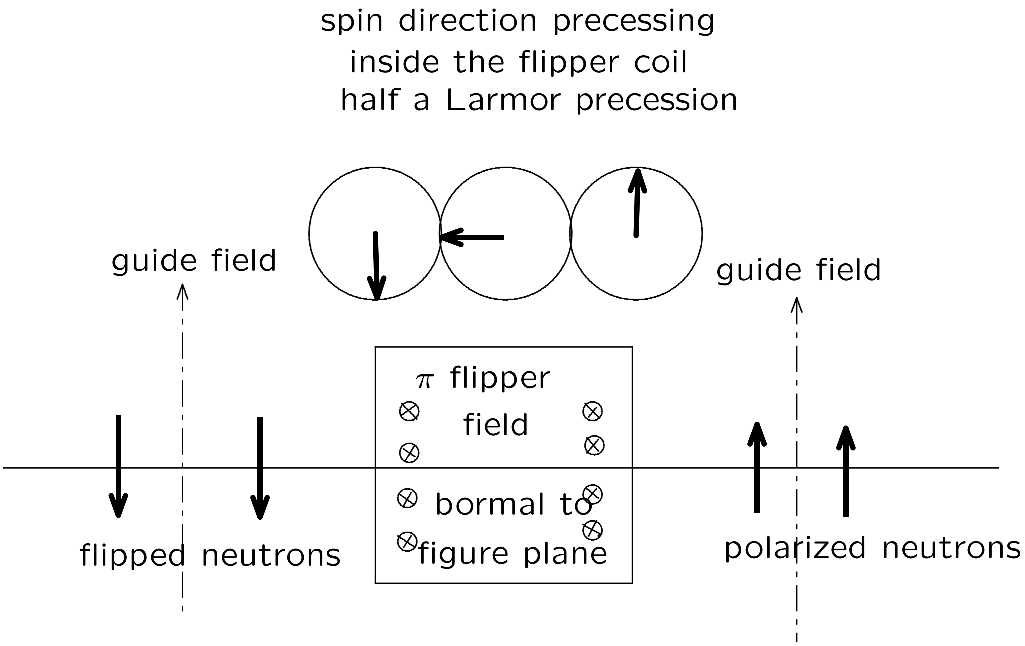
$$
\begin{aligned}
i\hbar\frac{\partial}{\partial t}\begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} &= \mu\vec{\sigma}\cdot\vec{B}\begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = \mu B(\vec{\sigma}\cdot\vec{n})\begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} \\
\frac{\partial}{\partial t}\begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} &= -i\frac{\omega_L}{2}\begin{pmatrix} \cos\vartheta & \sin\vartheta e^{-i\varphi} \\ \sin\vartheta e^{i\varphi} & \cos\vartheta \end{pmatrix}\begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}
\end{aligned}
$$

Separation of variables and integration yields

$$\begin{pmatrix} \psi_1(t) \\ \psi_2(t) \end{pmatrix} = e^{-i\frac{\omega_L t}{2}\vec{\sigma}\cdot\vec{n}}\begin{pmatrix} \psi_1(0) \\ \psi_2(0) \end{pmatrix}$$

This is a rotation of $\omega_L t$ around the axis $\vec{n}$, i.e. around the field $\vec{B}$ (precession). $\Longrightarrow$ **Precessing spin polarization**

Behaviour of the spin in a π flipper coil



Half a Larmor precession as a π-flipper

Currents in the xz-sudden-coil= Adjustment of the flipper currents

1. *first calculating the necessary current for half a Larmor precession for the pathlength L in the x-coil and the wavelength λ of the neutrons by* $H_\pi = \frac{67.825}{\lambda[nm]L[cm]}$ *mT*
2. *With this current in x-coil: current scan for the z-field to find the minimum count rate (compensates the guide field).*
3. *Fit a parabola the minimum of which is the best correction current. (Advantage: it uses also higher count rates)*
4. *iterate this for x and z coil until no change*

● only field in x-direction inside the coil ($\vartheta = 90^0$ and $\varphi = 0^0$). (guide field in z-direction compensated by z-coil)

●behaviour of the spin $|+> = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ inside the coil

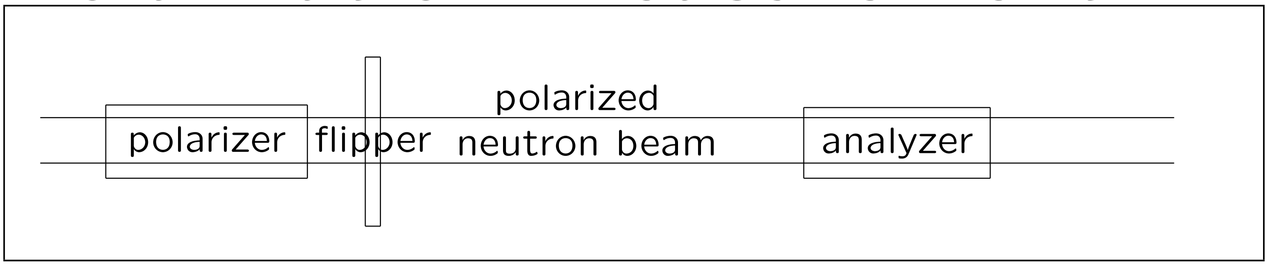
$$\begin{pmatrix} \psi_1(t) \\ \psi_2(t) \end{pmatrix} = e^{-i\frac{\omega_L t}{2}\sigma_x} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = e^{i\frac{\pi}{4}} \begin{pmatrix} \cos\frac{\omega_L t}{2} e^{-i\frac{\pi}{4}} \\ \sin\frac{\omega_L t}{2} e^{i\frac{\pi}{4}} \end{pmatrix}$$

i.e. spinor with ϑ changing, $\varphi = \pi/2$ fixed

● this is a precession of an incident spin $|+>$ around the x-axis in the y-z plane with the time dependent angle $\omega_L t$.

1. *with $\omega_L t = \pi$ neutron exits from the coil in reversed direction of the guide field on the outside of the coil.*
2. *This is exactly the behaviour of a* **flipper coil**.
3. *Entrance and exit from the coil: sudden transitions, the neutron remains in its state that it had before.*

Polarization measurement



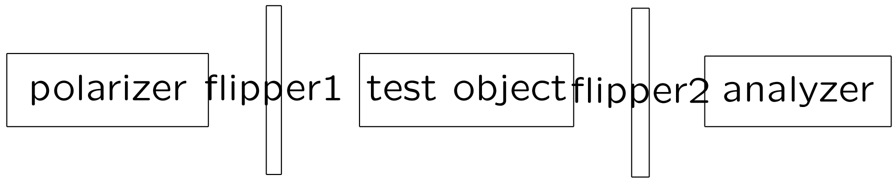
Determine the degree of polarization using flipper and analyzer

1. *measure count rate $I^{\uparrow}$ with spin not flipped*
2. *the intensity $I^{\downarrow}$ with spin flipped.*
3. *Their ratio (after background subtraction) gives the flipping ration $R = I^{\uparrow}/I^{\downarrow}$*
4. *and the polarization $P = (R-1)/(R+1)$.*

Cannot measure precessing spin polarization, only not precessing component.

Polarizing efficiency, flipper efficiency

Can be needed for correction purposes (see later)



Measurement of 1. polarizer efficiency in the position "test object". 2. the flipper efficiencies (no test object present)

1. *The* **polarizing efficiency P** *is the degree of polarization attained by an unpolarized beam on passing through the polarizer.*

2. *The* **flipper efficiency f** *can be defined as the fraction of spins reversed by the flipper.*

1. *The properties of a flipper can be given by a matrix representation as*

$$\underline{\underline{F}} = \begin{pmatrix} \epsilon & 1-\epsilon \\ 1-\epsilon & \epsilon \end{pmatrix}$$

2. *the properties of a polarizer by the matrix representation*

$$\begin{pmatrix} P_{11} & P_{12} \\ P_{21} & P_{22} \end{pmatrix}$$

.

