# Polarization elements.

O.Schärpf
Berchmanskolleg
Kaulbachstrasse 31a
80539 München, Germany

München, March 2, 2010

# Contents

# Chapter 1

# Experimenting with the neutron spin

The neutron has a magnetic moment of

$$\mu = -1.913 \cdot \mu_N \quad \text{with} \quad \mu_N = e\hbar/2m_p = 5.051 \cdot 10^{-27} JT^{-1} \tag{1.1}$$

In the following we want to 1. define polarization of a neutron beam including also precessing spin polarization 2. learn how to measure this polarization (also the precessing components), which is a linear process. 3. learn to understand,treat and measure the quadratic process of scattering, where also fluctuations are contributing.

We do this by experimentally preparing a precessing spin polarization and by preparing the tools for its measurement. This is done by visualizing the mathematical expressions like spinors, Pauli matrices, spin rotation operators, density matrix operations etc. by showing the corresponding experimental physical device to realize it or to measure it.

## 1.1 Tools for the preparation of a precessing spin polarization

Quantum mechanics gives us a probability density to find a particle in a state with orbit angular momentum, spin angular momentum, total angular momentum. But it gives neither information about the motion of the particle in its orbit, nor about the coordinate of the axis of rotation. All what it says can be visualized as if the orbit "precessed" in an unobservable way about the z-axis describable by a precession cone of the total $\vec{J}$, $\vec{L}$ or $\vec{S}$. In the case of the orbital behaviour one has at least with $\psi^*\psi$ a probability density of the particle in a state with the quantum number l,m. In the spin case only the fact is given that the particle such as the neutron or the electron has an internal angular momentum of $\hbar/2$, where the three components $s_x$, $s_y$, $s_z$ obey the commutation relations $[s_x, s_y] = i\hbar s_z$ or more generally $[s_i, s_j] = i\hbar\epsilon_{ijk}s_k$, with $i, j, k = x, y, z$, but no probability density of an orbit or of the spin directions or something similar is given. Such commutation relations are common to all angular momentum operators. In modern quantum mechanics angular momenta are often defined by such commutation relations, which are more general than the definition $\vec{p} \times \vec{r}$ which is not applicable to the spin. We want to consider some consequences of this commutator. What follows from this commutator with respect to the unobservable way the quantum mechanical spin behaves (not the expectation value of it), which we will describe using the words "as if it 'precessed' about the z-axis"? We want to understand the relationship between the indeterminacy relationship, the commutator and the visualization of the spin of a particle.(omitted because of space limitations).

We want to become acquainted with the different theoretical tools like spinors, Pauli spin matrices, density matrix formalism to describe the physical processes we are investigating. In

connection with this we want to understand the way how a spin flipper works in contrast to a spin rotator. These are the tools to be used in an instrument for polarization analysis measurements. An experimentalist must go to the limits of visualizability (= measureability) to be able to measure something. This is so as measurements always are in the range of classical physics, they represent the borderline between quantum mechanics and classical physics. For this reason the experimental physicist has to know this part of the theory better than the theoretician, who often does not need to care about measuring what he is treating formally. In the following we will always try to ask, what a certain formal process means physically, which is often just a sort of visualization.

### 1.1.1 Polarization and spinor

We use the Pauli two component spinor formalism . The wave function of the neutron with spin $\frac{1}{2}$ is described in quantum mechanics by a spinor

$$\boldsymbol{\psi(r)} = \begin{pmatrix} \psi_1(\mathbf{r}) \\ \psi_2(\mathbf{r}) \end{pmatrix}$$

In textbooks about quantum mechanics examples can rarely be found where the two components $\psi_1$ and $\psi_2$ are different functions of space coordinates . This is only the case if the Schrödinger equation includes terms which represent a strong force on magnetic moments, which is different for the two spin orientations. Examples for this are the Stern-Gerlach fields and also the magnetic helical structures of a Bloch wall for neutrons with gracing incidence [4, 5] or even the refraction of neutrons by a magnetic prism. This represents a sort of spin-orbit interaction. In this case the spin up and spin down components have different paths and the two components are separated in space. In the case of the Bloch wall the solution includes plane waves with 8 different wave vectors inside the wall. But those effects play a role only in very strong magnetic field inhomogeneities in ferromagnets. These act as strong forces on the magnetic dipoles of the neutron spin and change the path differently for the two components. In the following we use slowly varying magnetic fields, where the deviation of the neutron path is so small that the paths for both components are the same. Then we can factorize space and spin parts. Slowly varying field in this case is related to the wavelength of the neutron: If the size of the field inhomogeneities is on a length scale orders of magnitude larger then the neutron wavelength then only the magnetic field at the respective point or space region is sensed by the neutron. Space and time coordinates are then only coupled through the neutron velocity $\vec{v}$ with $\vec{r} = \vec{v}t$. Inhomogeneous magnetic fields along the neutron path then appear in spin space only as simple time dependent quantities $\vec{B}(\vec{v}t)$. Then the spinors are only functions of time.

First we want to visualize a constant spinor. We can write spin up $|+\rangle$ and spin down $|-\rangle$

$$|+\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \chi_+ \tag{1.2}$$

$$|-\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \chi_- \tag{1.3}$$

$$\langle +| = (1,0) = \chi_+^\dagger \tag{1.4}$$

$$\langle -| = (0,1) = \chi_-^\dagger \tag{1.5}$$

$$\chi = c_+\chi_+ + c_-\chi_- = \begin{pmatrix} c_+ \\ c_- \end{pmatrix} \tag{1.6}$$

Is there a relationship between the above used $\vec{s} = (s_x, s_y, s_z)$ in three dimensions and this spinor? This relationship between spinor space and cartesian space can be described using Pauli

spin matrices:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{1.7}$$

$$(\langle s_x\rangle, \langle s_y\rangle, \langle s_z\rangle) = \frac{\hbar}{2}(\chi^\dagger \sigma_x \chi, \chi^\dagger \sigma_y \chi, \chi^\dagger \sigma_z \chi) \tag{1.8}$$

which is the relationship between $\vec{s}$ and the spinor $\chi$. Attention has to be paid to the fact that this only connects $\langle s_x\rangle$, $\langle s_y\rangle$, $\langle s_z\rangle$ and not $s_x$, $s_y$, $s_z$.

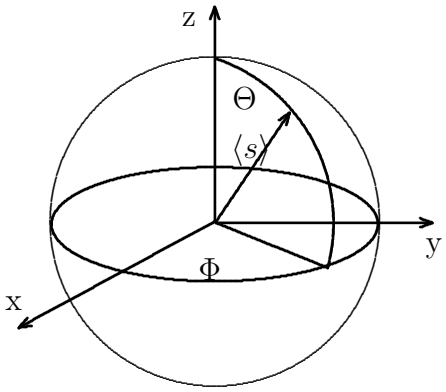



Figure 1.1: Spherical coordinates $(\vartheta, \varphi)$ of the polarization direction of the spin for the visualization of the spinor eq.(1.10)

If we wish to determine the $\chi$ which yields (see fig.1.1)

$$(\langle s_x\rangle, \langle s_y\rangle, \langle s_z\rangle) = \frac{\hbar}{2}(\cos\varphi \sin\vartheta, \sin\varphi \sin\vartheta, \cos\vartheta) \tag{1.9}$$

we find

$$\chi = \begin{pmatrix} \cos\frac{\vartheta}{2} \cdot e^{-i\frac{\varphi}{2}} \\ \sin\frac{\vartheta}{2} \cdot e^{i\frac{\varphi}{2}} \end{pmatrix} \tag{1.10}$$

In order to see this we calculate

$$\left(\cos\frac{\vartheta}{2}e^{i\frac{\varphi}{2}}, \sin\frac{\vartheta}{2}e^{-i\frac{\varphi}{2}}\right) \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \cos\frac{\vartheta}{2}e^{-i\frac{\varphi}{2}} \\ \sin\frac{\vartheta}{2}e^{i\frac{\varphi}{2}} \end{pmatrix} = \sin\vartheta\cos\varphi \tag{1.11}$$

and similarly for y and z-components.

These equations yield the relationships between the expectation values of the vector in the direction $(\varphi, \vartheta)$ in spherical coordinates to the corresponding vector in Cartesian coordinates and to the corresponding spinor in spinor space. In the following we will continuously use these relations to visualize the spinor, and often without much calculation. The process of eq.(1.8) is a strict relationship but it often results in unecessary complicated calculations which we can avoid by remembering the relationships (1.9) and (1.10).

### 1.1.2 Polarization and density matrix ($|P| < 1$ expressible)

How can one prepare a polarized beam? In textbooks this is nearly always done by a Stern-Gerlach magnet. In practice we do it using a magnetized mirror. Such a mirror represents just a simple potential well for one spin state. Inside of each material the neutrons of a neutron beam have

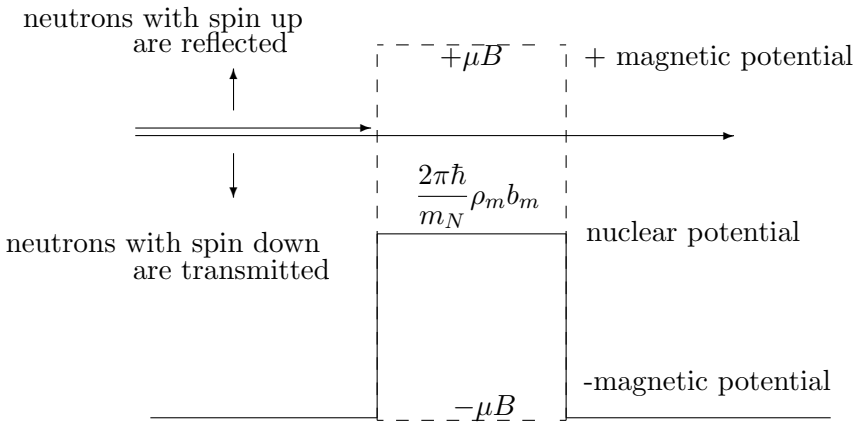



Figure 1.2: Nuclear and magnetic potential wells representing the way how a mirror polarizer works

another velocity than in free space. This can be described by a potential energy. A layer of material acts on a neutron beam like a potential well. If the material is ferromagnetic there is an additional contribution to this potential energy $V_M = \pm\mu_N \cdot B$ the sign depending on the orientation of the magnetic moment of the neutron in the magnetic induction B (see fig.1.2). In an unpolarized beam we have parallel and antiparallel spin components. As the spin and the magnetic moment of the neutron have opposite orientation those neutrons with parallel spin have a higher potential energy inside the magnetized layer. The others have a lower potential energy. If the size of the magnetic potential is just as high as the nuclear potential then only the spin state with a parallel spin sees a potential well. It is reflected, if its total energy is lower than the resulting potential well of the nuclear plus the magnetic contribution. The other component is transmitted or absorbed, if the substrate is made of absorbing material.

If we have a completely polarized neutron beam, we have particles in the state $\chi_+$ or $\chi_-$ in spinor space or particles with the spin direction (0,0,1) in cartesian space, the spin pointing in z-direction. This direction is determined by the quantization axes and is given by the direction of the magnetic field at the polarizer. The expectation values $\chi^\dagger\chi$ for a spinor as given by eq.(1.10) is always normalized to one. The 3d-vector 1.9 has the direction of the polarization of the beam, but it is not clear how with these spinors to express an incomplete polarization. A common factor still would describe a fully aligned spin, which would not be normalized. To describe an incomplete polarized beam one introduces a means of describing an ensemble of pure and mixed states by the density operator. We define with

$$\chi = \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} \qquad |c_1|^2 + |c_2|^2 = 1 \tag{1.12}$$

a new operator which is the dyadic product of $\chi$ and $\chi^\dagger$:

$$\rho = \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} (c_1^*, c_2^*) = \chi\chi^\dagger \tag{1.13}$$

$$\rho = \begin{pmatrix} |c_1|^2 & c_2^* c_1 \\ c_1^* c_2 & |c_2|^2 \end{pmatrix} \tag{1.14}$$

$$= \frac{1}{2}\left(\underline{1} + \vec{P}\cdot\vec{\underline{\sigma}}\right) \tag{1.15}$$

$$= \frac{1}{2}\begin{pmatrix} 1+P_z & P_x - iP_y \\ P_x + iP_y & 1-P_z \end{pmatrix} \tag{1.16}$$

$$= \frac{1}{2}\left(\underline{1} + \begin{pmatrix} \cos\vartheta & \sin\vartheta e^{-i\varphi} \\ \sin\vartheta e^{i\varphi} & -\cos\vartheta \end{pmatrix}\right) \tag{1.17}$$

with the properties

$$\text{Trace } \rho = \text{Tr}\rho = \sum_{i=1}^{2} \rho_{ii} = |c_1|^2 + |c_2|^2 = 1 \tag{1.18}$$

$$\rho^\dagger = \rho \tag{1.19}$$

i.e. $\rho$ is a Hermitian operator. We can immediately see that

$$|c_1|^2 = \frac{1}{2}(1+P_z) \tag{1.20}$$

$$|c_2|^2 = \frac{1}{2}(1-P_z) \tag{1.21}$$

$$P_z = |c_1|^2 - |c_2|^2 \tag{1.22}$$

$$P_x = c_1^* c_2 + c_2^* c_1 = 2\Re\left(c_1^* c_2\right) = 2\Re\left(c_2^* c1\right) \tag{1.23}$$

$$P_y = c_1^* c_2 - c_2^* c1 = 2\Im\left(c_1^* c_2\right) = 2\Im\left(c_2^* c1\right) \tag{1.24}$$

The density operator can be written as $\sum_m |m\rangle\langle m|$ and if $\text{Tr}\rho < 1$ then the probability of each state can be included and it is $\rho = \sum_m |m\rangle p_m \langle m|$. A completely polarized beam with polarization in z-direction $\vec{P} = (0,0,1)$ yields the density matrix

$$\rho = |+\rangle\langle +| = \begin{pmatrix} 1 \\ 0 \end{pmatrix}(1,0) = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \tag{1.25}$$

A completely polarized beam in positive or negative x-direction with $\vec{P} = (\pm 1, 0, 0)$ yields the density matrix

$$\rho = \frac{1}{2}\begin{pmatrix} 1+\cos\vartheta & \sin\vartheta e^{-i\varphi} \\ \sin\vartheta e^{i\varphi} & 1-\cos\vartheta \end{pmatrix} = \begin{pmatrix} \frac{1}{2} & \pm\frac{1}{2} \\ \pm\frac{1}{2} & \frac{1}{2} \end{pmatrix} \tag{1.26}$$

An unpolarized beam with $\vec{P} = 0$ has the density matrix

$$\rho = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix} \tag{1.27}$$

A partially polarized beam consisting of 50% of a beam polarized in +x-direction and of 50% polarized in +y-direction has the density matrix

$$\rho = 0.5 \cdot \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{pmatrix} + 0.5 \cdot \begin{pmatrix} \frac{1}{2} & -\frac{i}{2} \\ \frac{i}{2} & \frac{1}{2} \end{pmatrix} = \begin{pmatrix} \frac{1}{2} & \frac{1-i}{4} \\ \frac{1+i}{4} & \frac{1}{2} \end{pmatrix} \tag{1.28}$$

Using eq.(1.17) we see that this corresponds to a degree of polarization of $1/\sqrt{2} = 0.70$ in the direction (1,1,0). (prepairing is hard, analysis is easier)

A powerful relationship of the density matrix is the following: The ensemble average of an operator A (sometimes also called expectation value, but it should not be mixed up with the quantum

mechanical expectation value alone, it contains both sorts of averages: quantum mechanical and statistical, see below) is $\langle A\rangle$. In quantum mechanics it can be written as

$$\begin{aligned}
\langle A\rangle &= (c_1^*, c_2^*)\begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22}\end{pmatrix}\begin{pmatrix} c_1 \\ c_2\end{pmatrix} && (1.29)\\
&= (c_1^*, c_2^*)\begin{pmatrix} A_{11}c_1 + A_{12}c_2 \\ A_{21}c_1 + A22c_2\end{pmatrix} && (1.30)\\
&= A_{11}c_1^*c_1 + A_{12}c_1^*c_2 + A_{21}c_1c_2^* + A_{22}c_2c_2^* && (1.31)\\
&= \mathrm{Tr}\begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22}\end{pmatrix}\begin{pmatrix} c_1c_1^* & c_1c_2^* \\ c_1^*c_2 & c_2c_2^*\end{pmatrix} && (1.32)\\
&= \mathrm{Tr}\begin{pmatrix} A_{11}c_1c_1^* + A_{12}c_1^*c_2 & A_{11}c_1c_2^* + A_{12}c_2c_2^* \\ A_{21}c_1c_1^* + A_{22}c_1^*c_2 & A_{21}c_1c_2^* + A_{22}c_2c_2^*\end{pmatrix} && (1.33)\\
&= \mathrm{Tr}(A\rho) = \mathrm{Tr}(\rho A) && (1.34)
\end{aligned}$$

$$\boxed{\langle A\rangle = \mathrm{Tr}(\rho A) = \mathrm{Tr}(A\rho)} \qquad (1.35)$$

The reason why it is so powerful is that the trace does not depend on the quantum mechanical representation. So the trace of $\rho A$ can be evaluated using any convenient basis.

The statistical average plays a role if one has a statistical ensemble of N systems, for example with each system having its own spinor $\chi_\nu$ and its own density matrix $\rho_\nu$. Then one gets an average $\overline{\rho}$ by

$$\begin{aligned}
\overline{\rho} &= \frac{1}{N}\sum_{\nu=1}^{N}\rho_\nu = \frac{1}{2}[\begin{pmatrix}1\\0\end{pmatrix}0\\1\end{pmatrix} + ((\frac{1}{N}\sum_\nu P_\nu)\cdot\sigma))] && (1.36)\\
&= \frac{1}{2}(\underline{1} + (\overline{P}\cdot\sigma)) && (1.37)\\
\overline{\langle A\rangle} &= \frac{1}{N}\sum_{\nu=1}^{N}\langle A\rangle_\nu = \frac{1}{N}\sum_{\nu=1}^{N}\mathrm{Tr}_\sigma(\rho_\nu A) && (1.38)\\
&= \mathrm{Tr}(\overline{\rho}A) && (1.39)\\
\overline{P} &= \overline{\langle\sigma\rangle} = \frac{1}{N}\sum_{\nu=1}^{N}\langle\vec{\sigma}\rangle_\nu = \frac{1}{N}\sum_\nu \mathrm{Tr}(\rho_\nu\sigma) && (1.40)\\
&= \frac{1}{2}\mathrm{Tr}_\sigma[(\underline{1} + \overline{P}\cdot\sigma)\sigma] && (1.41)
\end{aligned}$$

As an example we determine the polarization for the mixture as given by eq.(1.28)

$$\langle\sigma_x\rangle = \mathrm{Tr}(\rho\sigma_x) = \mathrm{Tr}\begin{pmatrix} \frac{1}{2} & \frac{1-i}{4} \\ \frac{1+i}{4} & \frac{1}{2}\end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 0\end{pmatrix} = \mathrm{Tr}\begin{pmatrix} \frac{1-i}{4} & \frac{1}{2} \\ \frac{1}{2} & \frac{1+i}{4}\end{pmatrix} = \frac{1}{2} \qquad (1.42)$$

$$\begin{aligned}
\langle\sigma_y\rangle &= \frac{1}{2} && (1.43)\\
\langle\sigma_z\rangle &= 0 && (1.44)\\
\vec{P} &= (\frac{1}{2}, \frac{1}{2}, 0) && (1.45)
\end{aligned}$$

Another example, which we need later, is a beam consisting of neutrons with polarizations equally distributed over a range of $\phi = -\pi/10$ to $\phi = +\pi/10$ about the x-direction. $\vartheta$ shall be a fixed angle say $\pi/2$. In this case the density matrix is

$$\rho = \frac{1}{2}\begin{pmatrix} 1 & \langle e^{-i\varphi}\rangle \\ \langle e^{i\varphi}\rangle & 1 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1 & e^{-\frac{\langle\varphi^2\rangle}{2}} \\ e^{-\frac{\langle\varphi^2\rangle}{2}} & 1 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1 & 0.98 \\ 0.98 & 1 \end{pmatrix} \tag{1.46}$$

i.e. we have a reduced polarization of 98% even if the angular range of the polarization vector is 36 degrees. For the averaging of $\langle e^{i\varphi}\rangle$ we use

$$\begin{aligned} \langle e^{i\varphi}\rangle &= \langle\cos\varphi\rangle + i\langle\sin\varphi\rangle = \langle\cos\varphi\rangle + 0 && (1.47)\\ &= 1 - \frac{1}{2}\langle\varphi^2\rangle + \frac{1}{4!}\langle\varphi^4\rangle - \cdots && (1.48)\\ e^{-\frac{\langle\varphi^2\rangle}{2}} &= 1 - \frac{1}{2}\langle\varphi^2\rangle + \frac{1}{8}\langle\varphi^2\rangle^2 - \cdots && (1.49)\\ \langle\phi^2\rangle &= \frac{5}{\pi}\int_{-\pi/10}^{\pi/10}\phi^2 d\phi = \frac{5}{\pi}\cdot\frac{2}{3}\left(\frac{\pi}{10}\right)^3 && (1.50) \end{aligned}$$

There are also many other useful relationships involving the density matrix

$$\begin{aligned} \rho|\phi\rangle &= \chi\chi^\dagger|\phi\rangle = \chi(\chi^\dagger\phi) && (1.51)\\ \rho^2 &= \rho \quad \text{if } \rho \text{ is a pure state} && (1.52)\\ \vec{P}\underline{\sigma}\chi &= (2\rho-1)\chi = 2\rho\chi - \chi = 2\chi\chi^\dagger\chi - \chi = 2\chi - \chi = \chi && (1.53) \end{aligned}$$

i.e. $\vec{P}$ points in the direction of the spin of the particle. The time evolution of the ensembles is described by

$$i\hbar\frac{\partial\rho}{\partial t} = -[\rho, H] \tag{1.54}$$

The density matrix here is introduced because it is very powerful in the derivation of scattering cross sections for polarized beams. To describe the behaviour of the spin in a polarized beam itself it seems to be more complicated than the above simple spinor description. We will show the usefulness of the density matrix in connection with the derivation of the formulas for scattering cross sections. To understand the way a flipper or a spin rotator works it is easier to use the spinor formalism. But it can also be described using the density matrix formalism.

### 1.1.3 precession coil to rotate spinor in direction $\Theta, \Phi$

#### 1.1.3.1 Spin with direction ($\vartheta$,$\varphi$) in a constant magnetic field in z direction

We want now to apply the knowledge we have gained in the last section.

We want to see the behaviour of the polarization if the vector of the polarization with orientation $\Theta, \Phi$ enters into a magnetic field with (0,0,$B_z$) (see fig.(1.5) First we have to investigate how one can realize this. Normally the spin is kept parallel to the quantization axis by a guide field. Therefore initially the field and the spin are parallel behind the polarizer (see fig.1.5). As seen in figure 1.5 we use a rectangular coil where two mutually orthogonal rectangular coils are wound just one on top of another. In fig.1.5 this is indicated by showing pieces of these coils. The rest of it is cut away to show the windings. These coils must be large enough so that within the cross section of the beam we can expect a homogeneous region of the respective field components. Unfortunately it is not possible to have a sudden transition also in the y direction, the field lines can not just begin

at a wall, they must be closed ($\mathrm{div}\vec{B} = 0$ cannot be avoided). (They can also not just begin at a Meissner shield!). By selecting the currents in each of these coils one can rotate the field inside this rectangular coil in the xz plane into any desired direction. So we get an angle $\mu$ between field and polarization at the entrance of the coil. But $\varphi$ is either 0 or $\pi$.

The result of our following calculation will show that the spin precesses around this new field direction $\mu, 0$ inside the coil (see fig.1.6). By selecting the field direction and the field strength as given in the figure caption 1.6 we can move the polarization direction into any wanted direction at the exit of the sudden xz coil. There it suddenly will enter a field again in z direction. In this way we have prepared a beam with the polarization in direction $\Theta, \Phi$ in a constant magnetic field in z direction at the exit of the coil. i.e. a spinor with the initial condition

$$\chi = \begin{pmatrix} \cos\frac{\Theta}{2} e^{-i\frac{\Phi}{2}} \\ \sin\frac{\Theta}{2} e^{i\frac{\Phi}{2}} \end{pmatrix} \tag{1.57}$$

or in Cartesian space

$$(P_x, P_y, P_z) = (\cos\Phi\sin\Theta, \sin\Phi\sin\Theta, \cos\Theta) \tag{1.58}$$

or with the density matrix

$$\rho = \begin{pmatrix} \cos^2\frac{\Theta}{2} & \cos\frac{\Theta}{2}\sin\frac{\Theta}{2}e^{-i\Phi} \\ \cos\frac{\Theta}{2}\sin\frac{\Theta}{2}e^{i\Phi} & \sin^2\frac{\Theta}{2} \end{pmatrix} = \frac{1}{2}\left(\underline{1} + \begin{pmatrix} \cos\Theta & \sin\Theta e^{-i\Phi} \\ \sin\Theta e^{i\Phi} & -\cos\Theta \end{pmatrix}\right) \tag{1.59}$$

#### 1.1.3.2 Rotation in spinor space

In order to be able to visualize the behaviour of the polarization in a magnetic field with an initial spin of eq.(1.57) we need a simple way to describe the rotation in spinor space. The following will not be a rigorous mathematical demonstration but more an exercise to become acquainted with the spinor space and its visualization. For rigorous mathematics you have to consult the book of Dirac [2] or a book about Quantum Mechanics such as that of Sakurai [12]. A rotation around the z-axis by an angle $\varphi$ is affected by the following matrix

$$e^{i\frac{\varphi}{2}\sigma_z} \equiv \begin{pmatrix} e^{i\frac{\varphi}{2}} & 0 \\ 0 & e^{-i\frac{\varphi}{2}} \end{pmatrix} \tag{1.60}$$

We demonstrate this by showing

1. that this identity is valid and
2. that it represents a rotation around the z axis by the angle $\varphi$.

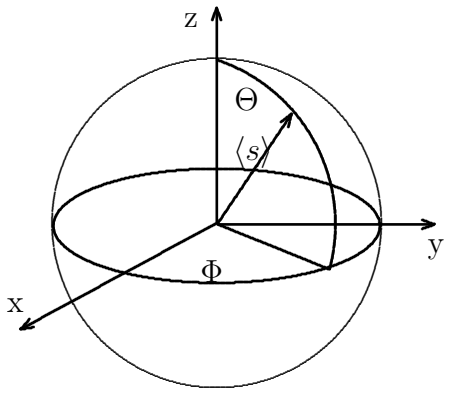



Figure 1.3: The initial conditions with polarization direction $\langle\vec{s}\rangle$ in direction $(\vartheta, \varphi)$ and field $\vec{B}$ in direction z is what we want.

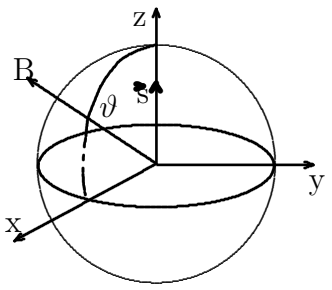



Figure 1.4: Angles of spin $\vec{s}$ and field $\vec{B}$ at the entrance of the sudden xz coil

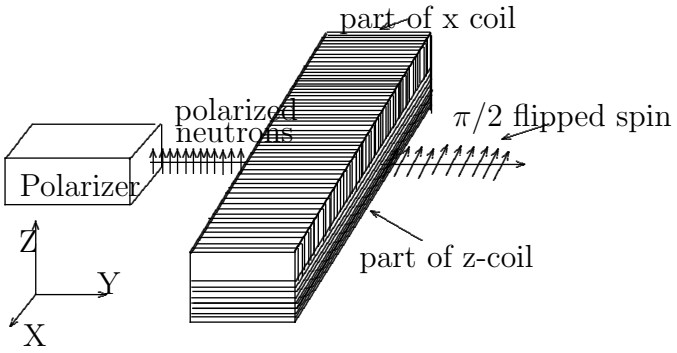
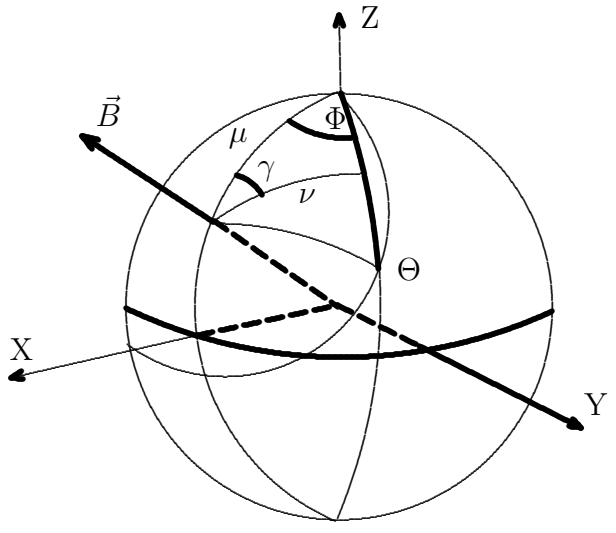
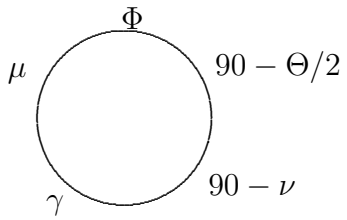



Figure 1.5: Visualization of the possibility to realize the initial condition that a polarized neutron begins in a defined way with a direction $(\Theta, \Phi)$ inclined with respect to a magnetic field $\vec{B}$. It enters suddenly through the walls of two orthogonal coils wound on top of each other as indicated in the figure. (See text)

**this identity is valid**

$$e^{i\frac{\varphi}{2}\sigma_z} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + i\frac{\varphi}{2}\sigma_z + i^2\frac{\varphi^2}{4}\cdot\frac{1}{2!}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \frac{i^3\varphi^3}{2^3\cdot 3!}\sigma_z + \frac{i^4\varphi^4}{2^4\cdot 4!}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad (1.61)$$




Nepers rule gives

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

$$\tan\mu = \frac{\tan\frac{\Theta}{2}}{\cos\Phi} \quad (1.55)$$

$$\cos\gamma = \sin\Phi\cdot\cos\frac{\Theta}{2} \quad (1.56)$$

Figure 1.6: Elementary geometry gives $\mu$ and $\gamma$ as functions of $\Theta$, $\Phi$ (Neper's rules). Adjusting the coil first as a flipper coil gives the current $I_\pi$ for a precession of 180 deg and $I_c$ to compensate the guide field inside the coil. By selecting the current $I = I_\pi \cdot \frac{2\gamma}{180}$ with $I_x = I\sin\mu$ in the sudden x-coil and $I_z = (I - I_c)\cos\mu$ in the z-coil we can manage any spin direction $\Theta, \Phi$ at the exit of the coils. Outside the coils $\vec{B}$ is in z direction.

$$= \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \cos\frac{\varphi}{2} + i\sigma_z \sin\frac{\varphi}{2} \tag{1.62}$$

$$= \begin{pmatrix} \cos\frac{\varphi}{2} & 0 \\ 0 & \cos\frac{\varphi}{2} \end{pmatrix} + i \begin{pmatrix} \sin\frac{\varphi}{2} & 0 \\ 0 & -\sin\frac{\varphi}{2} \end{pmatrix} \tag{1.63}$$

$$= \begin{pmatrix} e^{i\frac{\varphi}{2}} & 0 \\ 0 & e^{-i\frac{\varphi}{2}} \end{pmatrix} \tag{1.64}$$

**it represents a rotation around the z axis by the angle $\varphi$**

We can show this by using the fact that the relationship between the spinor space and the three dimensional space can be expressed by the Pauli spin matrices. If we want to transform the vector $\vec{P} = (x, y, z)$ by the application of the above rotation operator to $\vec{P'} = (x', y', z')$ then we have to transform it in the following way

$$\vec{P'}\sigma = \begin{pmatrix} z' & x' - iy' \\ x' + iy' & -z' \end{pmatrix} \tag{1.65}$$

$$= e^{i\frac{\varphi}{2}\sigma_z} \begin{pmatrix} z & x - iy \\ x + iy & -z \end{pmatrix} e^{-i\frac{\varphi}{2}\sigma_z} \tag{1.66}$$

$$= \begin{pmatrix} e^{i\frac{\varphi}{2}} & 0 \\ 0 & e^{-i\frac{\varphi}{2}} \end{pmatrix} \begin{pmatrix} z & x - iy \\ x + iy & -z \end{pmatrix} \begin{pmatrix} e^{-i\frac{\varphi}{2}} & 0 \\ 0 & e^{i\frac{\varphi}{2}} \end{pmatrix} \tag{1.67}$$

$$= \begin{pmatrix} e^{i\frac{\varphi}{2}} & 0 \\ 0 & e^{-i\frac{\varphi}{2}} \end{pmatrix} \begin{pmatrix} ze^{-i\frac{\varphi}{2}} & (x - iy)e^{i\frac{\varphi}{2}} \\ (x + iy)e^{-i\frac{\varphi}{2}} & -ze^{i\frac{\varphi}{2}} \end{pmatrix} \tag{1.68}$$

$$= \begin{pmatrix} z & (x - iy)e^{i\varphi} \\ (x + iy)e^{-i\varphi} & -z \end{pmatrix} \tag{1.69}$$

From this we see immediately

$$x' = x\cos\varphi + y\sin\varphi \tag{1.70}$$

$$y' = -x\sin\varphi + y\cos\varphi \tag{1.71}$$

$$z' = z \tag{1.72}$$

that it represents a rotation in three dimensional space around the z axis by an angle $\varphi$.

We can also show it by the effect of the rotation operator on the spinor

$$e^{i\frac{\gamma}{2}\sigma_z} \begin{pmatrix} \cos\frac{\vartheta}{2}e^{-i\frac{\varphi}{2}} \\ \sin\frac{\vartheta}{2}e^{i\frac{\varphi}{2}} \end{pmatrix} = \begin{pmatrix} e^{i\frac{\gamma}{2}} & 0 \\ 0 & e^{-i\frac{\gamma}{2}} \end{pmatrix} \begin{pmatrix} \cos\frac{\vartheta}{2}e^{-i\frac{\varphi}{2}} \\ \sin\frac{\vartheta}{2}e^{i\frac{\varphi}{2}} \end{pmatrix} = \begin{pmatrix} \cos\frac{\vartheta}{2}e^{-i\frac{(\varphi-\gamma)}{2}} \\ \sin\frac{\vartheta}{2}e^{i\frac{(\varphi-\gamma)}{2}} \end{pmatrix} \tag{1.73}$$

This shows that the application of the above rotation operator diminishes just the angle $\varphi$ i.e. it represents a rotation around the z axis in the clockwise sense.

Similarly one gets for **the rotation about x**

$$e^{i\frac{\chi}{2}\sigma_x} = \underline{1}\cos\frac{\chi}{2} + i\sigma_x \sin\frac{\chi}{2} = \begin{pmatrix} \cos\frac{\chi}{2} & i\sin\frac{\chi}{2} \\ i\sin\frac{\chi}{2} & \cos\frac{\chi}{2} \end{pmatrix} \tag{1.74}$$

and for the **rotation about the y axis**

$$e^{i\frac{\vartheta}{2}\sigma_y} = \underline{1}\cos\frac{\vartheta}{2} + i\sigma_y \sin\frac{\vartheta}{2} = \begin{pmatrix} \cos\frac{\vartheta}{2} & \sin\frac{\vartheta}{2} \\ -\sin\frac{\vartheta}{2} & \cos\frac{\vartheta}{2} \end{pmatrix} \tag{1.75}$$

Generally a **rotation around an axis $\vec{n}$ by an angle** $\omega$ we get the rotation operator

$$e^{i\frac{\omega}{2}\vec{n}\cdot\vec{\sigma}} = \underline{1}\cos\frac{\omega}{2} + i\sin\frac{\omega}{2}\vec{n}\cdot\vec{\sigma} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\cos\frac{\omega}{2} + i\sin\frac{\omega}{2}\begin{pmatrix} \cos\vartheta & \sin\vartheta e^{-i\varphi} \\ \sin\vartheta e^{i\varphi} & -\cos\vartheta \end{pmatrix} \tag{1.76}$$

with

$$\vec{n} = (\cos\varphi\sin\vartheta, \sin\varphi\sin\vartheta, \cos\vartheta) \tag{1.77}$$

### Some exercises to become acquainted with these spinors

1. Determine the direction $\vartheta, \varphi$ for an arbitrary spinor $\begin{pmatrix} a_1 \\ b_1 \end{pmatrix}$.

   **Solution:**

   $$\begin{pmatrix} a_1 \\ b_1 \end{pmatrix} = c_1\begin{pmatrix} \cos\frac{\vartheta}{2}e^{-i\frac{\varphi}{2}} \\ \sin\frac{\vartheta}{2}e^{i\frac{\varphi}{2}} \end{pmatrix} \quad \text{with} \quad \tan\frac{\vartheta}{2} = \frac{|b_1|}{|a_1|} \quad \text{and} \quad \varphi = \arg b_1 - \arg a_1 \tag{1.78}$$

2. Given the spinor $\chi = \begin{pmatrix} e^{i\alpha}\cos\delta \\ e^{i\beta}\sin\delta \end{pmatrix}$. a) Determine the polarization vector. b) determine the matrix which rotates it to $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$

   **Solution:**

   $$\vartheta = 2\delta; \quad \text{and} \quad \varphi = \beta - \alpha; \quad \text{with} \quad \vec{P} = (\sin 2\delta\cos(\beta-\alpha), \sin 2\delta\sin(\beta-\alpha), \cos 2\delta) \tag{1.79}$$

   By inspection one sees that one has to rotate by $\beta - \alpha$ around the z-axis and then by $2\delta$ around the x-axis. This yields the matrices

   $$e^{-i\frac{\beta+\alpha}{2}}\begin{pmatrix} \cos\delta & \sin\delta \\ -\sin\delta & \cos\delta \end{pmatrix}\begin{pmatrix} e^{i\frac{\beta-\alpha}{2}} & 0 \\ 0 & e^{-i\frac{\beta-\alpha}{2}} \end{pmatrix} = \underline{Q} \tag{1.80}$$

   Applying this to $\chi$ results in the required spinor as one can see by inspection.

## 1.1.4 Time dependent Schrödinger equation

### 1.1.4.1 The next steps:various flippers, CRYOPAD, SSPAD,

Now we want to see the behaviour of the spinor inside the coil with the field in $(\vartheta, \varphi)$ direction which represents a constant homogeneous magnetic field inside the coil of fig.1.5. This will indicate the way how various sorts of flippers work such as a $\pi/2$-flipper or a $\pi$-flipper. We will see how this can be used to completely measure a precessing spin. This gives us the understanding of a polarimeter for neutrons, which is realized with the CRYOPAD at the ILL and can be also done on an instrument like D7 after the addition of a $\pi/2$ flipper coil behind an adjustable guide field section between sample and analyzer, which we could call simplified spherical polarization analysis device (SSPAD), because it avoids complicated cryotechniques. After this we will derive the behaviour of a spin rotator which is a static field which changes the direction as a function of space coordinate (e.g. a helix). This is accomplished by the solution of the time dependent Schrödinger equation in a magnetic field with a helical geometry in space, which again can be realized by an appropriately wound coil. This helps us to understand what happens if we change the direction of the guide field of the neutron spin. Then we will shortly apply our knowledge to the uncertainty relationship for the spin and try to get out as much as possible from it (omitted because of space limitations). After this we have all the necessary elements to measure and to analyse the scattering of polarized neutrons. We still require some introduction into the theoretical concepts of the different sorts of scattering of polarized neutrons. This can be done by calculating the transition probabilities or by application of the density matrix formalism to polarized beam scattering.

#### 1.1.4.2 Spin behaviour in a constant homogeneous magnetic field

The description of a spin in a constant B-field can be obtained by using the time dependent Schrödinger equation. For this we need the potential of the spin in a magnetic field. The magnetic moment of the neutron is $\mu \cdot \vec{\sigma}$ with $\mu$ given by eq.(1.1 on page 5) and $\vec{\sigma}$ the Pauli spin matrices. The potential energy in the field $\vec{B}$ is then $V = -\mu\vec{\sigma} \cdot \vec{B}$. Omitting the dependence on $\vec{r}$ and concentrating on the spin only we can write down the time dependent Schrödinger equation of this problem (reason that this is possible see 1.1.1 on page 6):

$$i\hbar\frac{\partial}{\partial t}\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix} = \mu\vec{\sigma}\cdot\vec{B}\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix} \tag{1.81}$$

$$\frac{\partial}{\partial t}\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix} = \frac{\mu B}{i\hbar}\begin{pmatrix}\cos\vartheta & \sin\vartheta e^{-i\varphi}\\ \sin\vartheta e^{i\varphi} & \cos\vartheta\end{pmatrix}\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix} \tag{1.82}$$

$$= -i\frac{\omega_L}{2}\begin{pmatrix}\cos\vartheta & \sin\vartheta e^{-i\varphi}\\ \sin\vartheta e^{i\varphi} & \cos\vartheta\end{pmatrix}\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix} \tag{1.83}$$

$$= -\frac{i}{2}\begin{pmatrix}\omega_z & \omega_x - i\omega_y\\ \omega_x + i\omega_y & -\omega_z\end{pmatrix}\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix} \tag{1.84}$$

with

$$\omega_L = \frac{2\mu B}{\hbar} \tag{1.85}$$

$$\omega_x = \omega_L \sin\vartheta \sin\varphi \tag{1.86}$$

$$\omega_y = \omega_L \sin\vartheta \cos\varphi \tag{1.87}$$

$$\omega_z = \omega_L \cos\vartheta \tag{1.88}$$

Separation of variables yields

$$\frac{d\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix}}{\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix}} = -i\frac{\omega_L}{2}\begin{pmatrix}\cos\vartheta & \sin\vartheta e^{-i\varphi}\\ \sin\vartheta e^{i\varphi} & \cos\vartheta\end{pmatrix}dt \tag{1.89}$$

Integration gives

$$ln\begin{pmatrix}\psi_1(t)\\ \psi_2(t)\end{pmatrix} - ln\begin{pmatrix}\psi_1(0)\\ \psi_2(0)\end{pmatrix} = -i\frac{\omega_L}{2}\begin{pmatrix}\cos\vartheta & \sin\vartheta e^{-i\varphi}\\ \sin\vartheta e^{i\varphi} & \cos\vartheta\end{pmatrix}t \tag{1.90}$$

$$= -\frac{i}{2}\begin{pmatrix}\omega_z & \omega_x - i\omega_y\\ \omega_x + i\omega_y & -\omega_z\end{pmatrix}t \tag{1.91}$$

$$\begin{pmatrix}\psi_1(t)\\ \psi_2(t)\end{pmatrix} = e^{-i\frac{\omega_L t}{2}\begin{pmatrix}\cos\vartheta & \sin\vartheta e^{-i\varphi}\\ \sin\vartheta e^{i\varphi} & \cos\vartheta\end{pmatrix}}\begin{pmatrix}\psi_1(0)\\ \psi_2(0)\end{pmatrix} \tag{1.92}$$

With our knowledge of rotations in spinor space we see immediately that this represents a rotation of $\omega_L t$ around the axis $\vec{n}$, which has the direction $\vartheta, \varphi$ in space, i.e. around the field $\vec{B}$.