- P_{11} *gives the part of the incident beam which is transmitted without spin change. measured without flipper current*
- P_{12} *gives the part of the beam that is flipped from spin down to spin up. with flipper 1*
- P_{21} *the part flipped from spin up to spin down with flipper 2 ($P_{21} \neq P_{12}$ shows error in measurement)*
- P_{22} *is the part of spin down wich remains in spin down when transmitted through the polarizer. with both flippers.*

3. *Polarizer efficiency from*

$$\begin{pmatrix} A \\ B \end{pmatrix} = \frac{1}{\sqrt{2}} \cdot \begin{pmatrix} P_{11} + P_{12} \\ P_{21} + P_{22} \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} P_{11} & P_{12} \\ P_{21} & P22 \end{pmatrix} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

as the polarization from an unpolarized beam $\binom{1}{1}$

$$P = \frac{P_{11} + P_{12} - P_{21} - P_{22}}{P_{11} + P_{12} + P_{21} + P_{22}} = \frac{A - B}{A + B}$$

Determine flipper efficiency A flipper behind such a polarizer changes the spin of this beam in the following way:

$$\begin{pmatrix} A_f \\ B_f \end{pmatrix} = \begin{pmatrix} \epsilon & 1-\epsilon \\ 1-\epsilon & \epsilon \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} A\epsilon + B(1-\epsilon) \\ A(1-\epsilon) + B\epsilon \end{pmatrix}$$

with the polarization

$$P_f = \frac{A\epsilon + B(1-\epsilon) - A(1-\epsilon) - B\epsilon}{A\epsilon + B(1-\epsilon) + A(1-\epsilon) + B\epsilon}$$

$$= \frac{(1-2\epsilon)(B-A)}{A+B} = -(1-2\epsilon)P$$

With a second flipper (characterized by ϵ' instead of ϵ) one obtains for the flipper matrix of two flippers

$$\begin{pmatrix} \epsilon' & 1-\epsilon' \\ 1-\epsilon' & \epsilon' \end{pmatrix} \begin{pmatrix} \epsilon & 1-\epsilon \\ 1-\epsilon & \epsilon \end{pmatrix}$$

$$= \begin{pmatrix} 1-(\epsilon+\epsilon'-2\epsilon\epsilon') & \epsilon+\epsilon'-2\epsilon\epsilon' \\ \epsilon+\epsilon'-2\epsilon\epsilon' & 1-(\epsilon+\epsilon'-2\epsilon\epsilon') \end{pmatrix}$$

which has the same form as for one flipper, only with $\epsilon_{eff} = \epsilon + \epsilon' - 2\epsilon\epsilon'$ and using the same steps as above one obtains for the spinor after a polarizer and the two flippers

$$\begin{pmatrix} -(A-B)(\epsilon+\epsilon'-2\epsilon\epsilon') + A \\ (A-B)(\epsilon+\epsilon'-2\epsilon\epsilon') + B \end{pmatrix}$$

with the polarization

$$P_{ff'} \;=\; P[1 - 2(\epsilon + \epsilon' - 2\epsilon\epsilon')] \quad \text{with}$$

$$P = \frac{A - B}{A + B}$$

The analyzer always measures the spin up component. This yields countrates as

$$\begin{aligned} I^{\uparrow\uparrow} &= A \\ I^{\downarrow\uparrow} &= A\epsilon + B(1-\epsilon) \\ I^{\uparrow\downarrow} &= A\epsilon' + B(1-\epsilon') \\ I^{\downarrow\downarrow} &= A - (A-B)\epsilon_{eff} \end{aligned}$$

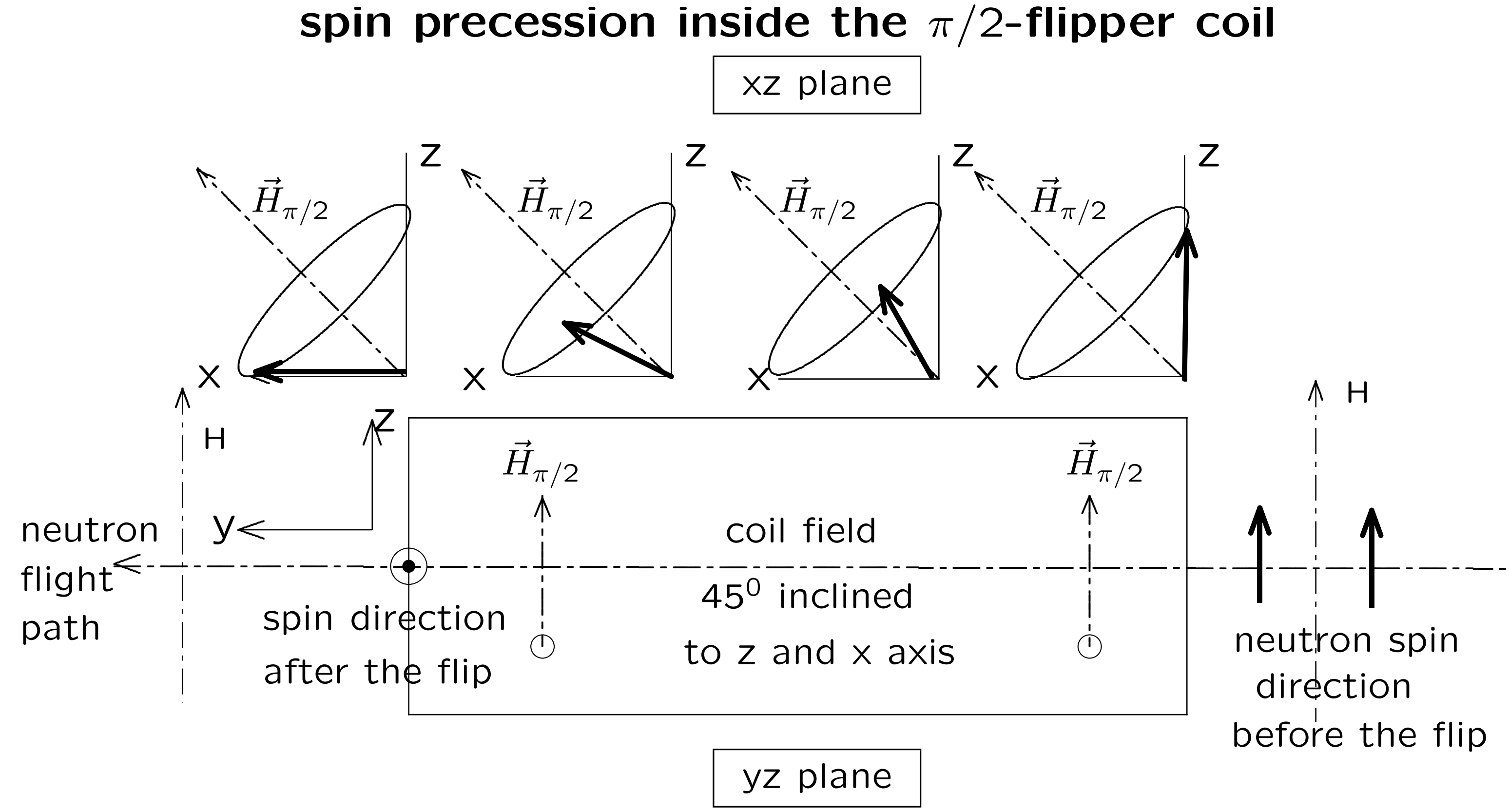
Combining these measured values one obtains the flipper efficiency:

$$\begin{aligned} \frac{I^{\uparrow\uparrow} - I^{\downarrow\downarrow}}{I^{\uparrow\uparrow} - I^{\uparrow\downarrow}} &= \frac{(A-B)\epsilon_{eff}}{(A-B)(1-\epsilon)} \\ &= \frac{\epsilon' + \epsilon - 2\epsilon\epsilon'}{1-\epsilon} \\ &= \frac{2\epsilon - 2\epsilon^2}{1-\epsilon} = 2\epsilon \end{aligned}$$

with the assumption that $\epsilon = \epsilon'$. One can measure these quantities for the polarizer and the analyzer and in this way come to very precise results.

$\pi/2$-flipper and its use

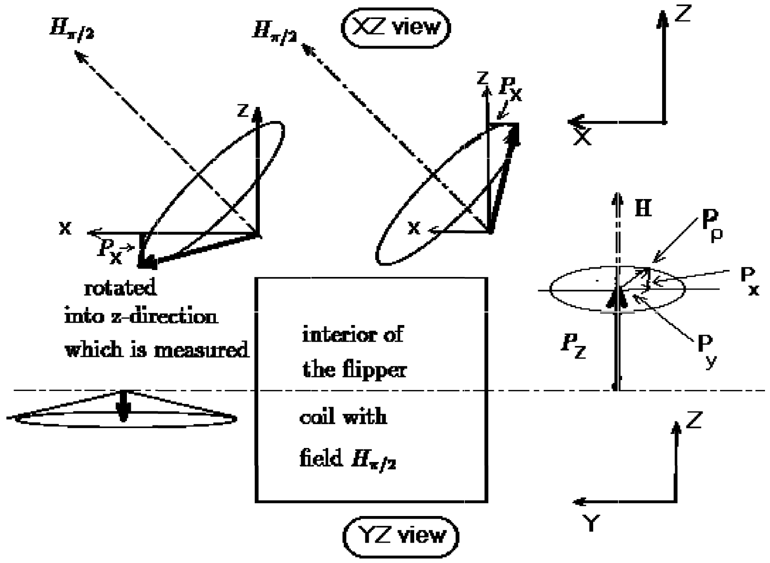
Behaviour of the neutron in a $\pi/2$ flipper