We include here only the spin but not the space behaviour. In [6, 7] also the space behaviour of a wave packet and the beam as a quantum mechanical current is included in the description, but here this would hide the essential behaviour under many practically empty formulas. If you have understood the essential things you can add this formalism yourself.

# Chapter 2

# Applications for measuring equipment

## 2.1 Behaviour of the spin in a $\pi$ flipper coil

We want to apply the solution eq.(1.92) for a field along the x-axis of our coil. For this we adjust the currents in the xz-sudden-coil of fig.1.5 so that the guide field in z-direction is compensated inside the coil and only a field in x-direction exists. This corresponds to $\vartheta = 90^0$ and $\varphi = 0^0$. With this we obtain

$$\vec{n}\vec{\sigma} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tag{2.1}$$

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

$$\begin{pmatrix} \psi_1(t) \\ \psi_2(t) \end{pmatrix} = e^{-i\frac{\omega_L t}{2}\sigma_x} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \tag{2.2}$$

$$= \begin{pmatrix} \cos\frac{\omega_L t}{2} & i\sin\frac{\omega_L t}{2} \\ i\sin\frac{\omega_L t}{2} & \cos\frac{\omega_L t}{2} \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \tag{2.3}$$

$$= \begin{pmatrix} \cos\frac{\omega_L t}{2} \\ i\sin\frac{\omega_L t}{2} \end{pmatrix} = e^{i\frac{\pi}{4}} \begin{pmatrix} \cos\frac{\omega_L t}{2} e^{-i\frac{\pi}{4}} \\ \sin\frac{\omega_L t}{2} e^{i\frac{\pi}{4}} \end{pmatrix} \tag{2.4}$$

With our knowledge of the visualization of a spinor from eq.(1.9) and fig.1.1 we can immediately visualize this as a precession of an incident spin $|+>$ with $\vartheta$ changing with time and $\varphi = \pi/2$ fixed i.e. around the x-axis in the y-z plane with the time dependent angle $\omega_L t$ (see fig.2.1). If we adjust the current in this coil so, that the time of flight through the coil is just the time needed for half a Larmour precession around the x-axis, the neutron exits from the coil with spin direction reversed with respect to the direction of the guide field. This is exactly the behaviour of a **flipper coil**. For this we only need dc-currents and it has nothing to do with a random process, as the word insinuates. It is the result of a classical spin precession. The transition from the guide field to inside of this coil and the transition from the inside of the coil to the guide field on the outside are sudden transitions, the neutron remains in its state that it had before.

The adjustment of the currents for such a flipper can be done in the easiest way by first calculating the necessary current for half a Larmor precession for the pathlength L in the coil and the wavelength $\lambda$ of the neutrons by

$$H_\pi = \frac{67.825}{\lambda[\text{Å}]L[cm]} \text{ Oerstedt} = \frac{67.825}{\lambda[nm]L[cm]} \text{ mT} \tag{2.5}$$

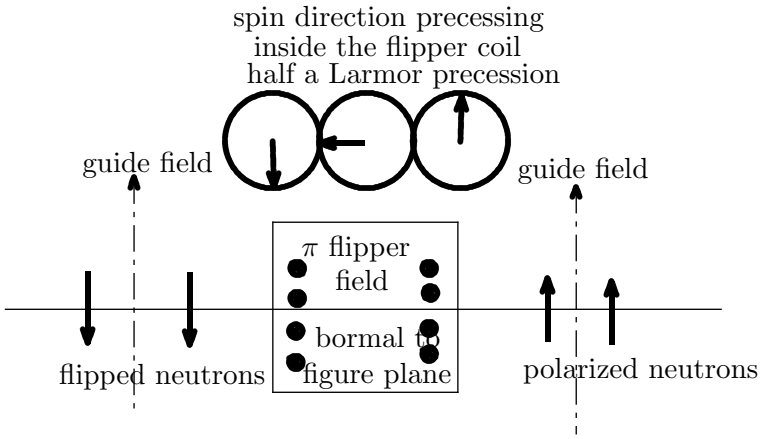



Figure 2.1: Half a Larmor precession as a $\pi$ flipper

Setting the x coil to this current value one then carries out a current scan for the field that compensates the guide field. This can then be fitted using a parabola and the minimum of the parabola is the best correction current. Then one can repeat this also for the x coil and then again for the z-coil until it does not change. The advantage of this method is that it uses also count rates which are not too small to find the minimum.

### 2.1.1 Polarization measurement

Using such a flipper coil and a second polarizing mirror as analyzer we are now able to determine the degree of polarization. For this we measure the intensity $I^{\uparrow\uparrow}$ with spin not flipped and the intensity $I^{\uparrow\downarrow}$ with spin flipped. Their ratio (after background subtraction) gives the flipping ration $R = I^{\uparrow\uparrow}/I^{\uparrow\downarrow}$ and the polarization $P = (R-1)/(R+1)$.

The measurement of polarization can be done with different degrees of sophistication. We use a polarizer, a flipper and a second polarizer as analyzer. Each of these elements has its imperfections. Sometimes (often in nuclear physics experiments) one needs the exact polarization of the beam at the target position. Then one has to separate the contributions to the imperfections of each of the elements. One has to determine the efficiencies of the polarizer, the analyzer, and the flipper separately. The **polarizing efficiency P** can be defined as the degree of polarization attained by an unpolarized beam on passing through the polarizer. The **flipper efficiency f** can be defined as the fraction of spins reversed by the flipper .

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

$$\underline{\underline{F}} = \begin{pmatrix} \epsilon & 1-\epsilon \\ 1-\epsilon & \epsilon \end{pmatrix} \tag{2.6}$$

the properties of a polarizer correspondingly by the matrix representation $\binom{P_{11}\,P_{12}}{P_{21}\,P_{22}}$. In this matrix $P_{11}$ gives the part of the incident beam which is transmitted without spin change. $P_{12}$ gives the part of the beam that is flipped from spin down to spin up. $P_{21}$ the part flipped from spin up to spin down and $P_{22}$ is the part of spin down wich remains in spin down when transmitted through the polarizer. These properties can be measured on a test set-up which has a polarizer and an analyzer and a flipper in front of the test object and a flipper behind the test object as shown in figure 2.2. The countrate without flipper currents gives $P_{11}$, with only flipper1 on we get $P_{12}$, with only flipper2 on we get $P_{21}$ and with both flippers on we get $P_{22}$. If $P_{21} \neq P_{12}$ we have a matrix

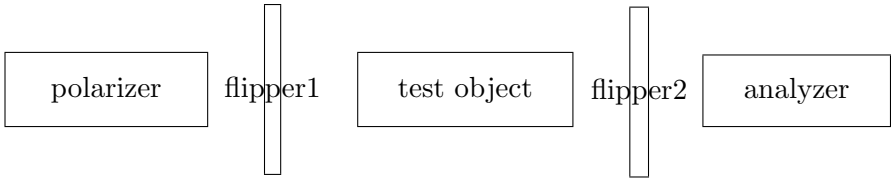



Figure 2.2: Measurement of the properties of a polarizer in the position "test object". When no test object is present one can measure the flipper efficiencies.

which is not conserving parity or perhaps an error in measurement. With these measurements we get the polarizer efficiency from

$$\begin{pmatrix} A \\ B \end{pmatrix} = \frac{1}{\sqrt{2}} \cdot \begin{pmatrix} P_{11}+P_{12} \\ P_{21}+P_{22} \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} P_{11} & P_{12} \\ P_{21} & P22 \end{pmatrix} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \tag{2.7}$$

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

$$P = \frac{P_{11}+P_{12}-P_{21}-P_{22}}{P_{11}+P_{12}+P_{21}+P_{22}} = \frac{A-B}{A+B} \tag{2.8}$$

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

$$\begin{pmatrix} A_f \\ B_f \end{pmatrix} = \begin{pmatrix} \epsilon & 1-\epsilon \\ 1-\epsilon & \epsilon \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} A\epsilon + B(1-\epsilon) \\ A(1-\epsilon) + B\epsilon \end{pmatrix} \tag{2.9}$$

with the polarization

$$P_f = \frac{A\epsilon + B(1-\epsilon) - A(1-\epsilon) - B\epsilon}{A\epsilon + B(1-\epsilon) + A(1-\epsilon) + B\epsilon} = \frac{(1-2\epsilon)(B-A)}{A+B} = -(1-2\epsilon)P \tag{2.10}$$

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

$$\begin{pmatrix} \epsilon' & 1-\epsilon' \\ 1-\epsilon' & \epsilon' \end{pmatrix} \begin{pmatrix} \epsilon & 1-\epsilon \\ 1-\epsilon & \epsilon \end{pmatrix} = \begin{pmatrix} 1-(\epsilon+\epsilon'-2\epsilon\epsilon') & \epsilon+\epsilon'-2\epsilon\epsilon' \\ \epsilon+\epsilon'-2\epsilon\epsilon' & 1-(\epsilon+\epsilon'-2\epsilon\epsilon') \end{pmatrix} \tag{2.11}$$

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

$$\begin{pmatrix} -(A-B)(\epsilon+\epsilon'-2\epsilon\epsilon') + A \\ (A-B)(\epsilon+\epsilon'-2\epsilon\epsilon') + B \end{pmatrix} \tag{2.12}$$

with the polarization

$$P_{ff'} = P[1-2(\epsilon+\epsilon'-2\epsilon\epsilon')] \quad \text{with} \tag{2.13}$$

$$P = \frac{A-B}{A+B} \tag{2.14}$$

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

$$I^{\uparrow\uparrow} = A \tag{2.15}$$

$$I^{\downarrow\uparrow} = A\epsilon + B(1-\epsilon) \tag{2.16}$$

$$I^{\uparrow\downarrow} = A\epsilon' + B(1-\epsilon') \tag{2.17}$$

$$I^{\downarrow\downarrow} = A - (A-B)\epsilon_{eff} \tag{2.18}$$

Combining these measured values one obtains the flipper efficiency:

$$\frac{I^{\uparrow\uparrow} - I^{\downarrow\downarrow}}{I^{\uparrow\uparrow} - I^{\uparrow\downarrow}} = \frac{(A-B)\epsilon_{eff}}{(A-B)(1-\epsilon)} \tag{2.19}$$

$$= \frac{\epsilon' + \epsilon - 2\epsilon\epsilon'}{1-\epsilon} \tag{2.20}$$

$$= \frac{2\epsilon - 2\epsilon^2}{1-\epsilon} = 2\epsilon \tag{2.21}$$

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. A similar procedure including 4 flippers and three polarizers for precision measurements of the polarization in an experimental set up is described in [8].

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

Assume that we need to rotate the incident spin of the neutron $|+>$ by $90^0$ so that afterwards it is normal to the guide field. We can use the same coil as above, but we have to adjust the field so that it is inclined by $45^0$ in the xz plane. If the field strength is the same as in the last section for the $\pi$-flipper, then the spin describes again half a Larmor precession on the path length inside the coil. We have a similar set of equations to solve which should now be easy to do. At the exit from the coil the neutron spin will then be in the xy-plane and precess around the guide field outside the coil.

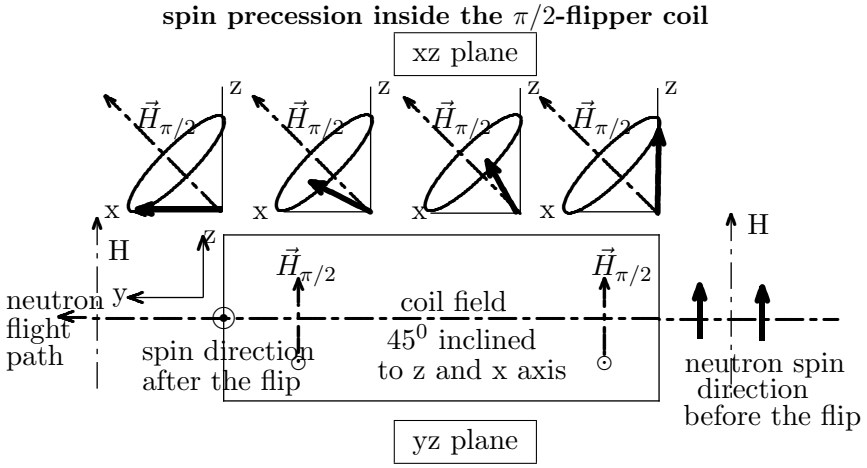



Figure 2.3: Half a Larmor precession as a $\pi/2$ flipper

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

Adjustment of the coil first as a $\pi$-flipper gives the current for $H_\pi$. The coil field for the $\pi/2$ coil must be set to $H_\pi/\sqrt{(}2)$. Then the correction coil is used to adjust the field so that the polarization $\vec{P}$ appears to be totally depolarized at the analyzer, i.e. that the counting rate is not changed if the spin is flipped using the $\pi$-coil (switching the current on or off).

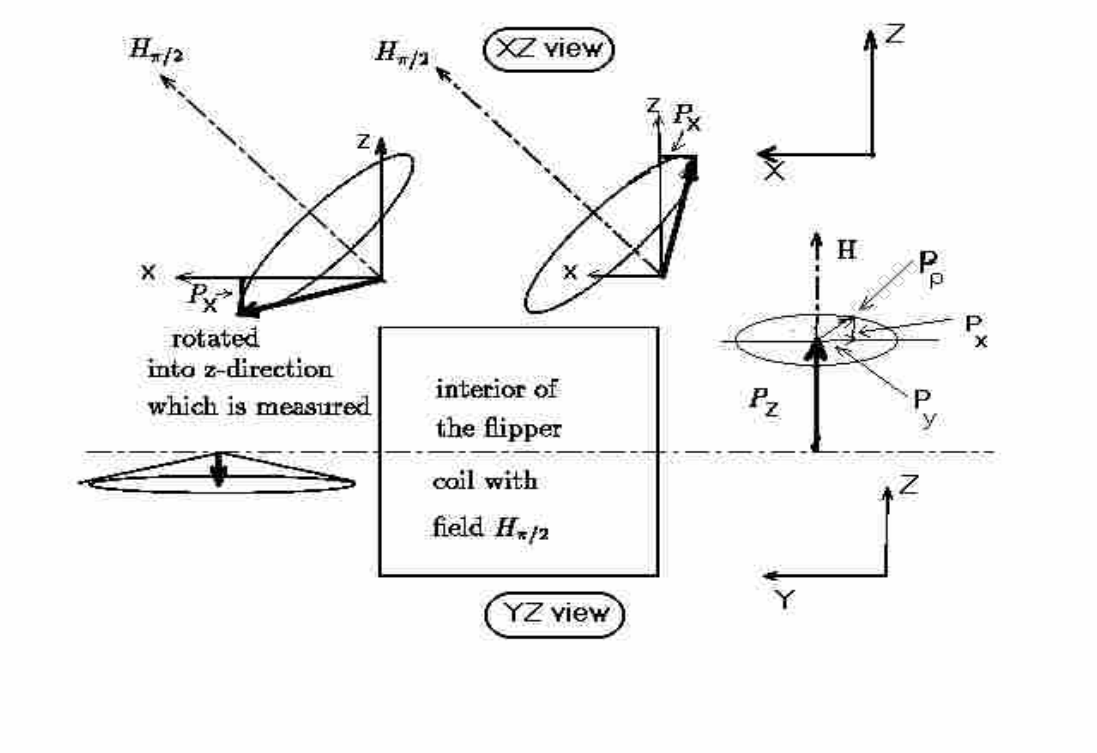



Figure 2.4: Measurement of one of the fluctuating components of the precessing spin polarization using the $\pi/2$ flipper at the entrance of the flipper. The yz-view shows at the right the precessing polarization with $(P_x, P_y, P_z)$. $P_z$, $P_\rho$, $P_x$ and $P_y$ are drawn. When it enters into the flipper coil it has e.g. the component $P_x$ as shown in xz-view of the figure. By the $\pi/2$ coil this is rotated in the z direction as shown in the figure. The spin polarization at the exit of the coil is beginning a precession around this component as shown on the left side of the figure.

### 2.2.2 Measurement of precessing spin polarization, CRYOPAD, SSPAD

By using such a $\pi/2$-flipper coil it is possible to determine the polarization for the case of a beam with precessing spin polarization, i.e. a polarization vector which is oriented in another direction compared to the field and which is therefore precessing in this field. Such a coil rotates the spin component which is normal to the initial z-direction and normal to the flight path into the z-direction. There it can be measured using a spin flipper and a spin analyzer (=a mirror that reflects only one spin) (see fig.2.4). The $\rho$-component of the polarization can be measured by the use of a varable guide field in front of the $\pi/2$-flipper. This can consist of a simple rectangular coil (see fig.2.5), which makes possible to shift the $\rho$-direction of the polarization into the x-direction by accelerating the precession without changing its cone angle. The $\rho$-direction is found when the $\pi/2$-flipped intensity is at a maximum. The $\pi$-flipper to measure the polarization has for such measurements to be between the $\pi/2$-flipper and the analyzer and this is possible for as many detectors as one can equip with the unit of fig. 2.5. If at the same position in space one analyses the polarization in three space directions by rotating $P_x$ with a $\pi/2$ flipper and $P_\rho$ with the variable guide field and a $\pi/2$-flipper into the z-direction where the x, the $\rho$ and the z-component $P_x$, $P_\rho$ and $P_z$ can be determined using a $\pi$-flipper and an analyzing mirror 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 of fig.1.5 or of the second coil of fig.2.5. This allows also to measure the full polarization in

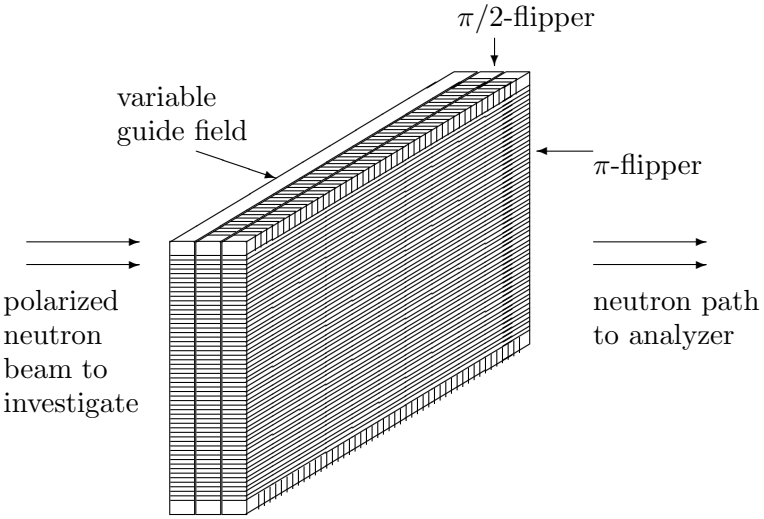



Figure 2.5: Unit to insert between sample and analyzer to measure the complete precessing spin polarization. The first coil is a variable guide field to shift the $\rho$-component into the x.direction without changing the cone angle. $\rho$-component is found when the $\pi/2$-flipped intensity is a maximum by variation of the current in coil 1. The third coil may be superfluous

the case of a precessing spin polarization and to see whether there is somewhere a depolarization in the scattering process

This is the way how a polarimeter works. Such polarimeters were developed around 1970 in three different laboratories [9, 10, 11] In this case the rotation of the spin by rotating it using a slowly rotating guide field, (which we describe in the following section), is not sufficient. This is only sufficient to measure the component of the polarization parallel to the guide field of a scattered beam. If one wants to measure the full polarization one has to use additionaly a $\pi/2$-flipper, a variable guide field and position a $\pi$ flipper in front of the analyzer.