Adjustment of the currents in a $\pi/2$-flipper

1. *Used set-up: polarizer, xz-coil, flipper, analyzer.*
2. *Adjust the xz-coil as a π-flipper: gives the current for H_π.*
3. *Set the x-coil field for the $\pi/2$ coil to $H_\pi/\sqrt{(}2)$.*
4. *Use the correction coil to adjust the z-field so that the beam appears to be totally depolarized at the analyzer, i.e. that the counting rate is not changed if the spin is flipped using the π-coil (switching its current on and off).*

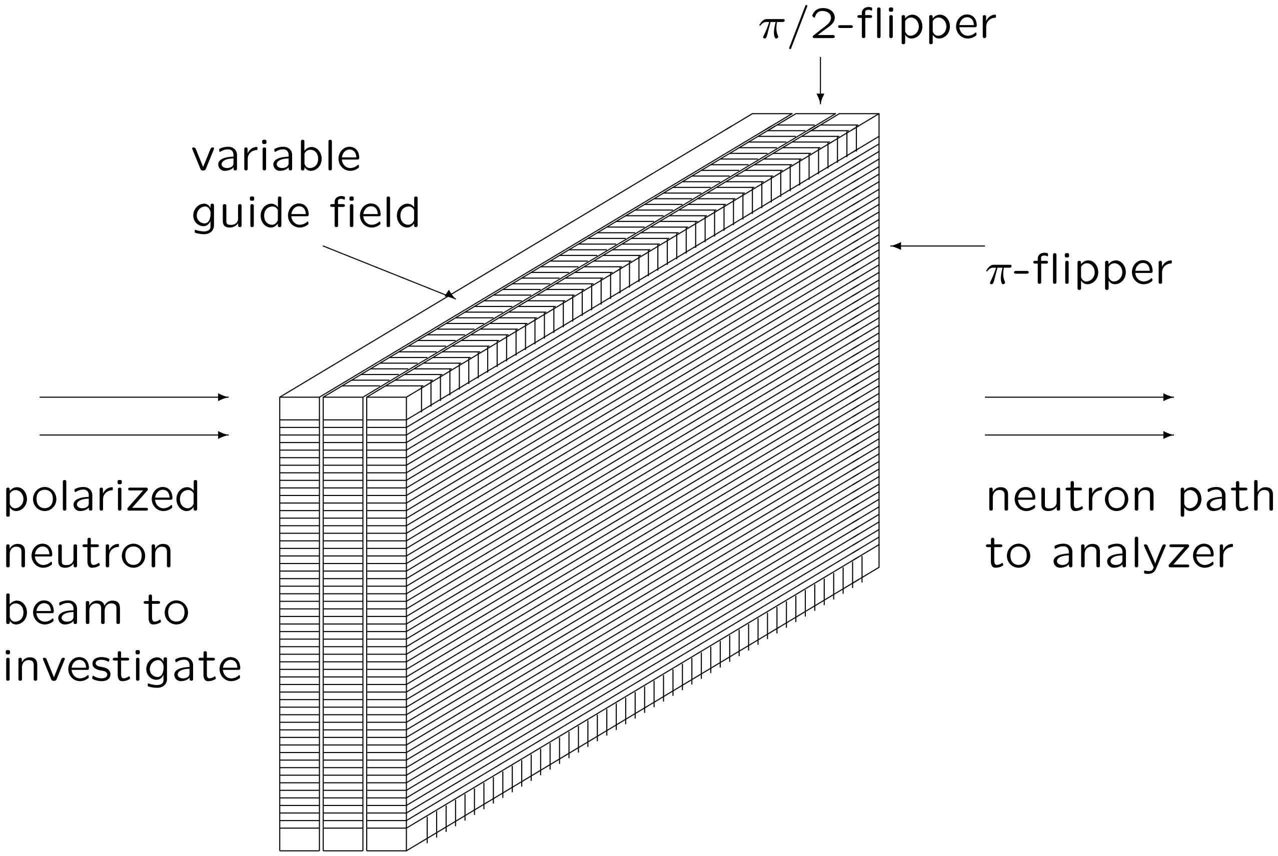
Measurement of precessing spin polarization, CRYOPAD, SSPAD



Such a $\pi/2$-flipper rotates that spin component which at the entrance of the coil is

1. *normal to the initial z-direction*
2. *and normal to the flight path i.e. the x-component*
3. *into the z-direction at the exit of the coil*
4. *i.e. into a component measurable in the usual way*

Unit to insert between sample and analyzer to measure the complete precessing spin polarization



1. *first coil is a variable guide section in front of the $\pi/2$-flipper. It shifts the ρ-direction of the polarization into the x-direction by accelerating the precession (changing ω_L) without changing the cone angle.*
2. *The ρ-direction is found when the $\pi/2$-flipped intensity is at a maximum by variation of the current in coil 1.*
3. *π-flipper between $\pi/2$-flipper and analyzer is not always necessary.*
4. *So at the same position in space one analyses the polarization in three space directions: P_x with a $\pi/2$ flipper, P_ρ with the variable guide field coil and the $\pi/2$-flipper and the z-component P_z*
5. *one obtains the direction and the modulus of $\vec{P}$ at the position in space which corresponds to the entrance point into the xz-flipper coil (Depolarization measurement).*
6. *To distinguish the x and y direction at the sample position, one can calibrate the setup by putting a known sample with only a component in x- or y-direction and look for*

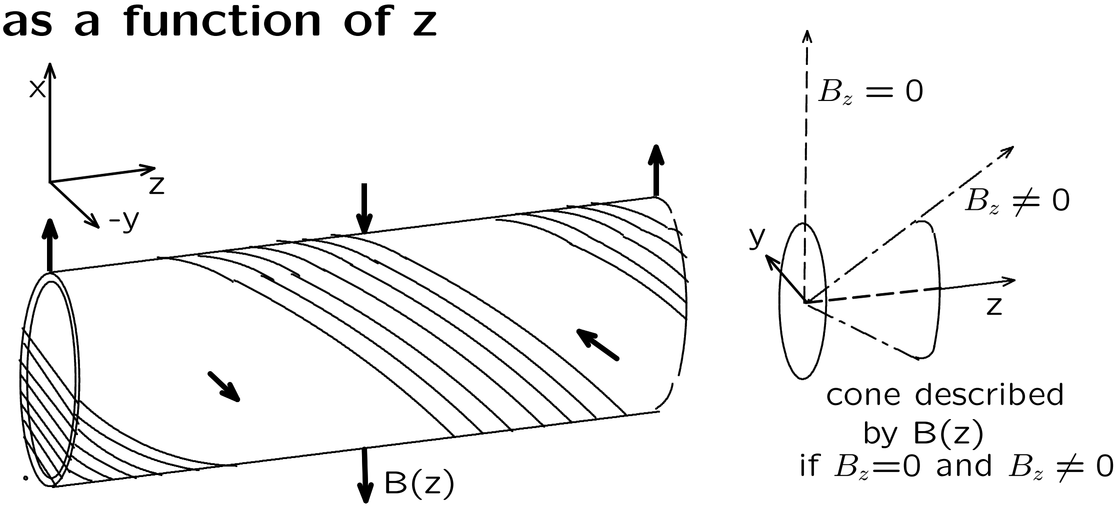
the current in the adjustable guide field that gives then the maximum. This corresponds then to the x or y at the sample position. Perhaps one could use a quartz sample inside a $\pi/2$-flipper coil to make this calibration.

7. *This unit changes the classical PA-instrument to SSPAD. There can be more such units in one instrument allowing multidetector application.*
8. *The fact that the finite size of the sample smeares the components normal to the guide field over a certain angular range does not make a problem, as we have seen for a range of* 36 deg. *The sample thickness giving such a smearing can be estimated with the help of the equation which gives the path length for the precession of π with the given fieldstrength and wavelenght. For* 36 deg *this would allow a pathlength in the sample of 8 mm for 1 mT and $\lambda = 0.15$ nm i.e. quite a large sample.*

J. Brown et al. have shown in many interesting papers how this possibility can be used in crystallography to clarify magnetic structures just by the analysis of the polarization matrix P_{ij}. They used the CRYOPAD which uses as flippers the so called cryoflipper, Meissner shields which separate regions of different field directions. They use a zero field region around the sample to avoid the necessity of a calibration.

Adiabatic spin rotator

Spin behaviour in a static magnetic field varying slowly as a function of z



1. *neutron flying in z-direction experiences a rotating field with $\omega = 2\pi \cdot v/L = 2\pi/L * 3956/\lambda[\AA]$ with L=length of the coil, λ=wavelength of the neutrons.*

2. *i.e. the helical magnetic induction $\vec{B} = B_1(\cos\omega t, -\sin\omega t, B_z)$*

1. *time dependent Schrödinger equation:*

$$\frac{\partial}{\partial t}\begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = \frac{\mu\vec{\sigma}\vec{B}}{i\hbar}\begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = -\frac{i}{2}\begin{pmatrix} \omega_z & \omega_1 e^{i\omega t} \\ \omega_1 e^{-i\omega t} & -\omega_z \end{pmatrix}\begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}$$

   i.e. time dependent coefficients. To get constant coefficients:

2. *transform this equation to a coordinate system rotating with the rotating field ω*

$$\begin{aligned} \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} &= e^{i\frac{\omega t}{2}\sigma_z}\begin{pmatrix} \varphi_1 \\ \varphi_2 \end{pmatrix} \\ \begin{pmatrix} \dot{\psi}_1 \\ \dot{\psi}_2 \end{pmatrix} &= i\frac{\omega}{2}\sigma_z e^{i\frac{\omega t}{2}\sigma_z}\begin{pmatrix} \varphi_1 \\ \varphi_2 \end{pmatrix} + e^{i\frac{\omega t}{2}\sigma_z}\begin{pmatrix} \dot{\varphi}_1 \\ \dot{\varphi}_2 \end{pmatrix} \\ &= e^{i\frac{\omega t}{2}\sigma_z}\left[\frac{i\omega}{2}\sigma_z\begin{pmatrix} \varphi_1 \\ \varphi_2 \end{pmatrix} + \begin{pmatrix} \dot{\varphi}_1 \\ \dot{\varphi}_2 \end{pmatrix}\right] \end{aligned}$$

3. *Inserting this yields*

$$e^{i\frac{\omega t}{2}\sigma_z}\left[\frac{i\omega}{2}\sigma_z\begin{pmatrix} \varphi_1 \\ \varphi_2 \end{pmatrix} + \begin{pmatrix} \dot{\varphi}_1 \\ \dot{\varphi}_2 \end{pmatrix}\right] = -\frac{i}{2}\begin{pmatrix} \omega_z & \omega_1 e^{i\omega t} \\ \omega_1 e^{-i\omega t} & -\omega_z \end{pmatrix} e^{i\frac{\omega t}{2}\sigma_z}\begin{pmatrix} \varphi_1 \\ \varphi_2 \end{pmatrix}$$

and we get

$$\begin{aligned} \frac{i\omega}{2}\sigma_z\begin{pmatrix} \varphi_1 \\ \varphi_2 \end{pmatrix} + \begin{pmatrix} \dot{\varphi}_1 \\ \dot{\varphi}_2 \end{pmatrix} &= -\frac{i}{2}e^{-i\frac{\omega t}{2}\sigma_z}\begin{pmatrix} \omega_z & \omega_1 e^{i\omega t} \\ \omega_1 e^{-i\omega t} & -\omega_z \end{pmatrix} e^{i\frac{\omega t}{2}\sigma_z}\begin{pmatrix} \varphi_1 \\ \varphi_2 \end{pmatrix} \\ &= \begin{pmatrix} \omega_z & \omega_1 \\ \omega_1 & -\omega_z \end{pmatrix}\begin{pmatrix} \varphi_1 \\ \varphi_2 \end{pmatrix} \end{aligned}$$

$$\begin{pmatrix} \dot\varphi_1 \\ \dot\varphi_2 \end{pmatrix} = -\frac{i}{2}\left[\begin{pmatrix} \omega & 0 \\ 0 & -\omega \end{pmatrix} + \begin{pmatrix} \omega_z & \omega_1 \\ \omega_1 & -\omega_z \end{pmatrix}\right]\begin{pmatrix} \varphi_1 \\ \varphi_2 \end{pmatrix}$$

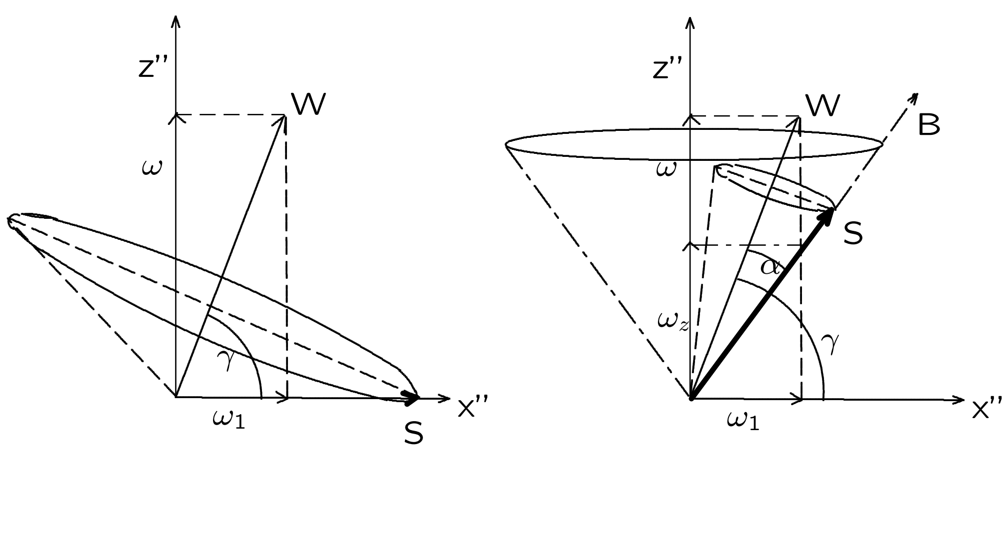
$$= -\frac{i}{2}\begin{pmatrix} \omega_z + \omega & \omega_1 \\ \omega_1 & -\omega_z - \omega \end{pmatrix}\begin{pmatrix} \varphi_1 \\ \varphi_2 \end{pmatrix}$$

differential equation with constant coefficients with the solution

$$\begin{pmatrix} \varphi_1(t) \\ \varphi_2(t) \end{pmatrix} = e^{-\frac{i}{2}\begin{pmatrix} \omega_z + \omega & \omega_1 \\ \omega_1 & -\omega_z - \omega \end{pmatrix}t}\begin{pmatrix} \varphi_1(0) \\ \varphi_2(0) \end{pmatrix} = e^{-\frac{iWt}{2}(\vec n\cdot\vec\sigma)}\begin{pmatrix} \varphi_1(0) \\ \varphi_2(0) \end{pmatrix}$$

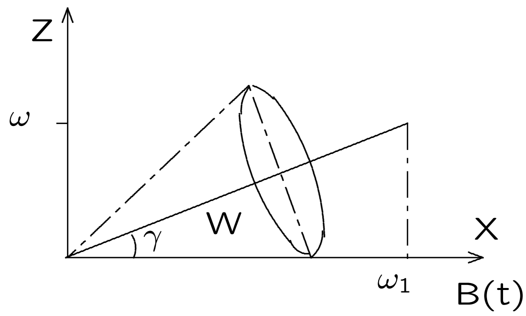
$\sin\gamma = \frac{\omega+\omega_z}{W}$ $\cos\gamma = \frac{\omega_1}{W}$ $W = \sqrt{\omega_1^2 + (\omega+\omega_z)^2}$ $\vec n = (\cos\gamma, 0, \sin\gamma)$

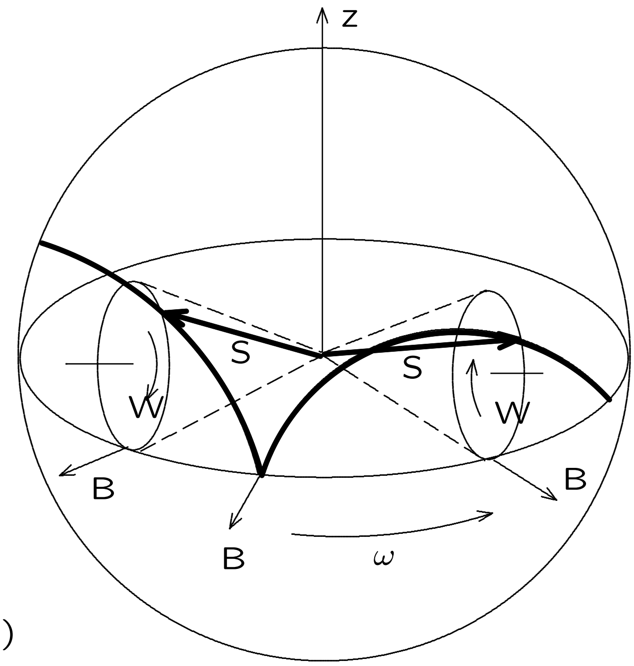
Complete solution: $\begin{pmatrix} \psi_1(t) \\ \psi_2(t) \end{pmatrix} = e^{\frac{i}{2}[-\omega t\sigma_z - \gamma\sigma_y - Wt\sigma_x + \gamma\sigma_y + \omega t\sigma_z]}\begin{pmatrix} \psi_1(0) \\ \psi_2(0) \end{pmatrix}$