During the discussion in a Summerschool in Jülich Dr.Schweika from Jülich made the remark, that one should insert the $\pi/2$-flipper with the varable guide field in front of the sample and adjust it so that at the center of the sample the spin direction points into the x, y, z direction with the field direction of the spinturn coil independently having the x, y, z direction. Then one can measure the full polarization matrix with 9 elements with all detectors equipped with analyzers simultaneously and even in time of flight mode of the instrument. This would be the most general way of measuring this matrix even with an applied field, i.e. without the necessity of a zero field.

The CRYOPAD fig.2.6 is a polarimeter, which enables the measurement of the three components of the polarization vector after scattering by a magnetic single crystal for each incident polarization vector component separately (in total 9 results for one scattering). 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 $P_{ij}$. This shows that it is interesting to be able to measure this matrix. In the papers of this group one can find often the statement that with a guide field at the sample all polarization components normal to the guide field arising by the magnetic scattering immediately begin to precess and are so unmeasurable. We have seen, that this is not true, they can be measured by adding a $\pi/2$-flipper coil somewhere between the sample and the analyzer and additionaly a piece of guide field with a coil to find the maximum of the polarization in the $\rho$-direction with $\rho = \sqrt{x^2 + y^2}$ = cylinder coordinate with guide field direction as cylinder axis. The angle of the precession cone remains namely constant on the whole way from the sample to the analyzer. 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 in section 1.1.2 on page 11. The sample thickness giving such a smearing can be estimated with the help of eq.(2.5 on page 17) which gives the path length

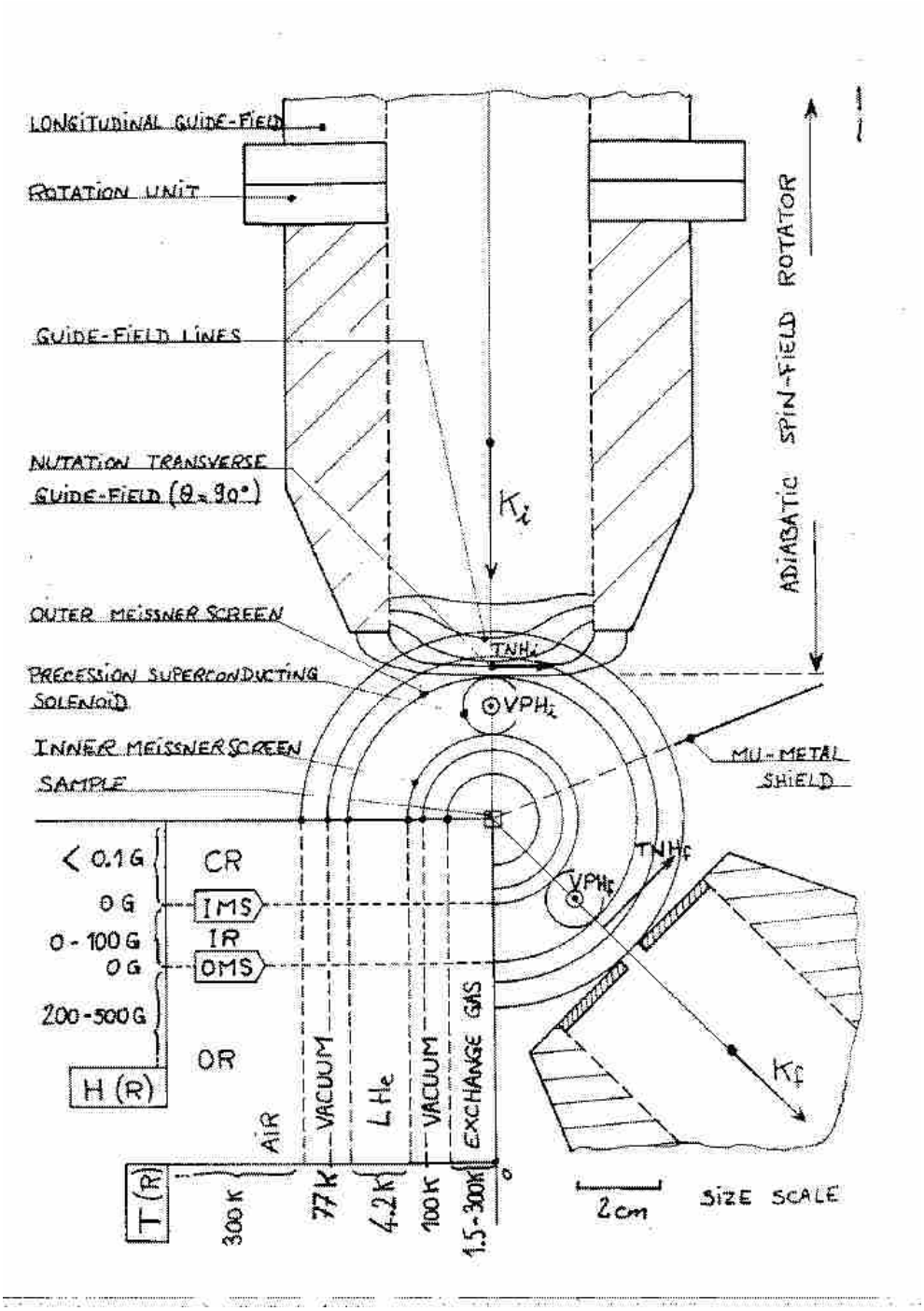



Figure 2.6: Construction of the CRYOPAD taken from [37]

for the precession of $\pi$ 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. With such a simple improvement one can change a 3d-polarization analysis instrument into a spherical polarimeter simultaneously avoiding all the uncertainities which arise from the strong (mutually interacting) fields of the adiabatic spin rotators contradicting the condition of no field at the sample position when the Meissner shield becomes superconducting, of mirror images of the field in

superconductors and from the small size of the rotation coils inside the Meissner shields and that one has no easy access to the interior of this shield in order to be able to control these fields, and all the problems with cryogenics. To distinguish the $P_x$ and $P_y$ 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. Perhaps one could use a quartz sample inside a $\pi/2$-flipper coil to calibrate the instrument. One can call such an instrument SSPAD = simplified spherical polarization analysis device. It makes possible measurements to determine all components of $P_{ij}$ as with the CRYOPAD. One could even think that the CRYOPAD could be simplified using only one Meissner shield, avoid the nutator by two sudden xz-coils (see fig.1.5 on page 13) to rotate the spin inside these coils into the wanted directions.

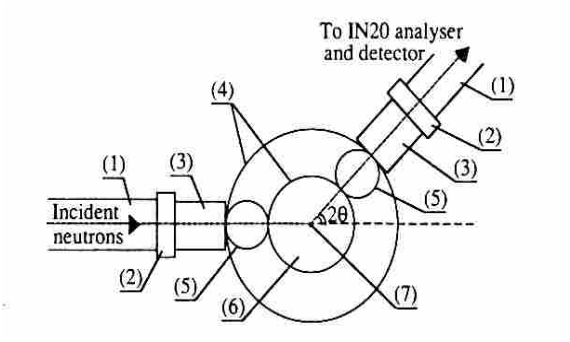



Figure 2.7: Schematic horizontal cross section of CRYOPAD. (1) axial guide field (150 Oe); (2) non-magnetic rotation unit; (3) adiabatic rotation (250 Oe); (4) concentric Meissner shields; (5) vertical superconducting solenoids - precession field (up to 100 Oe); (6) zero field chamber with variable temperature insert; (7) sample position

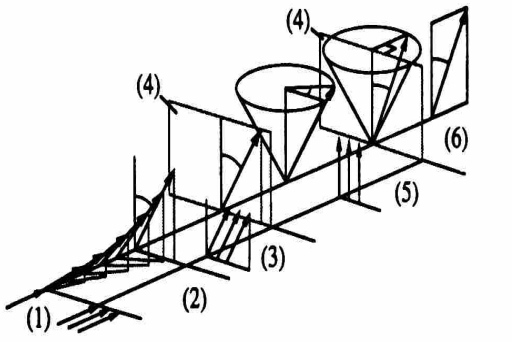



Figure 2.8: Polarization directions in different regions:(1) axially polarized incident neutrons (2) and (3) overlap, spin adiabatically rotated. (4) Meissner shields; (5) precession region; (6) zero field; (7) sample position

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

What happens if we change the direction of the guide field slowly can be investigated by solving the Schrödinger equation for polarized neutrons in the coil of fig.2.9. The neutron flies with constant velocity along the z-direction. It experiences a rotating field. We can also apply an additional field $B_z$ in z-direction. The effective field is

$$\vec{B} = (0, 0, B_z) + B_1(\cos\omega t, -\sin\omega t, 0) \tag{2.22}$$

The time dependent Schrödinger equation for this problem is

$$\frac{\partial}{\partial t}\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix} = \frac{\mu\vec{\sigma}\vec{B}}{i\hbar}\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix} = -\frac{i}{2}\begin{pmatrix}\omega_z & \omega_1 e^{i\omega t}\\ \omega_1 e^{-i\omega t} & -\omega_z\end{pmatrix}\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix} \tag{2.23}$$

We transform this equation to a coordinate system that rotates with the frequency the spin senses from the rotating field $\omega$ around the z-axis. This is accomplished by

$$\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix} = e^{i\frac{\omega t}{2}\sigma_z}\begin{pmatrix}\varphi_1\\ \varphi_2\end{pmatrix} \tag{2.24}$$

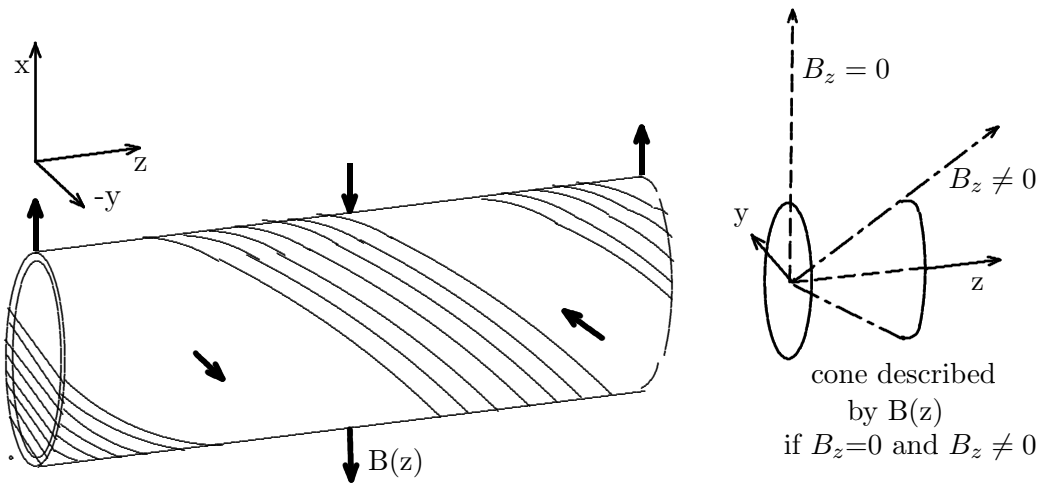



Figure 2.9: Coil to generate a helical magnetic field wound on the outside of a hollow cylinder. Depending on whether or not we apply a constant field along the z direction, on the right of the picture the cone is given which describes the magnetic induction B(z) either as a flat circle or as a cone

$$\begin{pmatrix} \dot{\psi}_1 \\ \dot{\psi}_2 \end{pmatrix} = i\frac{\omega}{2}\sigma_z e^{i\frac{\omega t}{2}\sigma_z}\begin{pmatrix} \varphi_1 \\ \varphi_2 \end{pmatrix} + e^{i\frac{\omega t}{2}\sigma_z}\begin{pmatrix} \dot{\varphi}_1 \\ \dot{\varphi}_2 \end{pmatrix} \tag{2.25}$$

$$= e^{i\frac{\omega t}{2}\sigma_z}\left[\frac{i\omega}{2}\sigma_z\begin{pmatrix} \varphi_1 \\ \varphi_2 \end{pmatrix} + \begin{pmatrix} \dot{\varphi}_1 \\ \dot{\varphi}_2 \end{pmatrix}\right] \tag{2.26}$$

Inserting this in eq.(2.23) yields

$$e^{i\frac{\omega t}{2}\sigma_z}\left[\frac{i\omega}{2}\sigma_z\begin{pmatrix} \varphi_1 \\ \varphi_2 \end{pmatrix} + \begin{pmatrix} \dot{\varphi}_1 \\ \dot{\varphi}_2 \end{pmatrix}\right] = -\frac{i}{2}\begin{pmatrix} \omega_z & \omega_1 e^{i\omega t} \\ \omega_1 e^{-i\omega t} & -\omega_z \end{pmatrix} e^{i\frac{\omega t}{2}\sigma_z}\begin{pmatrix} \varphi_1 \\ \varphi_2 \end{pmatrix} \tag{2.27}$$

$$\frac{i\omega}{2}\sigma_z\begin{pmatrix} \varphi_1 \\ \varphi_2 \end{pmatrix} + \begin{pmatrix} \dot{\varphi}_1 \\ \dot{\varphi}_2 \end{pmatrix}$$

$$= -\frac{i}{2}e^{-i\frac{\omega t}{2}\sigma_z}\begin{pmatrix} \omega_z & \omega_1 e^{i\omega t} \\ \omega_1 e^{-i\omega t} & -\omega_z \end{pmatrix} e^{i\frac{\omega t}{2}\sigma_z}\begin{pmatrix} \varphi_1 \\ \varphi_2 \end{pmatrix} \tag{2.28}$$

$$= \begin{pmatrix} e^{-i\frac{\omega t}{2}} & 0 \\ 0 & e^{i\frac{\omega t}{2}} \end{pmatrix}\begin{pmatrix} \omega_z & \omega_1 e^{i\omega t} \\ \omega_1 e^{-i\omega t} & -\omega_z \end{pmatrix}\begin{pmatrix} e^{i\frac{\omega t}{2}} & 0 \\ 0 & e^{-i\frac{\omega t}{2}} \end{pmatrix}\begin{pmatrix} \varphi_1 \\ \varphi_2 \end{pmatrix} \tag{2.29}$$

$$= \begin{pmatrix} e^{-i\frac{\omega t}{2}} & 0 \\ 0 & e^{i\frac{\omega t}{2}} \end{pmatrix}\begin{pmatrix} \omega_z e^{\frac{i\omega t}{2}} & \omega_1 e^{\frac{i\omega t}{2}} \\ \omega_1 e^{-\frac{i\omega t}{2}} & -\omega_z e^{-\frac{i\omega t}{2}} \end{pmatrix}\begin{pmatrix} \varphi_1 \\ \varphi_2 \end{pmatrix} \tag{2.30}$$

$$= \begin{pmatrix} \omega_z & \omega_1 \\ \omega_1 & -\omega_z \end{pmatrix}\begin{pmatrix} \varphi_1 \\ \varphi_2 \end{pmatrix} \tag{2.31}$$

$$\begin{pmatrix} \dot{\varphi}_1 \\ \dot{\varphi}_2 \end{pmatrix} = -\frac{i}{2}\left[\begin{pmatrix} \omega & 0 \\ 0 & -\omega \end{pmatrix} + \begin{pmatrix} \omega_z & \omega_1 \\ \omega_1 & -\omega_z \end{pmatrix}\right]\begin{pmatrix} \varphi_1 \\ \varphi_2 \end{pmatrix} \tag{2.32}$$

$$= -\frac{i}{2}\begin{pmatrix} \omega_z + \omega & \omega_1 \\ \omega_1 & -\omega_z - \omega \end{pmatrix}\begin{pmatrix} \varphi_1 \\ \varphi_2 \end{pmatrix} \tag{2.33}$$

This is a differential equation with constant coefficients which can be integrated by separation of variables as shown above eq.(1.92) with the solution

$$\begin{pmatrix} \varphi_1(t) \\ \varphi_2(t) \end{pmatrix} = e^{-\frac{i}{2}\begin{pmatrix} \omega_z+\omega & \omega_1 \\ \omega_1 & -\omega_z-\omega \end{pmatrix}t} \begin{pmatrix} \varphi_1(0) \\ \varphi_2(0) \end{pmatrix} \tag{2.34}$$

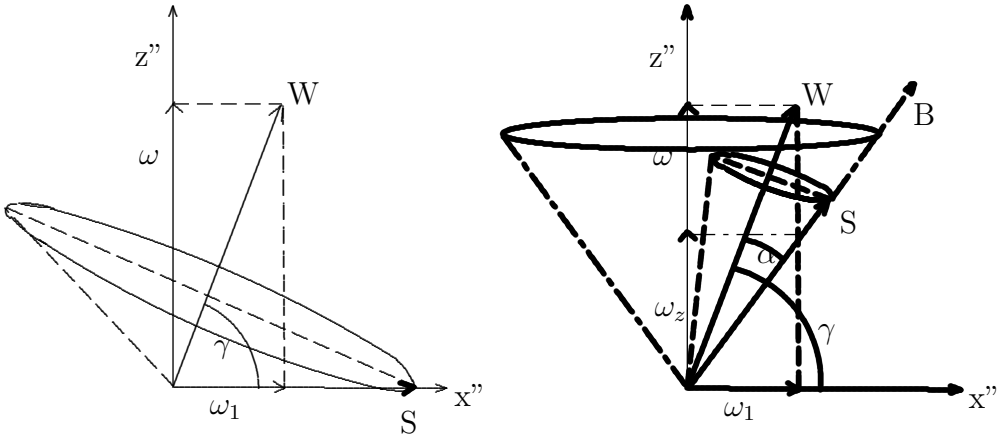



Figure 2.10: Definition of angles for the interpretation of the solution of the spin in a slowly varying field. If a constant field along the z axis is applied the initial spin direction is along the resultant field direction, as indicated on the right figure. The precession cone has then the apex angle $\alpha$ and is unrolling on the cone described by B. The equation is the same, and only the initial condition $\psi_1(0)$ and $\psi_2(2)$ will change.

We conjecture that the solution is equivalent to one obtained by a rotation about an axis which is inclined with respect to the coordinate axis. To investigate this possibility we have to try whether or not we can write the exponent using the form $\vec{n}\cdot\vec{\sigma}$. If we assume (see figure 2.10)

$$\sin\gamma = \frac{\omega+\omega_z}{W} \tag{2.35}$$

$$\cos\gamma = \frac{\omega_1}{W} \tag{2.36}$$

$$W = \sqrt{\omega_1^2+(\omega+\omega_z)^2} \tag{2.37}$$

we can rewrite the matrix in the exponent as

$$\begin{pmatrix} \omega_z+\omega & \omega_1 \\ \omega_1 & -\omega_z-\omega \end{pmatrix} = W\cdot\begin{pmatrix} \sin\gamma & \cos\gamma \\ \cos\gamma & -\sin\gamma \end{pmatrix} \tag{2.38}$$

$$= (\cos\gamma, 0, \sin\gamma)\cdot\vec{\sigma} = \vec{n}\cdot\vec{\sigma} \tag{2.39}$$

A rotation by $\gamma$ about the y-axis yields the solution as a simple precession around the x"-axis of the new system with the precession frequency W:

$$\begin{pmatrix} \varphi_1''(t) \\ \varphi_2''(t) \end{pmatrix} = e^{-i\frac{\gamma}{2}\sigma_y}\begin{pmatrix} \varphi_1(t) \\ \varphi_2(t) \end{pmatrix} \tag{2.40}$$

$$= e^{-i\frac{\gamma}{2}\sigma_y} e^{-i\frac{Wt}{2}\begin{pmatrix} \sin\gamma & \cos\gamma \\ \cos\gamma & -\sin\gamma \end{pmatrix}} e^{i\frac{\gamma}{2}\sigma_y} e^{-i\frac{\gamma}{2}\sigma_y} \begin{pmatrix} \varphi_1(0) \\ \varphi_2(0) \end{pmatrix} \tag{2.41}$$

$$= e^{-i\frac{Wt}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}} \begin{pmatrix} \varphi_1''(0) \\ \varphi_2''(0) \end{pmatrix} \tag{2.42}$$

$$= e^{-i\frac{Wt}{2}\sigma_x} \begin{pmatrix} \varphi_1''(0) \\ \varphi_2''(0) \end{pmatrix} \tag{2.43}$$

The complete solution with the explicit dependence on the initial spin direction at time 0 is finally obtained as:

$$\begin{pmatrix} \psi_1(t) \\ \psi_2(t) \end{pmatrix} = e^{\frac{i}{2}[-\omega t\sigma_z - \gamma\sigma_y - Wt\sigma_x + \gamma\sigma_y + \omega t\sigma_z]} \begin{pmatrix} \psi_1(0) \\ \psi_2(0) \end{pmatrix} \tag{2.44}$$

To visualize this solution we have to visualize all the transformations. The initial condition at the right is first transformed to the rotating system, then inclined by the angle $\gamma$ between the effective field direction (direction of W in fig.2.10) and the initial spin direction at time 0. This effective field direction depends on the different components of the rotation and the Lamor precession of the fields. This yields an effective precession frequency W. The spin precesses with angular velocity W in this rotating coordinate system around the axis inclined with angle $\gamma$. To see this precession in the laboratory system, we have to transform this precession around the inclined axis back to the laboratory frame. For this we bring the axis back to the direction inclined by $\gamma$ and then back to the fixed laboratory system. In this process and due to the geometrical conditions of the process the cone precessing with W is unrolling on the surface which is described by the field direction. It depends on the different signs on which side of this surface the precession cone is unrolling. Fig.2.11 shows the process for the case when $\omega_z = 0$.