Visualization of this precession in laboratory system

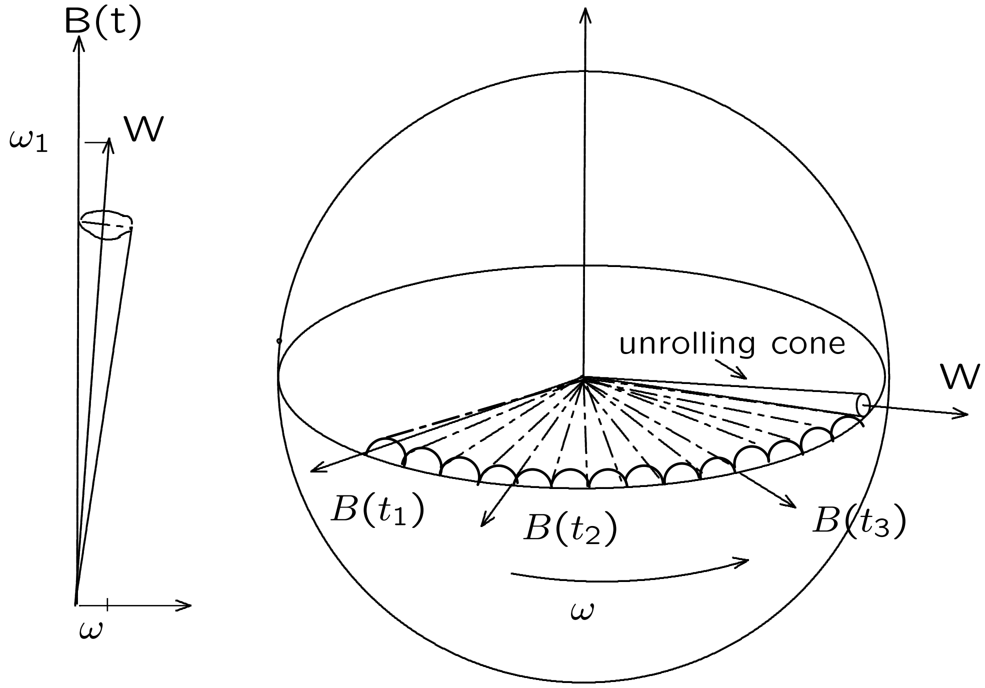
1. **Case 1:** $\omega \approx \omega_1$





transform this back to the laboratory frame $\Longrightarrow$ *inclination* γ $\Longrightarrow$ *not rotating system of the laboratory.*
Geometrical conditions: the cone precessing with W is unrolling without gliding on the surface described by the field direction. Field direction determines sense of precession and by this on which side of this surface the precession cone is unrolling. Figure: case $\omega_z = 0$.

2. **Case 2:** $\omega \ll \omega_1$; *ω_1 = Larmorfrequency for B_1*



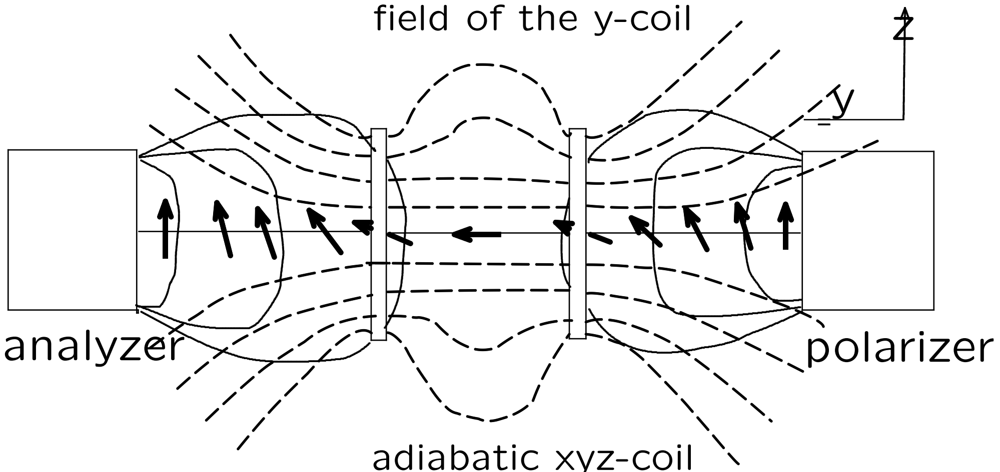
Maximum deviation of the spin from the field direction: angular diameter of the precession cone i.e.

$$2\gamma = \arccos\frac{\omega_1}{W}$$

or

$$2\alpha = 2|\arccos\frac{\omega_1}{W} - \arctan\frac{\omega_z}{\omega_1}|$$

Application: adiabatic spin rotator, xyz-coil



Rotation of the spin in the adiabatic y-coil: spin follows the direction of the guide field.

1. *Near the polarizer and analyzer the guide field is only H_z. At sample adjust z-coil for $H_z = 0$*
2. *then: superposition of the coil field and the stray field of the polarizers and analyzers.*
3. *sufficiently strong and slowly changing that the condition $\omega/\omega_1 \ll 1$ is fulfilled.*
4. *the spin or the axis of precessing polarization remains always parallel to the field direction and rotates with this field direction.*
5. *Before scattering spin rotated in three mutually orthogonal directions by three such coils.*
6. *After scattering field direction rotates back to the z direction and*
7. *takes with it the precession cone in case of precessing spin polarization*
8. *one can determine unambiguously the full (also processing) polarization of the beam after the scattering process simultaneously by* **many different detectors = in a multidetector instrument with full polarization analysis**.

More direct way to $d\sigma/d\Omega$ and $\vec{P}$ of scattered beam

1. *Born approximation for a beam of particles with spin:*

$$\Psi \approx e^{ikz}\chi^{(i)} + \frac{e^{ikr}}{r}\widehat{M}_{cc}(\vartheta,\varphi)\chi^{(i)} \qquad \textit{as } r \to \infty$$

with $\widehat{M}_{cc}(\vartheta,\varphi) = \langle \lambda' | V | \lambda \rangle$

2. *Density matrix of this outgoing spherically scattered wave in spin state* $\chi_c^f = \widehat{M}_{cc}\chi_c^{(i)}$*?*

$$\begin{aligned} \rho_c^{out} &= \chi_c^{(f)}\chi_c^{(f)\dagger} \\ &= \widehat{M}_{cc}\chi_c^{(i)}\chi_c^{(i)\dagger}\widehat{M}_{cc}^{\dagger} \\ &= \widehat{M}_{cc}\rho_c^{(i)}\widehat{M}_{cc}^{\dagger} \end{aligned}$$

- *This is the relationship between the outgoing and the incident density matrix*
- *in terms of the transition probability* $\widehat{M}_{cc}$*.*
- *also for beams which are unpolarized or partially polarized.*
- *The resultant beam is described by a density matrix which is the product of three* 2×2 *matrices.*

3. *Trace of* $\rho_c^{(out)}$ *gives the expectation value of the scattering matrix operator for the incident beam described by the density matrix* $\rho_c^{(in)}$*.*

$$\frac{d\sigma}{d\Omega} = \mathrm{Tr}\rho_c^{(out)} = \mathrm{Tr}(\widehat{M}_{cc}\rho_c^{(i)}\widehat{M}_{cc}^{\dagger})$$

4. Polarization of this outgoing beam:

$$\vec{P} = \frac{\mathrm{Tr}(\sigma\rho_c^{(out)})}{\mathrm{Tr}\rho_c^{(out)}} = \frac{\mathrm{Tr}(\sigma\widehat{M}_{cc}\rho^{(in)}\widehat{M}_{cc}^{\dagger})}{\mathrm{Tr}\rho_c^{(out)}}$$

Useful rules for Tr_σ of products of spin matrices:

$$\begin{aligned}
\text{Tr}(\sigma_\alpha) &= 0 \\
\text{Tr}(\sigma_\alpha\sigma_\beta) &= 2\delta_{\alpha\beta} \\
\text{Tr}(\sigma_\alpha\sigma_\beta\sigma_\gamma) &= i\sum_{\gamma''}\epsilon^{\alpha\beta\gamma''}\text{Tr}(\sigma_{\gamma''}\sigma_\gamma) = 2i\epsilon^{\alpha\beta\gamma} \\
\text{Tr}(\sigma_\alpha\sigma_\beta\sigma_\gamma\sigma_\delta) &= 2(\delta_{\alpha\beta}\delta_{\gamma\delta} - \delta_{\alpha\gamma}\delta_{\beta\delta} + \delta_{\alpha\delta}\delta_{\beta\gamma})
\end{aligned}$$

Some more sophisticated rules for Tr_σ

for the operators

$$\begin{aligned}
L_h &= \vec{S}_h \cdot (\vec{\sigma} - (\vec{e}\cdot\vec{\sigma})\vec{e}) \\
\vec{M}_h &= \vec{Q}_{\perp h} = \vec{S}_h - (\vec{e}\cdot\vec{S}_h)\vec{e} \text{ with } \vec{e} = \frac{\vec{\kappa}}{|\vec{\kappa}|}
\end{aligned}$$

a unit vector in the direction of the scattering vector. For these one can derive the additional rules

$$\begin{aligned}
\text{Tr}_\sigma(\vec{\sigma}L_h) &= 2\vec{M}_h \\
\text{Tr}_\sigma((\vec{P}\cdot\vec{\sigma})L_h) &= 2(\vec{M}_h\cdot\vec{P}) \\
\text{Tr}_\sigma((\vec{P}\cdot\vec{\sigma})\vec{\sigma}L_h) &= 2i(\vec{M}_h\times\vec{P}) \\
\text{Tr}_\sigma((\vec{P}\cdot\vec{\sigma})L_h\vec{\sigma}) &= -2i(\vec{M}_h\times\vec{P}) \\
\text{Tr}_\sigma(L_1L_2) &= 2(\vec{M}_1\cdot\vec{M}_2) \\
\text{Tr}_\sigma(L_1\vec{\sigma}L_2) &= -2i(\vec{M}_1\times\vec{M}_2) \\
\text{Tr}_\sigma((\vec{P}\cdot\vec{\sigma})L_1L_2) &= 2i(\vec{M}_1\times\vec{M}_2)\vec{P} \\
\text{Tr}_\sigma((\vec{P}\cdot\vec{\sigma})L_1\vec{\sigma}L_2) &= 2[(\vec{M}_1(\vec{M}_2\cdot\vec{P}) + (\vec{M}_1\cdot\vec{P})\vec{M}_2 \\
&\quad -\vec{P}(\vec{M}_1\cdot\vec{M}_2]
\end{aligned}$$

Density matrix formalism to determine cross sections

For me in Loveseys book this looked like magic. Apply some simple rules about traces of products of Pauli matrices give results otherwise to gain only with long calculations.
Why can this give physical results?

1. *$\underline{1}, \sigma_x, \sigma_y, \sigma_z$ are linearly independent and form a complete basis for the 2×2 matrices*
   i.e. any 2×2 matrix $\underline{A}$

   $$\underline{A} = \lambda_0 \underline{1} + \lambda_1 \sigma_x + \lambda_2 \sigma_y + \lambda_3 \sigma_z = \lambda_0 \underline{1} + |(\lambda_1, \lambda_2, \lambda_3)| \frac{(\lambda_1, \lambda_2, \lambda_3)}{|(\lambda_1, \lambda_2, \lambda_3)|}$$

   i.e. Each operator in the spinor space has the form

   $$\boxed{\frac{1}{2}\left(g\underline{1} + h\vec{n} \cdot \vec{\sigma}\right)}$$

   traces are only traces of products of Pauli matrices.

2. The second reason is that

   $$\overline{\langle A \rangle} = \mathrm{Tr}_\sigma(\overline{\rho} A)$$

   representation independent. We apply this to get the statistical average of the transition probability $\overline{\langle |\langle k's'\lambda'|V|ks\lambda\rangle|^2 \rangle} = \mathrm{Tr}_\sigma(\rho |\langle \lambda'|V|\lambda\rangle|^2)$ in spinor space used in the double differential neutron scattering cross section

   $$\left(\frac{\partial^2 \sigma}{\partial\Omega \partial E'}\right)_{ss'} = \left(\frac{m_n}{2\pi\hbar^2}\right)^2 \cdot \frac{k'}{k} \sum_{\lambda\lambda'} p_\lambda |\langle k's'\lambda'|V|ks\lambda\rangle|^2 \delta(\hbar\omega + E_\lambda - E_{\lambda'})$$

   V is the interaction between neutron and target: spinless target $h = 0$, nuclear spin $B(\vec{I} \cdot \sigma)$, magnetic interaction $(Q_\perp \cdot \sigma)$

Scattering of a polarized beam by a spinless target:

quartz measurement to determine the flipping ratio.

1. *for an aggregat of atoms without nuclear spins and without magnetism. The interaction potential has*

the form of a complex number $N_N e^{i\phi_N}$ e.g. crystallographic structure amplitude.

$$V_N(\vec{\kappa}) = V_N(\vec{k} - \vec{k}') = \frac{2\pi\hbar^2}{m_0} \sum_{\nu,j} b_j e^{i(\vec{k}-\vec{k}')(\vec{R}_\nu + \vec{d}_j)}$$

2. *Scattered intensity is obtained by*

$$\begin{aligned} \frac{d\sigma}{d\Omega} &= I^{\uparrow\uparrow} + I^{\uparrow\downarrow} \\ &= \mathrm{Tr}_\sigma(\rho \hat{N}^\dagger \hat{N}) \\ &= \frac{1}{2}\mathrm{Tr}_\sigma[(\underline{1} + \vec{P}\cdot\vec{\sigma})\hat{N}^\dagger \hat{N}] \\ &= \hat{N}^\dagger \hat{N} = N^2 \end{aligned}$$

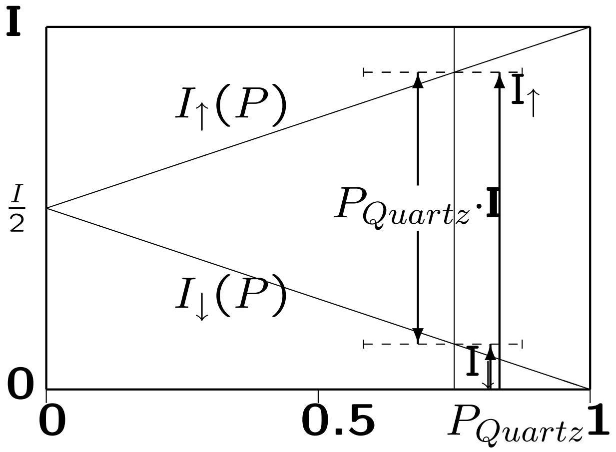
as $\mathrm{Tr}_\sigma(\underline{1}) = 2$ *and* $\mathrm{Tr}_\sigma(\vec{\sigma}) = 0$.

3. *For the polarization $\vec{P}_{out}$ of the outgoing beam with $\vec{P}_{in}$ as the polarization of the incident beam we get*

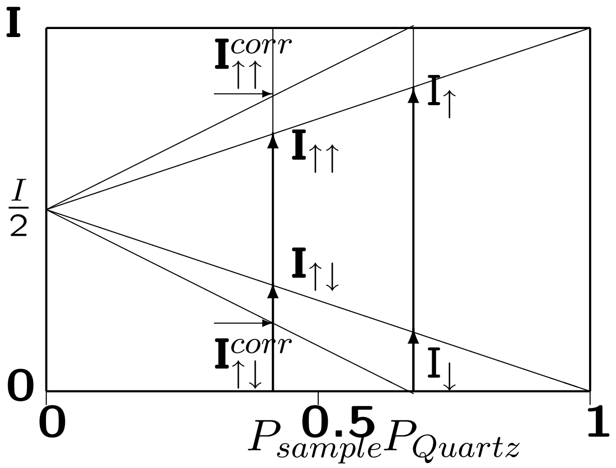
$$\begin{aligned} \vec{P}^{(out)}\frac{d\sigma}{d\Omega} &= I^{\uparrow\uparrow} - I^{\uparrow\downarrow} \\ &= \mathrm{Tr}_\sigma(\rho \hat{N}^\dagger \vec{\sigma} \hat{N}) \\ P_\beta^{(out)}\frac{d\sigma}{d\Omega} &= \frac{1}{2}\mathrm{Tr}_\sigma[(\underline{1} + P_\alpha^{(in)}\sigma_\alpha)\hat{N}^\dagger \sigma_\beta \hat{N}] \\ &= \frac{1}{2}\mathrm{Tr}_\sigma(\hat{N}^\dagger \sigma_\beta \hat{N} + P_\alpha^{(in)}\sigma_\alpha\sigma_\beta \hat{N} \dagger \hat{N}) \\ &= P_\alpha^{(in)}\delta_{\alpha\beta}\hat{N}^\dagger \hat{N} \\ &= P_\beta^{(in)}|\hat{N}|^2 \\ &= P_\beta^{(in)} N^2 \end{aligned}$$

as $\mathrm{Tr}\sigma_\alpha\sigma_\beta = \delta_{\alpha\beta}\mathrm{Tr}\begin{pmatrix}1&0\\0&1\end{pmatrix} = 2\delta_{\alpha\beta}$ *and* $\mathrm{Tr}\sigma = 0$.