### 2.3.1 Behaviour of the spin in a rotating guide field, adiabatic spin rotator

Figure 2.13 indicates the working of the adiabatic xyz coil as shown by the rotation of the spin in the y-coil. This behaviour as described above plays a role if one changes the direction of the spin by changing the direction of the guide field. The behaviour in fig.2.11 allows one to estimate the maximum deviation of the spin from the field direction. This maximum deviation between field direction and spin direction is the angular diameter of the precession cone i.e. $2\gamma = \arccos\omega_1/W$ or $2\alpha = 2|\arccos\omega_1/W - \arctan\omega_z/\omega_1|$.

In this case and in contrast to the sudden-xz coil in a polarimeter, the spin always remains parallel to the field direction (depending how well these conditions are fulfilled) and it rotates with this field direction. In figures 4.2 on page 49, 4.4 on page 55, 4.3 on page 54 this is used to rotate the spin on its way to the sample in three mutually orthogonal directions. After the scattering process the field direction is rotated back to the z direction and it takes with it that component of the spin, whose direction is not changed by the scattering process which is the cone axis of the resulting precessing spin polarization. In this manner one can unambiguously determine the polarization component parallel to that of the incident polarization of the beam after the scattering process and simultaneously for many different detectors. This is necessary if one wants to use a multidetector instrument with full polarization analysis. The scattering law of the sample and the kind of scattering (e.g. paramagnetic, nuclear spin incoherent) determine the behaviour of the polarization in the scattering process, the depolarization or the change of direction of the

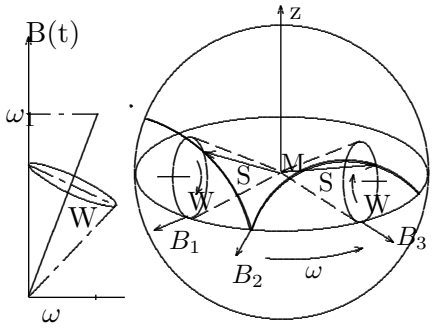



Figure 2.11: Behaviour of the neutron spin $\langle\vec{s}\rangle$ relative to the field direction $\vec{B}$ in the general case. The intersection of the field direction with the unit sphere describes the curve $B_1$, $B_2$, $B_3$. The intersection of the spin direction with the unit sphere describes a curve which originates by the unrolling of the cone with axis WM and with its apex in M. The apex angle is $2\gamma$ (see fig.2.10), in the conical case it would be $2\alpha$.

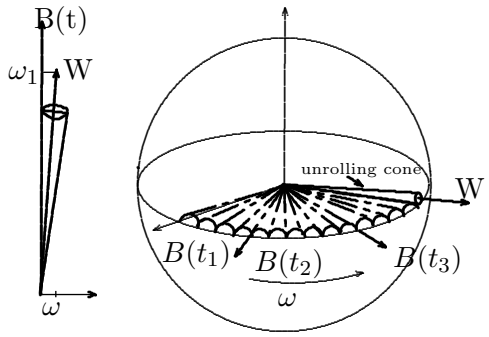



Figure 2.12: Behaviour of the neutron spin $\langle\vec{s}\rangle$ relative to the field direction $\vec{B}$ if the frequency $\omega$ is smaller than the Larmorfrequency

incident polarization. If you want to investigate the precessing polarization of the beam you need a polarimeter or you have to add a $\pi/2$-flipper coil and a section of variable guide field in an instrument as in figures 4.2 on page 49,4.4 on page 55, 4.3 on page 54.

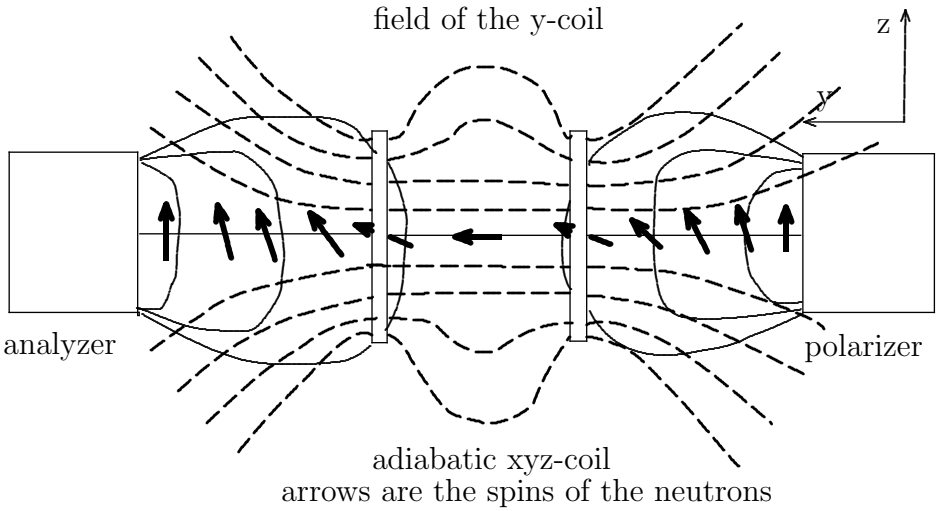



Figure 2.13: Way how the adiabatic xyz coil works, shown by the rotation of the spin in the y-coil. Near the polarizer and analyzer guide fields, which are far reaching fields decreasing with distance of the field sources, the spin has the z direction. The spin follows the direction of the field which results from the superposition of the coil field and the stray field of the analyzers. This is sufficiently strong and slowly changing that the condition $\omega/\omega_1 \ll 1$ is fulfilled. The figure shows only the effect of one of three mutually orthogonal coil pairs, which in the case of a cylinder symmetric arrangement of analysers and guide fields work also in the same way. (see figures 4.2 on page 49,4.4 on page 55,4.3 on page 54,

# Chapter 3

# Density matrix formalism to determine scattering cross sections

## 3.1 Introduction

In order to indicate how one has to proceed to obtain the necessary information using the density matrix formalism, we apply it to a calculation of the ensemble average of the cross section and to the polarization and show how we have to apply it to the xyz-method .

We first state some rules for Pauli spin matrices, which are very useful in connection with the density matrix. Then we define the scattering matrix and give some general properties of this scattering matrix. We apply these rules and properties to obtain the nuclear scattering cross section and the nuclear spin incoherent cross section and the dependence of the polarization for these sorts of scattering. Formulae as by Blume will be derived in a special chapter (chapter 5) after we have applied the transition probability method to determine the magnetic cross section. With the formulae of Blume we are able to discuss how the different contributions can be measured using the xyz method. We will see, where one needs a polarimeter to obtain results and whether or not the instrument D7 without modification is already sufficient for measuring all these cross sections or has to be changed by adding a $\pi/2$-flipper and a variable guide field section.

## 3.2 Compilation of rules for the Pauli spin matrices

### 3.2.1 some simple rules

First some useful rules for spin matrices:

$$\begin{aligned}
\{\sigma_\alpha, \sigma_\beta\} &= 2\delta_{\alpha\beta} && (3.1)\\
&= \sigma_\alpha\sigma_\beta + \sigma_\beta\sigma_\alpha && (3.2)\\
[\sigma_\alpha, \sigma_\beta] &= 2i\epsilon_{\alpha\beta\gamma}\sigma_\gamma && (3.3)\\
&= \sigma_\alpha\sigma_\beta - \sigma_\beta\sigma_\alpha && (3.4)\\
\sigma_1\sigma_2 &= -\sigma_2\sigma_1 = i\sigma_3 && (3.5)\\
\sigma^\alpha\sigma^\beta &= \delta^{\alpha\beta} + i\epsilon^{\alpha\beta\gamma}\sigma^\gamma && (3.6)\\
\sigma_\alpha^\dagger &= \sigma_\alpha && (3.7)\\
\det(\sigma_\alpha) &= -1 && (3.8)\\
\mathrm{Tr}(\sigma_\alpha) &= 0 && (3.9)
\end{aligned}$$

$$\vec{a}\cdot\vec{\sigma} = \sum_\gamma a_\gamma\sigma_\gamma = \begin{pmatrix} a_3 & a_1 - ia_2 \\ a1 + ia_2 & -a_3 \end{pmatrix} \tag{3.10}$$

$$\mathrm{Tr}(\sigma_\alpha\sigma_\beta) = 2\delta_{\alpha\beta} \tag{3.11}$$

$$\mathrm{Tr}(\sigma_\alpha\sigma_\beta\sigma_\gamma) = i\sum_{\gamma''}\epsilon^{\alpha\beta\gamma''}\mathrm{Tr}(\sigma_{\gamma''}\sigma_\gamma) \tag{3.12}$$

$$= 2i\epsilon^{\alpha\beta\gamma} \tag{3.13}$$

$$\mathrm{Tr}(\sigma_\alpha\sigma_\beta\sigma_\gamma\sigma_\delta) = 2(\delta_{\alpha\beta}\delta_{\gamma\delta} - \delta_{\alpha\gamma}\delta_{\beta\delta} + \delta_{\alpha\delta}\delta_{\beta\gamma}) \tag{3.14}$$

$$(\vec{a}\vec{\sigma})\cdot(\vec{b}\vec{\sigma}) = (\vec{a}\cdot\vec{b}) + i\vec{\sigma}\cdot(\vec{a}\times\vec{b}) \tag{3.15}$$

which can be derived as follows

$$(\vec{a}\vec{\sigma})(\vec{b}\vec{\sigma}) = (a^\alpha\sigma^\alpha)(b^\beta\sigma^\beta) = a^\alpha b^\beta\sigma^\alpha\sigma^\beta \tag{3.16}$$

$$= (\frac{1}{2}\{\sigma^\alpha,\sigma^\beta\} + \frac{1}{2}[\sigma^\alpha,\sigma^\beta])a^\alpha b^\beta \tag{3.17}$$

$$= (\delta^{\alpha\beta} + i\epsilon^{\alpha\beta\gamma}\sigma^\gamma)a^\alpha b^\beta \tag{3.18}$$

$$= [(\vec{a}\cdot\vec{b}) + i(\vec{a}\times\vec{b})\vec{\sigma}] \tag{3.19}$$

$$\tag{3.20}$$

Often a very useful rule for the treatment of functions of spin-$\frac{1}{2}$ matrices is the following:

- **Any function $f$ of the scalar $a + 2\vec{b}\vec{\sigma}$ linear in $\vec{\sigma}$**
- **can be converted into a linear function $f(a + 2\vec{b}\vec{\sigma}) = \alpha + 2\beta\frac{\vec{b}\vec{\sigma}}{b}$**
  - **with $\alpha = \frac{1}{2}[f(a+b) + f(a-b)]$ and**
  - **$\beta = \frac{1}{2}[f(a+b) - f(a-b)]$**
  - **with the eigenvalues $a \pm b$ of the operator $a + 2\vec{b}\vec{\sigma}$**
  - **and the eigenvalues $f(a \pm b)$ of the operator $f(a + 2\vec{b}\vec{\sigma})$**

The use of these rules often enables to treat the 2x2-matrices analytically.

### 3.2.2 Compilation of some more sophisticated rules for $\mathrm{Tr}_\sigma$

To average over the magnetic moment if it is spherically symmetric like in a paramagnet one has to avoid $\vec{Q}_\perp$ and formulate the equations using the normal component in the neutron magnetic moment. To treat the respectiv eqations one needs rules for the operators

$$L_h = \vec{S_h}\cdot(\vec{\sigma} - (\vec{e}\cdot\vec{\sigma})\vec{e}) \tag{3.21}$$

$$\vec{M}_h = \vec{Q}_{\perp h} = \vec{S}_h - (\vec{e}\cdot\vec{S}_h)\vec{e} \tag{3.22}$$

$$\vec{e} = \frac{\vec{\kappa}}{|\vec{\kappa}|} \tag{3.23}$$

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

$$\begin{aligned}
\mathrm{Tr}_\sigma(\vec{\sigma}L_h) &= 2\vec{M}_h && (3.24)\\
\mathrm{Tr}_\sigma((\vec{P}\cdot\vec{\sigma})L_h) &= 2(\vec{M}_h\cdot\vec{P}) && (3.25)\\
\mathrm{Tr}_\sigma((\vec{P}\cdot\vec{\sigma})\vec{\sigma}L_h) &= 2i(\vec{M}_h\times\vec{P}) && (3.26)\\
\mathrm{Tr}_\sigma((\vec{P}\cdot\vec{\sigma})L_h\vec{\sigma}) &= -2i(\vec{M}_h\times\vec{P}) && (3.27)\\
\mathrm{Tr}_\sigma(L_1L_2) &= 2(\vec{M}_1\cdot\vec{M}_2) && (3.28)\\
\mathrm{Tr}_\sigma(L_1\vec{\sigma}L_2) &= -2i(\vec{M}_1\times\vec{M}_2) && (3.29)\\
\mathrm{Tr}_\sigma((\vec{P}\cdot\vec{\sigma})L_1L_2) &= 2i(\vec{M}_1\times\vec{M}_2)\vec{P} && (3.30)\\
\mathrm{Tr}_\sigma((\vec{P}\cdot\vec{\sigma})L_1\vec{\sigma}L_2) &= 2[(\vec{M}_1(\vec{M}_2\cdot\vec{P})+(\vec{M}_1\cdot\vec{P})\vec{M}_2-\vec{P}(\vec{M}_1\cdot\vec{M}_2] && (3.31)
\end{aligned}$$

### 3.2.3 Some properties of the scattering matrix, which links the density matrix of the incident beam to that of the outgoing beam.

For me a long time the density matrix formalism looked like magic because e.g. Lovsey used it but without showing why it gives physical results. In the following I want to show the physical interpretation of the density matrix formalism, not only of the results but of the whole process i.e. I want to give the physical reasons why it works. Only then I can trust the results of this formalism. The Pauli spin matrices and the $2\times 2$ unit matrix are linearly independent and any $2\times 2$ matrix $\underline{A}$ can be represented as a linear combination

$$\begin{aligned}
\underline{A} &= \lambda_0\underline{1}+\lambda_1\sigma_x+\lambda_2\sigma_y+\lambda_3\sigma_z && (3.32)\\
&= \lambda_0\underline{1}+|(\lambda_1,\lambda_2,\lambda_3)|\frac{(\lambda_1,\lambda_2,\lambda_3)}{|(\lambda_1,\lambda_2,\lambda_3)|}\sigma && (3.33)
\end{aligned}$$

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

$$\boxed{\frac{1}{2}\left(g\underline{1}+h\vec{n}\cdot\vec{\sigma}\right)} \qquad (3.34)$$

like the density operator eq.(1.17). The scattering matrix, which describes the scattering by nuclei with a nuclear spin $(I_x,I_y,I_z)$ must then also have this form and also the scattering matrix describing the magnetic scattering and all interference terms must all have this general form.

First we want to investigate some properties of this scattering matrix. We describe the change of the spin state by the transformation

$$\chi_{c'}^{(f)}=\hat{M}_{c'c}\chi_c^{(i)} \qquad (3.35)$$

$\hat{M}_{c'c}$ is a $2\times 2$ matrix, which can also change the reference axes. In this case it would be $\hat{M}_{c'c}=\hat{R}_{c'c}\hat{M}_{cc}$ where $\hat{R}_{c'c}$ changes the reference axes from c to c' and $\hat{M}_{cc}$ is the scattering matrix for the system c. The most general form of this $\hat{M}_{cc}$ and assuming rotational invariance would then be

$$\hat{M}_{cc}=g\underline{1}+h_x\hat{\sigma}_x+h_y\hat{\sigma}_y+h_z\hat{\sigma}_z=g\underline{1}+\vec{h}\cdot\vec{\hat{\sigma}} \qquad (3.36)$$

Here g and $\vec{h}$ are complex quantities. The components of $\vec{h}$ and $\vec{\hat{\sigma}}$ are associated with the reference axes c. We assume these to be defined in the center of mass system. In an experiment $\vec{h}$ must be related to the scattering process. If the ingoing and outgoing wave vectors are $\vec{k}$ and $\vec{k}'$ we select

$$\vec{M} = \frac{(\vec{k}-\vec{k}')}{|\vec{k}-\vec{k}'|} \qquad (3.37)$$

$$\vec{N} = \frac{\vec{k}\times\vec{k}'}{|\vec{k}\times\vec{k}'|} \tag{3.38}$$

$$\vec{K} = \frac{\vec{k}+\vec{k}'}{|\vec{k}+\vec{k}'|} \tag{3.39}$$

three unit vectors, which form a Cartesian coordiante system. Taking the axes x,y,z along the vectors $\vec{M}$,$\vec{N}$, and $\vec{K}$, we can write

$$\vec{h}\cdot\vec{\hat{\sigma}} = h_x(\vec{M}\cdot\vec{\hat{\sigma}}) + h_y(\vec{N}\cdot\vec{\hat{\sigma}}) + h_z(\vec{K}\cdot\vec{\hat{\sigma}}) \tag{3.40}$$

The determination of the coefficients would correspond to a full polarimeter measurement measuring for each of three incident polarizations three components of the outgoing polarization.

In many cases additional symmetries occur such as parity conservation. Parity conservation postulates $\vec{M}\to-\vec{M}$, $\vec{N}\to\vec{N}$, $\vec{K}\to-\vec{K}$, $\vec{\hat{\sigma}}\to\vec{\hat{\sigma}}$. The consequence for the scattering process would then be $h_x = h_z = 0$, and writing for $h_y = h$ the general matrix is of the form

$$\hat{M}_{cc} = g\underline{1} + h(\vec{N}\cdot\vec{\hat{\sigma}}) \tag{3.41}$$

This is just the form we had assumed above for the general form of the scattering matrix. In this form g and h are related to scattering amplitudes describing the interaction of the incident neutrons with the target nuclei.

The use of polarimetry allows to identify processes in which the parity is not conserved as we did for example in [35, 36]. It may play a role if there are magnetic helices of only one helicity, because then parity is violated.

In the case of conservation of these symmetries the process of scattering of a beam with spin can be described further by applying the transformation with $\hat{M}_{cc}$ in the following way. For large values of r, we require that $\Psi$ may be written as the sum of an incoming plane wave in spin state $\chi_c^{(i)}$ and an outgoing spherically scattered wave in spin state $\chi_c^{(f)} = \hat{M}_{cc}\chi_c^{(i)}$. This results in the Born approximation for the case of a beam of particles with spin:

$$\Psi \approx e^{ikz}\chi^{(i)} + \frac{e^{ikr}}{r}\hat{M}_{cc}(\vartheta,\varphi)\chi^{(i)} \qquad \text{as } r\to\infty \tag{3.42}$$

We wish now to obtain the procedure for finding the density matrix of the resultant neutron beam after the scattering process by the scattering matrix of the form found above.

$$\rho_c^{out} = \chi_c^{(f)}\chi_c^{(f)\dagger} \tag{3.43}$$

$$= \hat{M}_{cc}\chi_c^{(i)}\chi_c^{(i)\dagger}\hat{M}_{cc}^{\dagger} \tag{3.44}$$

$$= \hat{M}_{cc}\rho_c^{(i)}\hat{M}_{cc}^{\dagger} \tag{3.45}$$

This is the relationship between the outgoing and the incident density matrix in terms of the scattering matrix $\hat{M}_{cc}$. This procedure also holds for beams which are unpolarized or partially polarized. The resultant beam is described by a density matrix which is the product of three $2\times2$ matrices.

If one takes the trace of $\rho_c^{(out)}$ one obtains the expectation value of the scattering matrix operator for the incident beam described by the density matrix $\rho_c^{(in)}$.

$$\frac{d\sigma}{d\Omega} = \mathrm{Tr}\rho_c^{(out)} = \mathrm{Tr}(\hat{M}_{cc}\rho_c^{(i)}\hat{M}_{cc}^{\dagger}) \tag{3.46}$$

Using $\rho_c^{out}$ one can obtain the polarization of the scattered beam (see eq.(1.40 on page 10)

$$\vec{P} = \frac{\mathrm{Tr}_\sigma(\sigma\rho_c^{(out)})}{\mathrm{Tr}_\sigma\rho_c^{(out)}} = \frac{\mathrm{Tr}_\sigma(\sigma\hat{M}_{cc}\rho_c^{(in)}\hat{M}_{cc}^\dagger)}{\mathrm{Tr}_\sigma(\hat{M}_{cc}\rho_c^{(in)}\hat{M}^\dagger)} \tag{3.47}$$

We now want to apply this to a simple example.