Correction for finite flipping ratio



$I_\uparrow$ and $I_\downarrow$ for the polarization P



$I_\uparrow$ and $I_\downarrow$ of the quartz and for the sample, and the flipping ratio corrected intensities of the sample $I^{corr}_{\uparrow\uparrow}$ and $I^{corr}_{\uparrow\downarrow}$. The correction relates the measured sample intensities to an ideal quartz scatterer

One has to be able to correct for the faults of the polarizers, charterized by the flipping ratio of the quartz sample.

$$\begin{aligned}
P_{Quartz} &= \frac{I_\uparrow - I_\downarrow}{I_\uparrow + I_\downarrow} = \frac{I_\uparrow / I_\downarrow - 1}{I_\uparrow / I_\downarrow + 1} = \frac{R_{quartz} - 1}{R_{quartz} + 1} \\
I^{corr}_{\uparrow\uparrow} + I^{corr}_{\uparrow\downarrow} &= I_{\uparrow\uparrow} + I_{\uparrow\downarrow} = I \\
\frac{I^{corr}_{\uparrow\uparrow} - I^{corr}_{\uparrow\downarrow}}{I} &= \frac{I_{\uparrow\uparrow} - I_{\uparrow\downarrow}}{I_\uparrow - I_\downarrow} \\
I^{corr}_{\uparrow\uparrow} - I^{corr}_{\uparrow\downarrow} &= \frac{I_{\uparrow\uparrow} - I_{\uparrow\downarrow}}{P_{Quartz}}
\end{aligned}$$

From this follows by some simple calculations

$$\begin{aligned}
I^{corr}_{\uparrow\uparrow} &= I_{\uparrow\uparrow} + \frac{1}{R_{quartz} - 1}(I_{\uparrow\uparrow} - I_{\uparrow\downarrow}) \\
I^{corr}_{\uparrow\downarrow} &= I_{\uparrow\downarrow} - \frac{1}{R_{quartz} - 1}(I_{\uparrow\uparrow} - I_{\uparrow\downarrow})
\end{aligned}$$

The correction for finite flipping ratio: measure the scattering of a fused quartz sample without spin flip $I_n^\uparrow$ and with spin flip $I_n^{\uparrow}$ for detector number n (after background correction). Determine R_n

$$R_n = \frac{I_n^{\uparrow}}{I_n^{\downarrow}}$$

and

$$(P_{pol} P_{anal} F_{flipper})_n = \frac{R_n - 1}{R_n + 1}$$

R_n serves also for the correction for finite flipping ratio of the measured data.

For the correction one can also use the polarizer and flipper efficiences determined before. Also a depolarization factor can be used if the sample has a known depolarization.

Scattering of polarized neutrons by a target with only nuclear spin incoherence: vanadium calibration

- absolute calibration: compare with a scatterer with known cross section and scattering behaviour.

- Vanadium is a nearly ideal incoherent scatterer, having a coherent scattering cross section of only 0.0184 barn and an incoherent cross section of 5.187 barn.

- incoherence: the angular scattering is isotropic.

- every detector should get the same scattered intensity if one has real single scattering behaviour and no absorption. But these latter effects can be corrected for.

- The incoherence results from interaction of the neutron with the nuclear spin of vanadium.

- For nuclear spin incoherent scattering the behaviour is given by two numbers b^+ and b^-

- which are the eigenvalues of the scattering length operator $\hat{b} = \bar{b} + \frac{1}{2} b_N \boldsymbol{I} \cdot \boldsymbol{\sigma}$. As $\boldsymbol{I} \cdot \boldsymbol{\sigma} = \mathbf{J^2} - \mathbf{I^2} - \frac{1}{4}\boldsymbol{\sigma}^2$ $= J(J+1) - I(I+1) - \frac{3}{4}$ this yields

$$\boldsymbol{I} \cdot \boldsymbol{\sigma} = I \quad \text{for} \qquad J = I + \frac{1}{2}$$
$$\boldsymbol{I} \cdot \boldsymbol{\sigma} = -(I+1) \quad \text{for} \qquad J = I - \frac{1}{2}$$

we obtain

$$b^+ = \bar{b} + \frac{1}{2} b_N I \tag{1}$$
$$b^- = \bar{b} - \frac{1}{2} b_N (I+1) \tag{2}$$
$$\bar{b} = \frac{(I+1)b^+ + I b^-}{2I+1} \tag{3}$$
$$b_N = \frac{2(b^+ - b^-)}{2I+1} \tag{4}$$

- density matrix method for the operator $\hat{B}(\boldsymbol{I} \cdot \boldsymbol{\sigma})$

- the nuclei are not polarized,i.e.

$$\langle I_x \rangle = \langle I_y \rangle = \langle I_z \rangle = 0$$
$$\langle I_x^2 \rangle = \langle I_y^2 \rangle = \langle I_z^2 \rangle = \frac{1}{3} I(I+1)$$

-

$$\frac{d\sigma}{d\Omega} = \text{Tr}(\rho \hat{B}^\dagger (\vec{\sigma} \cdot \vec{I}^\dagger) \hat{B} (\vec{\sigma} \cdot \vec{I}))$$
$$= \frac{1}{2} \text{Tr}[(\left(\begin{smallmatrix} 1 & 0 \\ 0 & 1 \end{smallmatrix}\right) + \sigma_\alpha P_\alpha^{(in)})(\sigma_\beta I_\beta^\dagger) \hat{B}^\dagger \hat{B} (\sigma_\gamma I_\gamma)]$$
$$= \frac{1}{2} \text{Tr}[\sigma_\beta \sigma_\gamma I_\beta^\dagger I_\gamma \hat{B}^\dagger \hat{B} + \hat{B}^\dagger \hat{B} \sigma_\alpha \sigma_\beta \sigma_\gamma P_\alpha^{(in)} I_\beta^\dagger I_\gamma]$$

$$
\begin{aligned}
&= \frac{1}{2}\hat{B}^\dagger \hat{B}[2\delta_{\beta\gamma} I_\beta^\dagger I_\gamma + 2i\epsilon_{\alpha\beta\gamma} P_\alpha^{(in)} I_\beta^\dagger I_\gamma] \\
&= \hat{B}^\dagger \hat{B}[I_\beta^\dagger I_\beta + i\vec{P}^{(in)}(\vec{I}^\dagger \times \vec{I})] \\
&= \hat{B}^\dagger \hat{B}[I(I+1) + i\vec{P}^{(in)}(\vec{I}^\dagger \times \vec{I})]
\end{aligned}
$$

- average over the nuclear spin orientation of $\vec{I}$. As $\vec{I}$ is an angular momentum, we know that $\vec{I}^\dagger = \vec{I}$ and that $\vec{I} \times \vec{I} = i\vec{I}$.

- the vector product expression is linear in nuclear spin so that it averages to zero for an unpolarized nuclear target. Therefore we obtain finally

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

Polarization if scattered by unpolarized nuclear spins

$$
\begin{aligned}
& P_\gamma^{(out)} \frac{d\sigma}{d\Omega} \\
&= \mathrm{Tr}(\rho \hat{B}^\dagger (\vec{\sigma} \cdot \vec{I}^\dagger) \sigma_\gamma (\vec{\sigma} \cdot \vec{I}) \hat{B}) \\
&= \frac{1}{2}\mathrm{Tr}[(\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \sigma_\alpha P_\alpha^{(in)})(\sigma_\beta I_\beta^\dagger)\sigma_\gamma(\sigma_\delta I_\delta)] \\
&= \frac{1}{2}\hat{B}^\dagger \hat{B}\mathrm{Tr}[\sigma_\beta \sigma_\gamma \sigma_\delta I_\beta^\dagger I_\delta + \sigma_\alpha \sigma_\beta \sigma_\gamma \sigma_\delta P_\alpha^{(in)} I_\beta^\dagger I_\delta] \\
&= \hat{B}^\dagger \hat{B}[i\epsilon_{\beta\gamma\delta} I_\beta^\dagger I_\delta + (\delta_{\alpha\beta}\delta_{\gamma\delta} \\
&\quad -\delta_{\alpha\gamma}\delta_{\beta\delta} + \delta_{\alpha\delta}\delta_{\beta\gamma}) P_\alpha^{(in)} I_\beta^\dagger I_\gamma] \\
&= \hat{B}^\dagger \hat{B}[-i(\vec{I}^\dagger \times \vec{I})_\gamma + (\vec{P}^{(in)} \cdot \vec{I}^\dagger) I_\gamma \\
&\quad +(\vec{P}^{(in)} \cdot \vec{I}) I_\gamma^\dagger - P_\gamma^{(in)} (\vec{I}^\dagger \cdot \vec{I})] \\
&= \hat{B}^\dagger \hat{B}[-i(\vec{I}^\dagger \times \vec{I})_\gamma - P_\gamma^{(in)} I(I+1) \\
&\quad +(\vec{P}^{(in)} \cdot \vec{I}^\dagger) I_\gamma + (\vec{P}^{(in)} \cdot \vec{I}) I_\gamma^\dagger]
\end{aligned}
$$