## 3.3 Application of the density matrix formalism to obtain nuclear coherent and nuclear spin incoherent scattering and their polarization

### 3.3.1 Scattering of a polarized beam by a spinless target: quartz measurement to determine the flipping ratio

We now apply these rules first for a spinless target, i.e. to an aggregat of atoms without nuclear spins and without magnetism. The scattering matrix has then the form of a complex number $N_N e^{i\phi_N}$ which in kinematic approximation is the result of the Fourier transform of the crystallographic structure. As is well known, the interaction of the neutron with a nucleus without nuclear spin is described by the expression for the scattering amplitude:

$$V_N(\vec{\kappa}) = V_N(\vec{k} - \vec{k}') = \frac{2\pi\hbar^2}{m_0}\sum_{\nu,j} b_j e^{i(\vec{k}-\vec{k}')(\vec{R}_\nu+\vec{d}_j)} \tag{3.48}$$

$\vec{k}$,$\vec{k}'$ are the wave vector of the incident and outgoing neutrons, $\vec{R}_\nu$ is the position of the origin of the unit cell $\nu$, $\vec{d}_j$ is the position of the atom j with scattering length $b_j$ in the unit cell $\nu$. Specializations of this general expression for single crystals, powder patterns, materials with short range order, liquids and amorphous materials will be derived when we need it to investigate such materials. The behaviour of this scattering amplitude in crystalline materials is the special topic of crystallography and all information about it is gathered in the international X-ray tables. Here we only need to know the most general form, which this expression can have for the scattering matrix. For the case where one has no symmetry center the above sum $V_N(\vec{\kappa})$ will be a complex number $\hat{N}$ with modulus N and phase $\phi_N$ or with real and imaginary parts $N^{(r)} = N\cos\phi_N$ and $N^{(i)} = N\sin\phi_N$. But $V_N^\dagger(\vec{\kappa})V_N(\vec{\kappa})$ is always real and positiv. Only the way to calculate this is changing in noncentro symmetric crystals as then in eq.(3.48) one has also an imaginary part. One can also split this into different factors like the lattice factor, the structure amplitude and the shape function. But without magnetic interaction terms and nuclear spin terms we have no term with the form $(\vec{\sigma}\cdot\vec{Op})$ with an operator $\vec{Op}$. So the scatterred intensity is obtained by

$$\frac{d\sigma}{d\Omega} = \mathrm{Tr}_\sigma(\rho\hat{N}^\dagger\hat{N}) \tag{3.49}$$

$$= \frac{1}{2}\mathrm{Tr}_\sigma[(\underline{1} + \vec{P}\cdot\vec{\sigma})\hat{N}^\dagger\hat{N}] \tag{3.50}$$

$$= \hat{N}^\dagger\hat{N} = N^2 \tag{3.51}$$

as $\mathrm{Tr}_\sigma(\underline{1}) = 2$ and $\mathrm{Tr}_\sigma(\vec{\sigma}) = 0$. For the polarization $\vec{P}_{out}$ of the outgoing beam with $\vec{P}_{in}$ as the polarization of the incident beam we get

$$\vec{P}_{out}\frac{d\sigma}{d\Omega} = \mathrm{Tr}_\sigma(\rho\hat{N}^\dagger\vec{\sigma}\hat{N}) \tag{3.52}$$

$$P_\beta^{(out)}\frac{d\sigma}{d\Omega} = \frac{1}{2}\mathrm{Tr}_\sigma[(\underline{1}+P_\alpha^{(in)}\sigma_\alpha)\hat{N}^\dagger\sigma_\beta\hat{N}] \quad (3.53)$$

$$= \frac{1}{2}\mathrm{Tr}_\sigma(\hat{N}^\dagger\sigma_\beta\hat{N}+P_\alpha^{(in)}\sigma_\alpha\sigma_\beta\hat{N}\dagger\hat{N}) \quad (3.54)$$

$$= P_\alpha^{(in)}\delta_{\alpha\beta}\hat{N}^\dagger\hat{N} \quad (3.55)$$

$$= P_\beta^{(in)}|\hat{N}|^2 \quad (3.56)$$

$$= P_\beta^{(in)}N^2 \quad (3.57)$$

as $\mathrm{Tr}\sigma_\alpha\sigma_\beta = \delta_{\alpha\beta}\mathrm{Tr}\left(\begin{smallmatrix}1&0\\0&1\end{smallmatrix}\right) = 2\delta_{\alpha\beta}$ and $\mathrm{Tr}\sigma = 0$.

This is nothing else but the fact that for pure nuclear coherent scattering the scattered beam has the differential scattering cross section $\frac{d\sigma}{d\Omega} = \hat{N}^\dagger\hat{N}$ and the polarization of the scattered beam is the same as that of the incident beam. If the incident beam is polarized in the x direction then also the outgoing beam is polarized in the x direction, and correspondingly for y and z. For quartz we have such a scattering, which has no nuclear spin incoherent and no magnetic cross section. Fused quartz is characterized by broad diffuse scattering as it behaves like a frozen liquid. It enables to measure the polarization product properties of the analyzers in a broad angular range, which is needed for the correction of the results of the multidetector for finite flipping ratio.

### 3.3.2 Correction for finite flipping ratio

Any reliable results of a measurement should not depend on the properties of the measuring equipment. But if one measures with bad polarizers and analyzers one gets other results than with good ones. So one has to be able to correct for this faults. The quality of the equipment can be charterized by the flipping ratio of the scattering by a purely coherent scatterer, and for this we use a quartz sample. The polarization is not a linear function but in the way it is visualized in fig.3.1 and 3.2 one can use simple rules of elementary geometry of proportionality to correct the flipped and nonflipped scattering intensities of the sample. From fig.3.2 one sees immediately that

$$P_{Quartz} = \frac{I_\uparrow - I_\downarrow}{I_\uparrow + I_\downarrow} \quad (3.58)$$

$$= \frac{I_\uparrow/I_\downarrow - 1}{I_\uparrow/I_\downarrow + 1} \quad (3.59)$$

$$= \frac{R_{quartz}-1}{R_{quartz}+1} \quad (3.60)$$

$$I_{\uparrow\uparrow}^{corr} + I_{\uparrow\downarrow}^{corr} = I_{\uparrow\uparrow} + I_{\uparrow\downarrow} = I \quad (3.61)$$

$$\frac{I_{\uparrow\uparrow}^{corr} - I_{\uparrow\downarrow}^{corr}}{I} = \frac{I_{\uparrow\uparrow} - I_{\uparrow\downarrow}}{I_\uparrow - I_\downarrow} \quad (3.62)$$

$$I_{\uparrow\uparrow}^{corr} - I_{\uparrow\downarrow}^{corr} = \frac{I_{\uparrow\uparrow} - I_{\uparrow\downarrow}}{P_{Quartz}} \quad (3.63)$$

From this follows by some simple calculations

$$I_{\uparrow\uparrow}^{corr} = I_{\uparrow\uparrow} + \frac{1}{R_{quartz}-1}(I_{\uparrow\uparrow} - I_{\uparrow\downarrow}) \quad (3.64)$$

$$I_{\uparrow\downarrow}^{corr} = I_{\uparrow\downarrow} - \frac{1}{R_{quartz}-1}(I_{\uparrow\uparrow} - I_{\uparrow\downarrow}) \quad (3.65)$$

which one can also immediately see in fig.3.2 applying simple geometric rules.

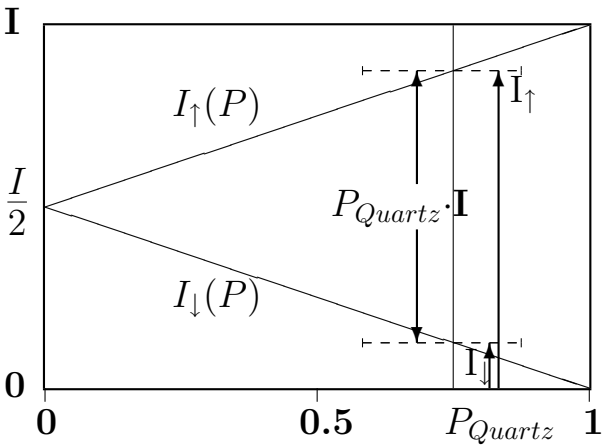



Figure 3.1: Vizualization for the intensities $I_\uparrow$ and $I_\downarrow$ for the polarization with a flipping ratio 7

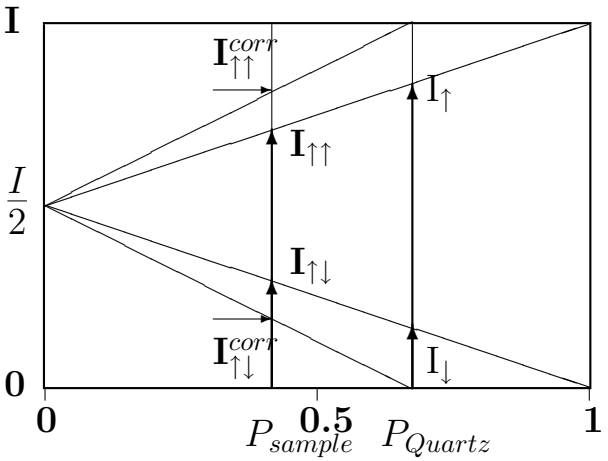



Figure 3.2: Vizualization of the background corrected intensities $I_\uparrow$ and $I_\downarrow$ of the quartz for the flipping ratio about 4, the measured and background corrected intensities for the sample and the flipping ratio corrected intensities of the sample $I^{corr}_{\uparrow\uparrow}$ without flip, and $I^{corr}_{\uparrow\downarrow}$ with flip. The correction assumes that the quartz should only scatter without flip and relates the measured sample intensities to an ideal quartz scatterer

The correction for finite flipping ratio is then done in following way: For the three polarization directions x,y,z we measure the scattering of a fused quartz sample with and without spin flip. As we know from the above discussion that this scattering does not change the polarization we use these scattered intensities without spin flip $I^\uparrow_n$ and with spin flip $I^\uparrow_n$ for detector number n (after background correction) to determine the properties of the measuring set-up of this detector. These properties are contained in the product $P_{polarizer}P_{analyzer}F_{flipper}$ with $P_{polarizer}$=polarization efficiency of the polarizer, $P_{analyzer}$=polarization efficiency of the analyzer and $F_{flipper}$= flipper efficiency (see 2.1.1 on page 18). As a measure for this "polarization product" we use the flipping ratio $R_n$ for each detector n given by

$$R_n = \frac{I^\uparrow_n}{I^\downarrow_n} \tag{3.66}$$

From this we can determine the polarization product for each detector

$$(P_{pol}P_{anal}F_{flipper})_n = \frac{R_n - 1}{R_n + 1} \tag{3.67}$$

$R_n$ serves also for the correction for finite flipping ratio of the measured data. This flipping ratio contains all polarization losses by depolarizations in the polarizer, the analyzer the guide fields and the imperfections of the polarizer, the analyzer and the flipper.

The correction for detector n can then be performed by using eq.(3.64) and eq.(3.65). In the literature you can also find the application of eq.(3.64,3.65) with $R_{quartz}$ replaced by the flipping ratio of the sample. From the above figures you can see immediately the nonesense of such a correction. It would only calculate the intensity that would have been measured without polarization analysis but with losses by the transition of the beam through polarizer and analyzer, which you can have easier by just adding the (backgroud corrected) intensities with and without flip.

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

For absolute calibration measurements one normally uses the scattering of a standard scatterer whose cross section and scattering behaviour is well known. 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. Because of the incoherence the angular scattering is isotropic, so one knows that 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 of the scattering of vanadium results from interaction of the neutron with the nuclear spin of vanadium. For nuclear spin incoherent scattering the behaviour of the scattering length is given by two numbers $b^+$ and $b^-$ which are the eigenvalues of the scattering length operator $\hat{b} = \overline{b} + \frac{1}{2} b_N \boldsymbol{I} \cdot \boldsymbol{\sigma}$ . 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

$$\boldsymbol{I} \cdot \boldsymbol{\sigma} = I \quad \text{for} \qquad J = I + \frac{1}{2} \tag{3.68}$$

$$\boldsymbol{I} \cdot \boldsymbol{\sigma} = -(I+1) \quad \text{for} \qquad J = I - \frac{1}{2} \tag{3.69}$$

we obtain

$$b^+ = \overline{b} + \frac{1}{2} b_N I \tag{3.70}$$

$$b^- = \overline{b} - \frac{1}{2} b_N (I+1) \tag{3.71}$$

$$\overline{b} = \frac{(I+1)b^+ + I b^-}{2I+1} \tag{3.72}$$

$$b_N = \frac{2(b^+ - b^-)}{2I+1} \tag{3.73}$$

As an example that shows that the available values in tables are often questionable: In the table we find for vanadium which is 99.5% $^{51}V$ with $I = \frac{7}{2}$ the values $b^+ = 5.11 fm$ and $b^- = -7.52 fm$ and this gives $\overline{b} = -0.4156 fm$ and $b_N = 3.158 fm$. This should give the known nuclear incoherent cross section of vanadium, but it does not. Perhaps the authors which measured the values used other definitions of $b^+$ and $b^-$. In fact one can find different definitions in the literature. It is a factor 2 which is lost. What is really measured is only the difference. The values itself are then calculated using other informations.

We apply the density matrix method now to the case with only the operator $\hat{B}(\boldsymbol{I} \cdot \boldsymbol{\sigma})$ with $\hat{B} = \frac{1}{2} b_N$ but we assume that the nuclei are not polarized,i.e.

$$\langle I_x \rangle = \langle I_y \rangle = \langle I_z \rangle = 0 \tag{3.74}$$

$$\langle I_x^2 \rangle = \langle I_y^2 \rangle = \langle I_z^2 \rangle = \frac{1}{3} I(I+1) \tag{3.75}$$

$$\frac{d\sigma}{d\Omega} = \mathrm{Tr}(\rho \hat{B}^\dagger (\vec{\sigma} \cdot \vec{I}^\dagger) \hat{B} (\vec{\sigma} \cdot \vec{I}) \tag{3.76}$$

$$= \frac{1}{2}\mathrm{Tr}[(\left(\begin{smallmatrix}1&0\\0&1\end{smallmatrix}\right)+\sigma_\alpha P_\alpha^{(in)})(\sigma_\beta I_\beta^\dagger)\hat{B}^\dagger\hat{B}(\sigma_\gamma I_\gamma)] \tag{3.77}$$

$$= \frac{1}{2}\mathrm{Tr}[\sigma_\beta\sigma_\gamma I_\beta^\dagger I_\gamma\hat{B}^\dagger\hat{B}+\hat{B}^\dagger\hat{B}\sigma_\alpha\sigma_\beta\sigma_\gamma P_\alpha^{(in)}I_\beta^\dagger I_\gamma] \tag{3.78}$$

$$= \frac{1}{2}\hat{B}^\dagger\hat{B}[2\delta_{\beta\gamma}I_\beta^\dagger I_\gamma+2i\epsilon_{\alpha\beta\gamma}P_\alpha^{(in)}I_\beta^\dagger I_\gamma] \tag{3.79}$$

$$= \hat{B}^\dagger\hat{B}[I_\beta^\dagger I_\beta+i\vec{P}^{(in)}(\vec{I}^\dagger\times\vec{I})] \tag{3.80}$$

$$= \hat{B}^\dagger\hat{B}[I(I+1)+i\vec{P}^{(in)}(\vec{I}^\dagger\times\vec{I})] \tag{3.81}$$

Now we have to 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 $\vec{I}\times\vec{I}=i\vec{I}$. This shows that the vector product expression in eq.(3.81) is linear in nuclear spin so that it averages to zero for an unpolarized nuclear target. Therefore we obtain finally

$$\boxed{\frac{d\sigma}{d\Omega}=\hat{B}^\dagger\hat{B}I(I+1)} \tag{3.82}$$

For the polarization of the beam scattered by unpolarized nuclear spins we obtain

$$P_\gamma^{(out)}\frac{d\sigma}{d\Omega} = \mathrm{Tr}(\rho\hat{B}^\dagger(\vec{\sigma}\cdot\vec{I}^\dagger)\sigma_\gamma(\vec{\sigma}\cdot\vec{I})\hat{B}) \tag{3.83}$$

$$= \frac{1}{2}\mathrm{Tr}[(\left(\begin{smallmatrix}1&0\\0&1\end{smallmatrix}\right)+\sigma_\alpha P_\alpha^{(in)})(\sigma_\beta I_\beta^\dagger)\sigma_\gamma(\sigma_\delta I_\delta)] \tag{3.84}$$

$$= \frac{1}{2}\hat{B}^\dagger\hat{B}\mathrm{Tr}[\sigma_\beta\sigma_\gamma\sigma_\delta I_\beta^\dagger I_\delta+\sigma_\alpha\sigma_\beta\sigma_\gamma\sigma_\delta P_\alpha^{(in)}I_\beta^\dagger I_\delta] \tag{3.85}$$

$$= \hat{B}^\dagger\hat{B}[i\epsilon_{\beta\gamma\delta}I_\beta^\dagger I_\delta+(\delta_{\alpha\beta}\delta_{\gamma\delta}-\delta_{\alpha\gamma}\delta_{\beta\delta}+\delta_{\alpha\delta}\delta_{\beta\gamma})P_\alpha^{(in)}I_\beta^\dagger I_\gamma] \tag{3.86}$$

$$= \hat{B}^\dagger\hat{B}[-i(\vec{I}^\dagger\times\vec{I})_\gamma+(\vec{P}^{(in)}\cdot\vec{I}^\dagger)I_\gamma+(\vec{P}^{(in)}\cdot\vec{I})I_\gamma^\dagger-P_\gamma^{(in)}(\vec{I}^\dagger\cdot\vec{I})] \tag{3.87}$$

$$= \hat{B}^\dagger\hat{B}[-i(\vec{I}^\dagger\times\vec{I})_\gamma-P_\gamma^{(in)}I(I+1)+(\vec{P}^{(in)}\cdot\vec{I}^\dagger)I_\gamma+(\vec{P}^{(in)}\cdot\vec{I})I_\gamma^\dagger] \tag{3.88}$$

Now we average again over nuclear spin orientations and obtain by using eqs.(3.74-3.75)

$$(\vec{P}^{(in)}\cdot\vec{I}^\dagger)I_\gamma = (P_x^{(in)}I_x^\dagger+P_y^{(in)}I_y^\dagger+P_z^{(in)}I_z^\dagger)I_\gamma=\frac{1}{3}P_\gamma^{(in)}I(I+1) \tag{3.89}$$

$$(\vec{P}^{(in)}\cdot\vec{I})I_\gamma^\dagger = (P_x^{(in)}I_x+P_y^{(in)}I_y+P_z^{(in)}I_z)I_\gamma^\dagger=\frac{1}{3}P_\gamma^{(in)}I(I+1) \tag{3.90}$$

With this we obtain

$$P_\gamma^{(out)}\frac{d\sigma}{d\Omega} = \hat{B}^\dagger\hat{B}P_\gamma^{(in)}I(I+1)[\frac{1}{3}+\frac{1}{3}-1] \tag{3.91}$$

$$= -\frac{1}{3}P_\gamma^{(in)}I(I+1)\hat{B}^\dagger\hat{B} \tag{3.92}$$

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

$$\frac{d\sigma}{d\Omega} = I_\gamma^{\uparrow\uparrow}+I_\gamma^{\uparrow\downarrow}=\hat{B}^\dagger\hat{B}I(I+1) \tag{3.93}$$

$$P_\gamma^{(out)}\frac{d\sigma}{d\Omega} = \frac{I_\gamma^{\uparrow\uparrow}-I_\gamma^{\uparrow\downarrow}}{I_\gamma^{\uparrow\uparrow}+I_\gamma^{\uparrow\downarrow}}(I_\gamma^{\uparrow\uparrow}+I_\gamma^{\uparrow\downarrow})=I_\gamma^{\uparrow\uparrow}-I_\gamma^{\uparrow\downarrow}=-\frac{1}{3}\hat{B}^\dagger\hat{B}I(I+1) \tag{3.94}$$

for $\gamma$ = x,y or z. Solving this two equations for the intensity without spin flip $I_\gamma^{\uparrow\uparrow}$ and for the intensity with spin flip $I_\gamma^{\uparrow\downarrow}$ we obtain immediately

$$I_\gamma^{\uparrow\uparrow} = \frac{1}{3}|B|^2I(I+1) \tag{3.95}$$

$$I_\gamma^{\uparrow\downarrow} = \frac{2}{3}|B|^2I(I+1) \tag{3.96}$$

The physical meaning of this is that 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 with one third without flip and two third with flip of the neutrons in the polarized beam.

These results will be used in the next chapter where we derive formulas for magnetic scattering and include nuclear scattering without derivation. In the next chapter we wish to derive the cross section for magnetic scattering using the xyz method, and employ the method of tansition probability calculation, (this method to calculate the polarization behaviour is complimentary). This method should also be known. In the literature this method is also very often used. There we derive the general form of magnetic scattering, which differs from nuclear spin scattering by the fact that only the component of the magnetic moment which is orthogonal to the scattering vector contributes to the scattering. This is the first topic of the next chapter. Then we develope a method for describing the behaviour of the spin if the quantization axis is changed from the z to the x or y direction. With these methods we calculate the transition probabilities for spin flip and non spin flip scattering for these quantization axes and their relationship to the magnetic correlation functions $M_{\mu\nu}$ with $\mu, \nu = x, y, z$. We apply the results to get formulas for powder and single crystal samples which will be used in the following chapters. To demonstrate the advantages of the density matrix method, we will also use it to first derive the same results. After this we will then use it to find the behaviour for more general cases and interpret these results by visualizing the respective behaviour for pure magnetic scattering and for interference terms and including the case of non centro symmetric systems. These play a role especially for Bragg scattering by more complicated spin structures as they were investigated with the CRYOPAD (see chapter 5.6).

### 3.3.4 Summary about the density matrix formalism

One can see that the density matrix method offers a simple and very effective method to treat spin problems. One only has to use some simple rules for the calculation of the traces of combinations of Pauli spin matrices. This strength results from the law we found in eq.(1.35 on page 10) and the fact that the Pauli spin matrices combined with the $2 \times 2$ unit matrix form a complete system to express all hermitian $2 \times 2$ matrices. They are all of the form $A\left(\begin{smallmatrix}1&0\\0&1\end{smallmatrix}\right) + B(\vec{\sigma}\vec{O})$. To interpret the results one has to use the relationships of eq.(3.93 on page 39, 3.94). I myself learned these things when I collaborated with Boris Toperverg on diffuse scattering by the roughness in multilayers, where we treated the multilayer system using the pseudo spin $\frac{1}{2}$ method.

# Bibliography


[1] Sakurai, J.J. *Modern Quantum Mechanics* Benjamin/Cummings Publishing Company, Menlo Park, California 1985

[2] Dirac, P.A.M. *Spinors in Hilbert Space* Plenum Press, New York and London 1974

[3] Goldstein, H. *Klassische Mechanik* Akademische Verlagsgesellschaft, Frankfurt am Main 1972

[4] Schärpf, O., *J. Appl. Cryst.* **11**, 631, (1978)

[5] Schärpf, O., Strothmann, H., *Physica Scripta* **T24**, 58, (1988)

[6] Mezei, F. *Journal de Physique* **45**, (1984), C3-223

[7] Mezei, F. in *Imaging Processes and Coherence in Physics* Schlenker, M. et al. editors, Springer Verlag, Heidelberg (1980) p.282.

[8] Serebrov, A.P., Aldushchenkov, A.V., Lasakov, M.S., Kuznetsov, I.A., Stepanenko, I.V. *Nuclear Instruments and Methods* **A 357**, (1995), 503

[9] Reckveldt, M.Th., *J. de Physique* **32**, (1971), C579

[10] Mezei, F. *Z.Physik* **255**, (1972), 146

[11] Okorokov, A.I., Runov, V.V., Volkov, V.I., Gukasov, A.G.: *JETP* **69**, (1975), 590

[12] Sakurai, J.J. *Modern Quantum Mechanics* Benjamin/Cummings Publishing Company, Menlo Park, 1985

[13] Capellmann,H., J.Magn.Magn.Materials.28,250(1982)

[14] Emery,V.J.: Phys.Rev.Lett.58,2794(1987)

[15] Lovesey,S.W.:Theory of neutron scattering from condensed matter. Vol. 2: Polarization effects and magnetic scattering. Oxford: Clarendon Press 1986

[16] Capellmann,H., Vieira,V.: Phys.Rev.B25,3333(1982)

[17] Brink, D.M., Satchler, G.R. *Angular momentum* Clarendon Press, Oxford 1971

[18] Brussaard, P.J., Tolhoek, H.A. *Physica* **23**, (1957) 955

[19] Brenig, W. *Annalen der Physik* **5**, (1996) 123

[20] Zhou, C., Schulz, H.J. *Phys. Rev.B* **52**, (1995) R11557

[21] Aharonov, Y., Albert, D.Z., Casher, A., Vaidman, L. *Physics Letters A* **124**, (1987) 199

[22] Aharonov, Y., Albert, D.Z., Vaidman, L. *Phys. Rev. Lett.* **60**, (1988) 1351

[23] Busch, P. *Physics Letters A* **130**, (1988) 323

[24] Golub, R., Gähler, R. *Physics Letters A* **136**, (1989) 178

[25] Golub, R., Gähler, R. *Nuclear Instrum. and Methods* **A284**, (1989) 188

[26] Rose, M.E. *Elementary theory of angular momentum* John Wiley & sons, New York 1967 (5.th edition)

[27] Schertler, K., Thoma, M.H., *Annalen der Physik* **5**, 103, (1996)

[28] Edmonds, A.R. *Angular momentum in quantum mechanics* Princeton University Press, Princeton, New Jersey 1974

[29] Robson, B.A. *The theory of polarization phenomena* Clarendon Press, Oxford 1974

[30] Abragam, A., Winter, J.M., *Phys.Rev. Letters* **1** (1958), 374

[31] Donally, B.L., Clapp, Th., Sawyer, W., Schultz, M. *Phys. Rev. Letters* **12**, 502

[32] Clausnitzer, G., Fick, D. *Nuclear Instruments and Methods* **47** (1967), 171

[33] Beurtey, R. in *Polarized Targets and Ion Sources* Proceedings of the International Conference on Polarized Targets and Ion sources, Saclay, France (1966), Edited by La Direction de la Physique d'Etudes Nucléaires de Saclay, Boite postale Nr.2, 91 Gif-sur-Yvette

[34] DeKieviet, M., Dubbers, D., Schmidt, Ch., Scholz, D., Spinola, U. *Phys. Rev. Letters* **75** (1995), 1919

[35] Heckel, B., Ramsey, N.F., Green, K., Greene, G.L., Gähler, R., Schärpf, O., Forte, M., Dress, W., Miller, P.D., Golub, R., Byrne, J., Pendlebury, J.M, *Physics Letters B*, **119**, 298, (1982)

[36] Heckel, B., Forte, M., Schärpf, O., Green, K., Greene, G.L., Ramsey, N.F., Byrne, J., Pendlebury, J.M., *Phys. Rev. C* **29**, 2389, (1984)

[37] F.Tasset, *Physica B*, **156 & 157**, 627 (1989)

# Chapter 4

# Theory of the XYZ-difference method using polarized neutrons for the separation of coherent, spin incoherent and magnetic scattering cross sections and employing a multidetector: Requirements for such an instrument.

## 4.1 Abstract

Equations are derived for the polarization analysis using 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.

## 4.2 Introduction

Experiments with polarized neutrons and especially with polarization analysis always suffer from intensity problems. The application of multidetectors similar to experiments without polarization analysis can help to overcome such problems. However in the $\parallel$-$\perp$ difference method [1] the need to rotate the polarization into the direction parallel to the scattering vector prevents its application in a multidetector. We want to derive equations which show how a polarization analysis experiment for paramagnetic and antiferromagnetic scatterers and a multidetector instrument has to be carried out. Then we want to demonstrate how the using method can be implemented in a real instrument. We demonstrate this using the example of the existing instrument D7 at the ILL in Grenoble.

[0] first published as O.Schärpf, H.Capellmann, in *phys. stat. sol. (a)* **135**, (1993), 359

## 4.3 XYZ-Difference method

First we re-derive the ∥-⊥-method and afterwards we generalize it to the xyz-difference method, which can be used for the simultaneous measurements of a multidetector polarization analysis experiment.

The double differential neutron scattering cross section is given by the relation

$$\left(\frac{\partial^2\sigma}{\partial\Omega\partial E'}\right)_{ss'} = \left(\frac{m_n}{2\pi\hbar^2}\right)^2 \cdot \frac{k'}{k}\sum_{\lambda\lambda'} p_\lambda | < k's'\lambda'|V|ks\lambda > |^2\delta(\hbar\omega + E_\lambda - E_{\lambda'}) \tag{4.1}$$

$$\left(\frac{\partial^2\sigma}{\partial\Omega\partial E'}\right) = \left(\frac{m_n}{2\pi\hbar^2}\right)^2 \cdot \frac{k'}{k}\sum_{\lambda\lambda'} p_\lambda \mathrm{Tr}_\sigma(\rho|\langle k'\lambda'|V|k\lambda\rangle|^2)\delta(\hbar\omega + E_\lambda - E_{\lambda'}) \tag{4.2}$$

where quantum numbers without prime correspond to the initial states, quantum numbers with primes correspond to final states, k,s are the quantum numbers for the neutron, $\lambda$ are the quantum numbers of the target. V is the interaction between neutron and target.

Eq.(4.2) we get by factorizing the spin part $\langle s'|$, $|s\rangle$ and write it as the density matrix $\rho = \sum |s\rangle\langle s|$

$$\sum_{ss'} |\langle k's'\lambda'|V|ks\lambda\rangle|^2 = \sum_{ss'} |\langle s'|\langle k'\lambda'|V|k\lambda\rangle|s\rangle|^2 = \mathrm{Tr}_\sigma(\rho|\langle k'\lambda'|V|k\lambda\rangle|^2)$$

Eq.(4.2) does not give the transition probability s to s' directly but by $\mathrm{Tr}_\sigma(\rho\sigma|\langle k'\lambda'|V|k\lambda\rangle|^2)$ as shown in 3.47 on page 35.

For magnetic scattering the magnetization density of the electrons $\mathbf{M_e(r)}$ interacts with the dipole field of the neutron. This density of the magnetization of the electrons has an orbital part $\mathbf{M_L(r)}$ and a spin part $\mathbf{M_S(r)}$

$$\mathbf{M_e(r)} = \mathbf{M}_\mathrm{L}(\mathbf{r}) + \mathbf{M}_\mathrm{S}(\mathbf{r}) = \mathbf{M_L(r)} - \mathrm{g}\mu_\mathrm{B}\mathbf{S}(\mathbf{r}) \tag{4.3}$$

The dipole field of the neutron $\mathbf{B}_\mathrm{n}(\mathbf{r})$ is

$$\boldsymbol{B_n(r)} = \boldsymbol{\nabla_r} \times \left(\boldsymbol{\nabla_r} \times \frac{\boldsymbol{\mu_n}}{|\boldsymbol{r_n} - \boldsymbol{r}|}\right) \tag{4.4}$$

with $\boldsymbol{\mu_n} = \boldsymbol{\gamma\mu_N}$, $\gamma = -1.9132$, $\mu_N$ = nuclear magneton, g=gyromagnetic ratio of the electron, $\mu_B = \frac{e\hbar}{2m_ec}$ = Bohr magneton.

So one finally has (index e corresponds to electron, index n to neutron respectively)

$$\hat{V}_e = \frac{1}{4\pi\mu_B}\mathbf{M}_e(\mathbf{r})\mathbf{B}_n(\mathbf{r}) \tag{4.5}$$

The matrix element of $\frac{1}{|\mathbf{r}_n - \mathbf{r}|}$ relative to $\mathbf{r}_n$ is

$$< k'|\frac{1}{\mathbf{r}_n - \mathbf{r}}|k >= e^{i\boldsymbol{\kappa}\,\boldsymbol{\cdot}\,\boldsymbol{r}}\int \frac{e^{i\boldsymbol{\kappa}\cdot(\mathbf{r_n}-\mathbf{r})}}{|\mathbf{r_n} - \mathbf{r}|}d^3r_n = \frac{e^{i\boldsymbol{\kappa}\,\boldsymbol{\cdot}\,\boldsymbol{r}}}{\kappa^2} \tag{4.6}$$

with $\boldsymbol{\kappa} = \boldsymbol{k} - \boldsymbol{k'}$. So we get with $\boldsymbol{e} = \boldsymbol{\kappa}/|\boldsymbol{\kappa}|$ unit vector in direction of $\boldsymbol{\kappa}$

$$< k'|\mathbf{B}_n(\mathbf{r})|k >= \frac{1}{\kappa^2}\boldsymbol{\kappa} \times (\boldsymbol{\mu}_n \times \boldsymbol{\kappa})e^{i\boldsymbol{\kappa}\,\boldsymbol{\cdot}\,\boldsymbol{r}} = \gamma\mu_N\mu_B e^{i\boldsymbol{\kappa}\,\boldsymbol{\cdot}\,\boldsymbol{r}}(\boldsymbol{\sigma_n} - (\boldsymbol{e}\,\boldsymbol{\cdot}\,\boldsymbol{\sigma_n})\boldsymbol{e}) \tag{4.7}$$

and

$$< k'|\mathbf{M_e(r)} \cdot \mathbf{B}_n(\mathbf{r})|k >= \mathbf{M_e(r)} \cdot \frac{\boldsymbol{\kappa}}{\kappa} \times (\boldsymbol{\mu}_n \times \frac{\boldsymbol{\kappa}}{\kappa})e^{i\boldsymbol{\kappa}\,\boldsymbol{\cdot}\,\boldsymbol{r}} = \mathbf{M_e(r)} \cdot \boldsymbol{\mu}_{n\perp}e^{i\boldsymbol{\kappa}\,\boldsymbol{\cdot}\,\boldsymbol{r}} \tag{4.8}$$

with

$$\boldsymbol{\mu}_{n\perp} = \frac{\boldsymbol{\kappa}}{\kappa} \times (\boldsymbol{\mu}_n \times \frac{\boldsymbol{\kappa}}{\kappa}) = \mu_n(\boldsymbol{\sigma_n} - (\boldsymbol{e} \cdot \boldsymbol{\sigma_n})\boldsymbol{e}) \tag{4.9}$$

For a crystal with magnetic atoms with $|\mathbf{M}_\nu|$ Bohr magnetons $\mu_B$ in the direction $\mathbf{M}_\nu/|\mathbf{M}_\nu|$ at the positions $(x_\nu, y_\nu, z_\nu)$ and the scattering vector in the direction (h,k,l) gathering from (4.1) and (4.5) all factors as $4\pi\frac{m_n}{2\pi\hbar^2}\mu_B\mu_N\gamma = \gamma\frac{e^2}{2m_ec^2} = \gamma\frac{r_0}{2} = 0.2695 \cdot 10^{-12}cm$ this results in the magnetic structure amplitude

$$\mathbf{F}^{mag}_{hkl} = 0.2695 \cdot 10^{-12} \cdot \sum_{\substack{magn.\ atoms\ \nu \\ in\ unit\ cell}} \mathbf{M}_\nu f_\nu(hkl) e^{2\pi i(hx_\nu + ky_\nu + lz_\nu)}[cm] = (A_1, A_2, A_3) \tag{4.10}$$

$\mathbf{M}_\nu$ measured in units of $\mu_B$, $f_\nu(hkl)$ is the form factor of the magnetic atom $\nu$, $r_0 = \frac{e^2}{m_ec^2}$ is the classical electron radius.

$$\mathbf{F}^{mag}_{\perp hkl} = (A_1, A_2, A_3) - \frac{[(\frac{h}{a}, \frac{k}{b}\frac{l}{c}) \cdot (A_1, A_2, A_3)](\frac{h}{a}, \frac{k}{b}\frac{l}{c})}{\frac{k^2}{b^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}}$$

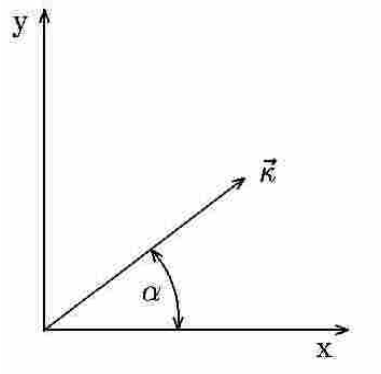



Figure 4.1: Geometry of equation (4.11) and the equations (4.27 on page 48) et seq.. x and y axes must be in the scattering plane. These directions are determined by the field direction of the adiabatic spin turner coil pair, which is selected as x direction and correspondingly that for the y direction.

For the following we choose the axis such that the scattering vector $\boldsymbol{\kappa} = \boldsymbol{k} - \boldsymbol{k'}$ lies in the x,y plane. For the multidetector instrument to be discussed different detectors have angles $\alpha$ with respect to the x-axis (determined by the direction of the field in the spin turner coils, see fig.4.1) i.e. $\frac{\boldsymbol{\kappa}}{\kappa} = (\cos\alpha, sin\alpha, 0)$. Therefore

$$\boldsymbol{\mu}_{n\perp} = \frac{\boldsymbol{\kappa}}{\kappa^2} \times (\boldsymbol{\mu}_n \times \boldsymbol{\kappa}) = (\mu_x \sin^2\alpha - \mu_y \sin\alpha\cos\alpha, \mu_y \cos^2\alpha - \mu_x \sin\alpha\cos\alpha, \mu_z) \tag{4.11}$$

and

$$\begin{aligned} \boldsymbol{M_e} \cdot \boldsymbol{\mu}_{n\perp} &= M_x(\mu_x \sin^2\alpha - \mu_y \sin\alpha\cos\alpha) + M_y(\mu_y \cos^2\alpha - \mu_x \sin\alpha\cos\alpha) + M_z\mu_z \\ &= \mu_x(M_x \sin^2\alpha - M_y \sin\alpha\cos\alpha) + \mu_y(M_y \cos^2\alpha - M_x \sin\alpha\cos\alpha) + \mu_z M_z \\ &= \boldsymbol{\mu}_n \cdot \mathbf{M}_{\mathbf{e}\perp}. \end{aligned} \tag{4.12}$$

$\mathbf{M_e}(\mathbf{r})$ is the magnetization density of the electron and $\boldsymbol{\mu}_n = -\gamma\frac{e\hbar}{2m_nc}\boldsymbol{\sigma}_n = -\gamma\mu_N\boldsymbol{\sigma}_n$ is the magnetic moment of the neutron, $\boldsymbol{\sigma}_n$ are the Pauli spin matrices for the neutron spin.

For the presentation of the xyz difference method it will be convenient to introduce raising or lowering operators with respect to all three axes:

$$\overset{x}{\mu}_\pm = \frac{1}{2}(\mu_y \pm i\mu_z) \qquad \overset{y}{\mu}_\pm = \tfrac{1}{2}(\mu_z \pm i\mu_x) \qquad \overset{z}{\mu}_\pm = \frac{1}{2}(\mu_x \pm i\mu_y) \tag{4.13}$$

Eigenstates to $\mu_\nu = -\gamma\mu_N\sigma_\nu$; $\nu$ =x,y,z are indexed as $|\overset{\nu}{\uparrow}>$ and $|\overset{\nu}{\downarrow}>$. E.g. $\sigma_x|\overset{x}{\uparrow}>=|\overset{x}{\uparrow}>$; $\sigma_x|\overset{x}{\downarrow}>=-|\overset{x}{\downarrow}>$; $\sigma_y|\overset{y}{\uparrow}>=|\overset{y}{\uparrow}>$ etc. with $|\overset{x}{\uparrow}>=\frac{1}{\sqrt{2}}\{|\overset{z}{\uparrow}>+|\overset{z}{\downarrow}>\}$, $|\overset{x}{\downarrow}>=\frac{i}{\sqrt{2}}\{-|\overset{z}{\uparrow}>+|\overset{z}{\downarrow}>\}$, $|\overset{y}{\uparrow}>=\frac{1}{\sqrt{2}}\{|\overset{z}{\uparrow}>+i|\overset{z}{\downarrow}>\}$, $|\overset{y}{\downarrow}>=\frac{1}{\sqrt{2}}\{i|\overset{z}{\uparrow}>+|\overset{z}{\downarrow}>\}$.

A flip operation is possible for polarizations in all three directions x, y or z. It corresponds to the fact that for the spin up/down at the polarizer the spin at the analyzer is down/up. This spin flip is described by operations as $\overset{x}{\sigma}_+|\overset{x}{\downarrow}>=|\overset{x}{\uparrow}>$ and $\overset{x}{\sigma}_-|\overset{x}{\uparrow}>=|\overset{x}{\downarrow}>$ etc. for the other directions, yielding

$$<\overset{x}{\uparrow}|\overset{x}{\sigma}_+|\overset{x}{\downarrow}>=1 \qquad <\overset{x}{\downarrow}|\overset{x}{\sigma}_+|\overset{x}{\downarrow}>=0 \qquad <\overset{x}{\downarrow}|\overset{x}{\sigma}_-|\overset{x}{\uparrow}>=1 \tag{4.14}$$

etc. This admits a generalization by allowing operations using mixtures of eigenstates as e.g.

$$<\overset{z}{\downarrow}|\sigma_x|\overset{y}{\uparrow}>=\frac{1}{\sqrt{2}} \qquad <\overset{z}{\uparrow}|\sigma_y|\overset{y}{\uparrow}>=\frac{1}{\sqrt{2}} \qquad <\overset{y}{\downarrow}|\sigma_z|\overset{x}{\uparrow}>=-\frac{1+i}{2} \tag{4.15}$$

etc. Such relationships are needed for the generalized polarization analysis [18] where one measures the x, y or z component of the polarization **P'** after scattering for the incident polarization $\mathbf{P}=(1,0,0)$, $(0,1,0)$ or $(0,0,1)$, respectively. The density matrix method does not need all this specializations, it is representation independent and yields all combinations, also those containing mixtures of eigenstates in one go, as we will see in chapter 5 on page 61.