- Now we average again over nuclear spin orientations and obtain

$$
(\vec{P}^{(in)} \cdot \vec{I}^\dagger) I_\gamma = (P_x^{(in)} I_x^\dagger + P_y^{(in)} I_y^\dagger + P_z^{(in)} I_z^\dagger) I_\gamma
$$

$$= \frac{1}{3}P_\gamma^{(in)}I(I+1)$$

$$(\vec{P}^{(in)}\cdot\vec{I})I_\gamma^\dagger = (P_x^{(in)}I_x + P_y^{(in)}I_y + P_z^{(in)}I_z)I_\gamma^\dagger$$

$$= \frac{1}{3}P_\gamma^{(in)}I(I+1)$$

With this we obtain

$$\vec{P}^{(out)}\frac{d\sigma}{d\Omega} = \hat{B}^\dagger\hat{B}\vec{P}^{(in)}I(I+1)[\frac{1}{3}+\frac{1}{3}-1]$$

$$= -\frac{1}{3}\vec{P}^{(in)}I(I+1)\hat{B}^\dagger\hat{B}$$

- To understand the physical meaning of this result we have to know that

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

$$\vec{P}^{(out)}\frac{d\sigma}{d\Omega} = \frac{I^{\uparrow\uparrow}-I^{\uparrow\downarrow}}{I^{\uparrow\uparrow}+I^{\uparrow\downarrow}}(I^{\uparrow\uparrow}+I^{\uparrow\downarrow}) = I^{\uparrow\uparrow}-I^{\uparrow\downarrow}$$

$$= -\frac{1}{3}\hat{B}^\dagger\hat{B}I(I+1)$$

- Solving this two equations for the intensity without spin flip $I^{\uparrow\uparrow}$ and for the intensity with spin flip $I^{\uparrow\downarrow}$ we obtain immediately

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

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

- irrespective of the incident polarization direction (i.e. P in x or y or z direction) the outgoing scattering resulting from unpolarized nuclear spins is always
  - one third without flip and
  - two third with flip of the neutrons in the polarized beam.

Application to paramagnetic powder scattering

[Derivation of $\vec{P}' = -\vec{e}(\vec{e}\cdot\vec{P})$]

we use

$$\vec{M}_e \cdot \vec{\mu}_{n\perp} = \vec{\mu}_n \cdot \vec{M}_{e\perp}$$

1. - *With $\vec{S}_i$ the operator of the electron magnetization including all factors and sums*
   - *$\vec{M}_i = \vec{S}_i - (\vec{e}\cdot\vec{S}_i)\vec{e}$ its normal component to the unit vector $\vec{e}$ in the direction of the scattering vector,*
   - *$L_i = \vec{S}_i \cdot (\vec{\sigma} - (\vec{e}\cdot\vec{\sigma})\vec{e})$ describing the interaction of the neutron with the electron magnetization*
2. *the polarization of the neutron beam scattered by L_i is*

$$\begin{aligned}\vec{P}^{out} &= \frac{\mathrm{Tr}_\sigma(\rho L^\dagger \vec{\sigma} L)}{\mathrm{Tr}_\sigma(\rho L^\dagger L)} \\ &= \frac{\frac{1}{2}\mathrm{Tr}_\sigma(L^\dagger\vec{\sigma}L + (\vec{P}\cdot\vec{\sigma})L^\dagger\vec{\sigma}L)}{\frac{1}{2}\mathrm{Tr}_\sigma(L^\dagger L + (\vec{P}\cdot\vec{\sigma})L^\dagger L)} \\ &= \frac{-i(\vec{M}^\dagger\times\vec{M}) + \vec{M}^\dagger(\vec{M}\cdot\vec{P}) + (\vec{M}^\dagger\cdot\vec{P})\vec{M} - \vec{P}(\vec{M}^\dagger\cdot\vec{M})}{(\vec{M}^\dagger\cdot\vec{M}) + i(\vec{M}^\dagger\times\vec{M})\vec{P}}\end{aligned}$$

the last line by applying the rules for Tr.

For a paramagnet without helical structures the cross product in the nominator and denominator disappear and we get

$$\vec{P}^{out} = \frac{\vec{M}^\dagger(\vec{M}\cdot\vec{P}) + (\vec{M}^\dagger\cdot\vec{P})\vec{M} - \vec{P}(\vec{M}^\dagger\cdot\vec{M})}{(\vec{M}^\dagger\cdot\vec{M})}$$

Now we have to average $\vec{M}^\dagger$ and $\vec{M}$ and the products containing them over the random orientations of the atomic spins $\vec{S}^\dagger$,$\vec{S}$. For random orientation we have

$$\begin{aligned}\langle(\vec{S}^\dagger\cdot\vec{S})\rangle &= S(S+1) \\ &= \langle S_x^\dagger S_x\rangle + \langle S_y^\dagger S_y\rangle + \langle S_z^\dagger S_z\rangle\end{aligned}$$

$$
\begin{aligned}
\langle S_\nu^\dagger S_\nu \rangle &= \frac{1}{3} S(S+1) \text{ with } \nu\text{=x,y,z} \\
\langle S_x \rangle &= \langle S_y \rangle = \langle S_z \rangle = \langle S_\nu^\dagger \rangle = 0
\end{aligned}
$$

With these the average of the first product is

$$
\begin{aligned}
\langle (\vec{S}^\dagger - (\vec{e} \cdot \vec{S}^\dagger)\vec{e})[(\vec{S} \cdot \vec{P}) \\
-(\vec{e} \cdot \vec{S})(\vec{e} \cdot \vec{P})] \rangle &= \langle \vec{S}^\dagger (\vec{S} \cdot \vec{P}) \rangle - \langle \vec{S}^\dagger (\vec{e} \cdot \vec{S})(\vec{e} \cdot \vec{P}) \rangle \\
&\quad - \langle (\vec{e} \cdot \vec{S}^\dagger)\vec{e}(\vec{S} \cdot \vec{P}) \rangle + \langle (\vec{e} \cdot \vec{S}^\dagger)\vec{e}(\vec{e} \cdot \vec{S})(\vec{e} \cdot \vec{P}) \rangle \\
&= \frac{1}{3} S(S+1)[\vec{P} - (\vec{e} \cdot \vec{P})\vec{e} - (\vec{e} \cdot \vec{P})\vec{e} + (\vec{e} \cdot \vec{P})\vec{e} \\
&= \frac{1}{3} S(S+1)[\vec{P} - (\vec{e} \cdot \vec{P})\vec{e}]
\end{aligned}
$$

We used for this

$$
\begin{aligned}
\langle \vec{S}^\dagger (\vec{S} \cdot \vec{P}) \rangle &= \langle (S_x^\dagger, S_y^\dagger, S_z^\dagger)(S_x P_x + S_y P_y + S_z P_z) \rangle \\
&= \frac{1}{3} S(S+1)(P_x, P_y, P_z) \\
&= \langle (\vec{S}^\dagger \cdot \vec{P}) \vec{S} \rangle \\
\langle \vec{S}^\dagger (\vec{e} \cdot \vec{S}) \rangle &= \frac{1}{3} S(S+1)(e_x, e_y, e_z) \\
\langle (\vec{e} \cdot \vec{S}\dagger)(\vec{S} \cdot \vec{P}) \rangle &= \frac{1}{3} S(S+1)(\vec{e} \cdot \vec{P}) \\
\langle (\vec{e} \cdot \vec{S}^\dagger)(\vec{e} \cdot \vec{S}) \rangle &= \frac{1}{3} S(S+1)
\end{aligned}
$$

The average of the second expression gives the same. The third expression and the denominator can be averaged in one go

$$
\begin{aligned}
\langle (\vec{M}^\dagger \cdot \vec{M}) \rangle &= \langle (\vec{S}^\dagger - (\vec{e} \cdot \vec{S}^\dagger)\vec{e}) \cdot (\vec{S} - (\vec{e} \cdot \vec{S})\vec{e}) \rangle \\
&= \langle (\vec{S}^\dagger \cdot \vec{S}) - (\vec{S}^\dagger \cdot \vec{e})(\vec{e} \cdot \vec{S}) \\
&\quad -(\vec{e} \cdot \vec{S}^\dagger)(\vec{e} \cdot \vec{S}) + (\vec{e} \cdot \vec{S}^\dagger)(\vec{e} \cdot \vec{S}) e^2 \rangle \\
&= \langle (\vec{S}^\dagger \cdot \vec{S}) - (\vec{S}^\dagger \cdot \vec{e})(\vec{e} \cdot \vec{S}) \rangle \\
&= S(S+1) - \frac{1}{3} S(S+1) \\
&= \frac{2}{3} S(S+1)
\end{aligned}
$$

So we get for $\vec{P}^{out}_{paramagnetic}$ finally

$$\vec{P}^{out}_{paramagnet} = \frac{\frac{1}{3}S(S+1)[\vec{P} - (\vec{e}\cdot\vec{P})\vec{e} + \vec{P} - (\vec{e}\cdot\vec{P})\vec{e} - 2\vec{P}]}{\frac{2}{3}S(S+1)} = -(\vec{e}\cdot\vec{P})\vec{e}$$