### 4.3.1 The $\|-\perp$ method

#### 4.3.1.1 Magnetic part of the neutron cross section

For the $\|$-$\perp$ method the polarization is rotated successively parallel and perpendicular to the scattering vector and by taking the difference of these two measurements one separates the magnetic scattering from the other sorts of scattering. This method uses a single detector and the rotation of $\boldsymbol{\kappa}$ parallel to the x-axis can be achieved by setting $\alpha = 0$ in eq.(4.11) or (4.12). For the xyz difference method this will be generalized to arbitrary angles at a later stage. For $\alpha = 0$

$$\boldsymbol{M_e}\cdot\boldsymbol{\mu}_{n\perp} = \mu_y M_y + \mu_z M_z = -\gamma\mu_N(\sigma_{ny}M_{ey} + \sigma_{nz}M_{ez}) \tag{4.16}$$

Defining $\overset{x}{M}_\pm(\mathbf{r})$, $\overset{y}{M}_\pm(\mathbf{r})$ and $\overset{z}{M}_\pm(\mathbf{r})$ analogically to the $\overset{\nu}{\mu}_\pm$ operators, eq.(4.16) can also be written as

$$\boldsymbol{M_e}\cdot\boldsymbol{\mu}_{n\perp} = (\overset{x}{M}_+\overset{x}{\mu}_- + \overset{x}{M}_-\overset{x}{\mu}_+) = -\gamma\mu_N(\overset{x}{M}_+\overset{x}{\sigma}_- + \overset{x}{M}_-\overset{x}{\sigma}_+) \tag{4.17}$$

Remembering that $\mathbf{M_e}(\mathbf{r})$ is still a function of $\mathbf{r}$ and thereby also $M_x(\mathbf{r})$, $M_y(\mathbf{r})$, $M_z(\mathbf{r})$ and $\overset{\nu}{M}_\pm(\mathbf{r})$ one obtains for the magnetic part of the function $\Gamma^{\|}_{ss'}(\mathbf{r},\omega)$:

$$\begin{aligned}(\gamma\mu_N)^2\Gamma^{\|}_{ss'}(\mathbf{r},\omega) &= \sum_{\lambda\lambda'} p_\lambda|<\lambda' s'|\boldsymbol{M_e}\cdot\boldsymbol{\mu}_{n\perp}|\lambda s>|^2\delta(\hbar\omega+E_\lambda-E_{\lambda'}) \\ &= \sum_{\lambda\lambda'} p_\lambda|<\lambda' s'|\overset{x}{M}_+\overset{x}{\mu}_- + \overset{x}{M}_-\overset{x}{\mu}_+|\lambda s>|^2\delta(\hbar\omega+E_\lambda-E_{\lambda'}) \\ &= (\gamma\mu_N)^2\sum_{\lambda\lambda'} p_\lambda|<\lambda' s'|\overset{x}{M}_+\overset{x}{\sigma}_- + \overset{x}{M}_-\overset{x}{\sigma}_+|\lambda s>|^2\delta(\hbar\omega+E_\lambda-E_{\lambda'})\end{aligned} \tag{4.18}$$

**A.Spin flip scattering.**

Let us now investigate the spin flip neutron scattering cross section for the polarization parallel to the scattering vector i.e.

### $\boldsymbol{P} \parallel \boldsymbol{\kappa} \parallel \boldsymbol{e_x} = (1,0,0)$

If we can neglect spin orbit coupling the $\overset{\nu}{\sigma}_{\pm}$ operators can be applied separately and so one obtains from (4.18)

$$\begin{aligned}\Gamma^{\parallel}_{\uparrow\downarrow}(\mathbf{r},\omega) &= \sum_{\lambda\lambda'} p_\lambda |<\lambda'|\overset{x}{M}_+|\lambda>|^2 \delta(\hbar\omega + E_\lambda - E\lambda') \\ &= \int \ll \overset{x}{M}_+(\mathbf{r},t)\ \overset{x}{M}_-(0,0) \gg e^{i\omega t} dt \\ &= M_{yy}(\mathbf{r},\omega) + M_{zz}(\mathbf{r},\omega) + i(M_{zy}(\mathbf{r},\omega) - M_{yz}(\mathbf{r},\omega))\end{aligned} \tag{4.19}$$

and similarly

$$\Gamma^{\parallel}_{\downarrow\uparrow}(\mathbf{r},\omega) = M_{yy}(\mathbf{r},\omega) + M_{zz}(\mathbf{r},\omega) - i(M_{zy}(\mathbf{r},\omega) - M_{yz}(\mathbf{r},\omega))$$

The double brackets indicate thermal (i.e. $\sum_\lambda p_\lambda \ldots$) and quantum mechanical average (i.e. $\sum_{\lambda'} < \lambda|M_+|\lambda' >< \lambda'|exp(itE_{\lambda'})M_- exp(-itE_\lambda)|\lambda >$). In the following, intermediate steps will be omitted and we will always write immediately the time Fourier transform $M_{xx}(\mathbf{r},\omega)$ etc. of the corresponding correlation functions, or for brevity $\ll \ldots \gg$, especially in the longer formulae in eq.(4.27) et seq. and where no special abbreviations are in use. The factor i in (4.19 on page 47) signals a phase shift of $\frac{\pi}{2}$. It disappears when multiplied by a similar factor i resulting from the Fourier transform of an odd part of a correlation function, as e.g. $M_{zy} - M_{yz}$ for a helical structure. The resulting cross section is of course a real expression.

For polarization normal to the scattering vector i.e.

### $\boldsymbol{P} \perp \boldsymbol{\kappa} \parallel \boldsymbol{e_z} = (0,0,1)$

$$\begin{aligned}\Gamma^{\perp}_{\uparrow\downarrow}(\mathbf{r},\omega) &= \sum_{\lambda\lambda'} p_\lambda |<\lambda'|M_y|\lambda>|^2 \delta(\hbar\omega + E_\lambda - E_{\lambda'}) \\ &= M_{yy}(\mathbf{r},\omega) = \Gamma^{\perp}_{\downarrow\uparrow}(\mathbf{r},\omega)\end{aligned} \tag{4.20}$$

By taking the difference (as mentioned above) one obtains:

$$\begin{aligned}\Gamma^{\parallel}_{\uparrow\downarrow}(\mathbf{r},\omega) - \Gamma^{\perp}_{\uparrow\downarrow}(\mathbf{r},\omega) &= M_{zz}(\mathbf{r},\omega) + i(M_{zy}(\mathbf{r},\omega) - M_{yz}(\mathbf{r},\omega)) \\ \Gamma^{\parallel}_{\downarrow\uparrow}(\mathbf{r},\omega) - \Gamma^{\perp}_{\downarrow\uparrow}(\mathbf{r},\omega) &= M_{zz}(\mathbf{r},\omega) - i(M_{zy}(\mathbf{r},\omega) - M_{yz}(\mathbf{r},\omega))\end{aligned} \tag{4.21}$$

**B.Non-spin flip scattering**

For $\boldsymbol{P} = \boldsymbol{P_x} \parallel \boldsymbol{\kappa}$: in the non-spinflip scattering cross section one obtains analogously

$$\Gamma^{\parallel}_{\uparrow\uparrow}(\mathbf{r},\omega) = 0 \tag{4.22}$$

for $\boldsymbol{P} \parallel \boldsymbol{e_z} \perp \boldsymbol{\kappa}$

$$\Gamma^{\perp}_{\uparrow\uparrow}(\mathbf{r},\omega) = M_{zz}(\mathbf{r},\omega) \tag{4.23}$$

and the difference is here

$$\Gamma^{\perp}_{\uparrow\uparrow}(\mathbf{r},\omega) - \Gamma^{\parallel}_{\uparrow\uparrow}(\mathbf{r},\omega) = M_{zz}(\mathbf{r},\omega) \tag{4.24}$$

$\Gamma^{i}_{ss'}(\mathbf{r},\omega)$ derived above are functions which can be used to express the double differential cross section by combining eq.(4.1),(4.5) and including the factor $e^{i\boldsymbol{\kappa}\cdot\boldsymbol{r}}$ from eq.(4.8) to perform the spatial Fourier transform, taking into account the fact that $\mathbf{M_e}(\mathbf{r})$ is a function of $\mathbf{r}$. This yields

the magnetic part (indicated by the sign $\hat{}$ ) of the dynamical scattering function $\hat{S}^i_{ss'}(\boldsymbol{\kappa},\omega)$ as a function of $\boldsymbol{\kappa}$ and $\omega$ in addition to a form factor $f(\boldsymbol{\kappa})^2$ which describes the Fourier transform of the magnetization density. For the sake of simplicity these processes of the spatial Fourier transform have not been included above, and they will also not be included in the following derivations. This is done in order to avoid the essential physics being hidden behind pure formalism, which is assumed to be known and which is not essential for the aims of this paper. It will be assumed as performed when one finally needs the dynamical structure factor. Fourier transforming $\Gamma^i_{ss'}(\mathbf{r},\omega)$ as derived above to determine $\hat{S}^i_{ss'}(\boldsymbol{\kappa},\omega)$, one obtains the double differential cross section

$$\left.\frac{\partial^2\sigma}{\partial\omega\partial\Omega}\right|^i_{ss'} = \left(\frac{r_0\gamma}{2}\right)^2 \frac{k'}{k}\hat{S}^i_{ss'}(\boldsymbol{\kappa},\omega)f^2(\boldsymbol{\kappa}) \tag{4.25}$$

for i=$\parallel,\perp$. The differential cross section is obtained from the integral over $\omega$ defined as

$$\left.\frac{d\sigma}{d\Omega}\right|^i_{ss'} = \left(\frac{r_0\gamma}{2}\right)^2 \int \frac{k'(\omega)}{k}\hat{S}^i_{ss'}(\boldsymbol{\kappa},\omega)f^2(\boldsymbol{\kappa})d\omega \tag{4.26}$$

with i=$\parallel$, $\perp$.

## 4.4 General case of multidetectors

For the case of a multidetector instrument like that in fig.4.2 it is not possible to fulfil simultaneously the condition of the polarization parallel to the scattering vector for all detectors. In this case the method described above has to be modified in the following manner: we assume the general geometry of fig.4.2, eqs.(4.11) and (4.12) and discuss again the various cross sections. However, for the case of multidetectors the expressions become longer:

### 4.4.1 Spin flip cross sections (magnetic part only)

The polarization is defined as a vector with $\mathbf{P} = (P_x, P_y, P_z) = P_x\mathbf{e}_x + P_y\mathbf{e}_y + P_z\mathbf{e}_z$ the magnitude of which describes the degree of polarization according to $|\mathbf{P}| = \frac{n_\uparrow - n_\downarrow}{|n_\uparrow + n_\downarrow|}$. Polarization in x-direction (which can be achieved by putting the field in the spin rotation coil of fig.4.2 in the direction to be taken as x-direction) is then designated by $P_x = 1$ or $\mathbf{P}$=(1,0,0) or $\mathbf{P} \parallel \mathbf{e}_x$.

#### 4.4.1.1 Polarization in x-direction

Because $<\overset{x}{\downarrow}|\sigma_x|\overset{x}{\uparrow}>= 0$ the only remaining contribution in eq.(4.12) is

$$\begin{aligned}(\gamma\mu_N)^2\Gamma^x_{\uparrow\downarrow}(\mathbf{r},\omega) &= \sum_{\lambda\lambda'} p_\lambda |<\lambda'\overset{x}{\downarrow}|\mu_y(M_y\cos^2\alpha - M_x\sin\alpha\cos\alpha) + \\ &\quad \mu_z M_z|\lambda\overset{x}{\uparrow}>|^2\delta(\hbar\omega + E_\lambda - E_{\lambda'})\end{aligned} \tag{4.27}$$

which with $\overset{x}{\mathrm{A}}_\pm = M_y\cos^2\alpha - M_x\sin\alpha\cos\alpha \pm iM_z$ can be written as

$$\begin{aligned}\Gamma^x_{\uparrow\downarrow}(\mathbf{r},\omega) &= \sum_{\lambda\lambda'} p_\lambda |<\lambda'\overset{x}{\downarrow}|(\overset{x}{\sigma}_+\overset{x}{\mathrm{A}}_- + \overset{x}{\sigma}_-\overset{x}{\mathrm{A}}_+)|\lambda\overset{x}{\uparrow}>|^2\delta(\hbar\omega + E_\lambda - E_{\lambda'}) \\ &= \sum_{\lambda\lambda'} p_\lambda |<\lambda'|\overset{x}{\mathrm{A}}_+|\lambda>|^2\delta(\hbar\omega + E_\lambda - E_{\lambda'})\end{aligned} \tag{4.28}$$

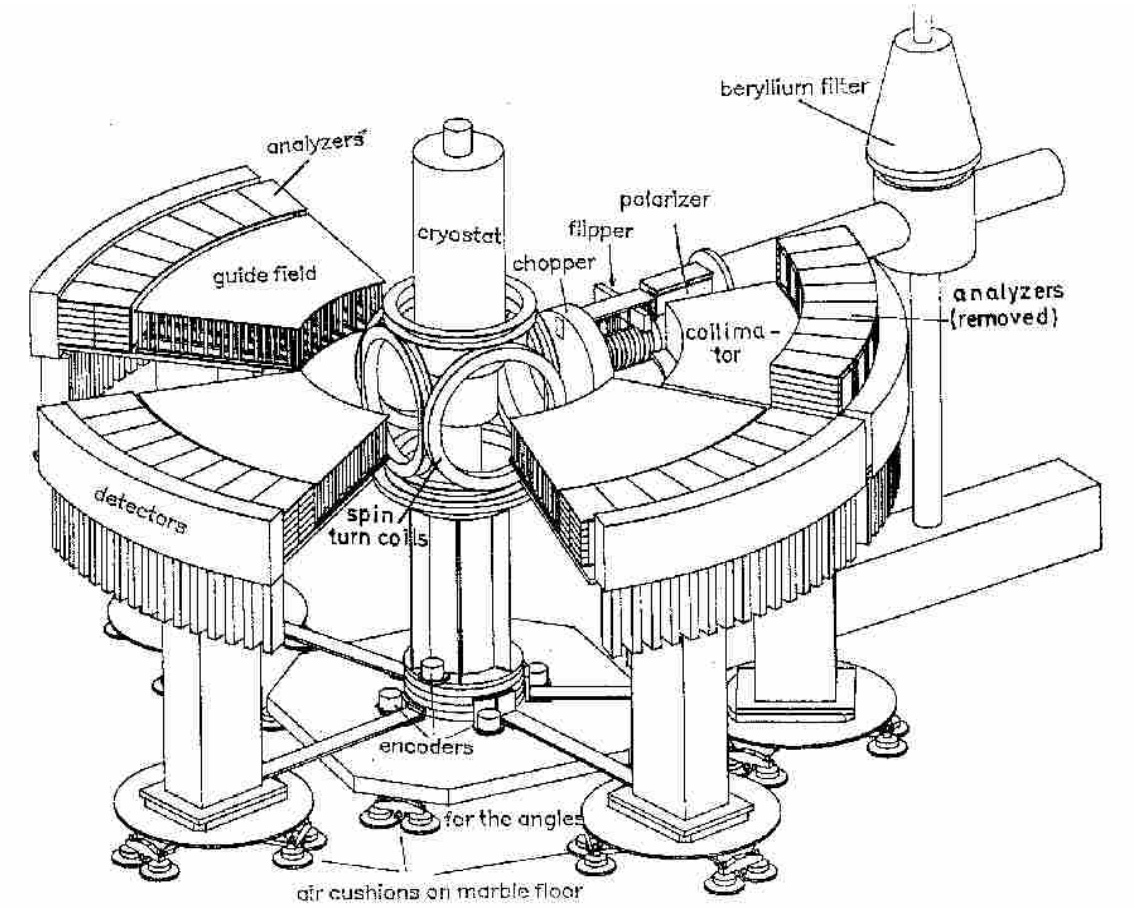



Figure 4.2: Multipurpose instrument D7 at the Institute Laue Langevin in Grenoble. At the right one bank is shown in the non-analyzing version with analyzers removed by the pneumatic elevators and the collimator inserted instead of the guide fields in front of the analyzers on the other banks. The neutrons arrive from the monochromator through the beryllium filter, the polarizer, the flipper and the chopper to the sample in the cryostat. From there they are scattered and arrive through the guide fields at the analysers and detectors. With the spin turner coils the polarization of the neutrons can be rotated in the x, y or z direction.

As in (4.19) $<\overset{x}{\downarrow} \mid \overset{x}{\sigma}_- \mid \overset{x}{\uparrow}>= 1$ and all other terms involving $\overset{x}{\sigma}_+$ are zero. If we can neglect spin orbit coupling we can evaluate the above matrix element with respect to the spin variables. This results in

$$
\begin{aligned}
&\Gamma^x_{\uparrow\downarrow}(\mathbf{r},\omega) \\
&\quad = \ll \overset{x}{\hat{A}}_- \overset{x}{\hat{A}}_+ \gg \\
&\quad = \ll (M_y\cos^2\alpha - M_x\sin\alpha\cos\alpha)(M_y\cos^2\alpha - M_x\sin\alpha\cos\alpha) \gg + \ll M_zM_z \gg \\
&\qquad -i \ll M_z(M_y\cos^2\alpha - M_x\sin\alpha\cos\alpha) \gg +i \ll (M_y\cos^2\alpha - M_x\sin\alpha\cos\alpha)M_z \gg \\
&\quad = \ll M_yM_y \gg \cos^4\alpha + \ll M_xM_x \gg \sin^2\alpha\cos^2\alpha + \ll M_zM_z \gg \\
&\qquad -(\ll M_xM_y \gg + \ll M_yM_x \gg)\sin\alpha\cos^3\alpha - i[\ll (M_zM_y - M_yM_z \gg)\cos^2\alpha \\
&\qquad +(\ll M_xM_z - M_zM_x \gg)\sin\alpha\cos\alpha]
\end{aligned}
\tag{4.29}
$$

(Remember that the correlation functions $\ll M_xM_x \gg$ etc. are always to be understood as $M_{xx}(\mathbf{r},\omega)$ etc. (see remarks eq.(4.19))). In determining $\Gamma^x_{\downarrow\uparrow}$ we obtain $\ll \overset{x}{\text{Å}}_+ \overset{x}{\text{Å}}_- \gg$ and thereby the same expression as in (4.29). However –i is replaced by +i in the phase shifted part.

#### 4.4.1.2 Polarization in y direction

With $P_y = 1$ or $\mathbf{P} = (0,1,0)$ and

$$\overset{y}{\text{Å}}_\pm = M_z \pm i(M_x \sin^2\alpha - M_y \sin\alpha\cos\alpha)) \tag{4.30}$$

$$\begin{aligned}
\Gamma^y_{\uparrow\downarrow}(\mathbf{r},\omega) &= \ll \overset{y}{\text{Å}}_- \overset{y}{\text{Å}}_+ \gg \\
&= \ll M_zM_z \gg + \ll M_xM_x \gg \sin^4\alpha + \ll M_yM_y \gg \sin^2\alpha\cos^2\alpha \\
&\quad -(\ll M_xM_y \gg + \ll M_yM_x \gg)\sin^3\alpha\cos\alpha - i[(\ll M_xM_z \gg \\
&\quad - \ll M_zM_x \gg)\sin^2\alpha + (\ll M_zM_y \gg - \ll M_yM_z \gg)\sin\alpha\cos\alpha]\}
\end{aligned} \tag{4.31}$$

Also here for $\Gamma^y_{\downarrow\uparrow}$ we obtain the same expression as in (4.31) but instead of –i we have to write +i. See also (4.40).

#### 4.4.1.3 Polarization in z direction

$$\begin{aligned}
(\gamma\mu_N)^2\Gamma^z_{\uparrow\downarrow}(\mathbf{r},\omega) &= \sum_{\lambda\lambda'} p_\lambda | < \lambda' \overset{z}{\uparrow} | \mu_x(M_x\sin^2\alpha - M_y\sin\alpha\cos\alpha) \\
&\quad +\mu_y(M_y\cos^2\alpha - M_x\sin\alpha\cos\alpha | \lambda \overset{z}{\downarrow} > |^2 \delta(\hbar\omega + E_\lambda - E_{\lambda'})
\end{aligned} \tag{4.32}$$

and with

$$\overset{z}{\text{Å}}_\pm = (M_x\sin^2\alpha - M_y\sin\alpha\cos\alpha) \pm i(M_y\cos^2\alpha - M_x\sin\alpha\cos\alpha) \tag{4.33}$$

this yields

$$\begin{aligned}
\Gamma^z_{\uparrow\downarrow}(\mathbf{r},\omega) &= \ll \overset{z}{\text{Å}}_- \overset{z}{\text{Å}}_+ \gg \\
&= \ll M_xM_x \gg (\sin^4\alpha + \sin^2\alpha\cos^2\alpha) + \ll M_yM_y \gg \cos^2\alpha \\
&\quad +(\ll M_xM_y \gg + \ll M_yM_x \gg)\sin\alpha\cos\alpha)\}
\end{aligned} \tag{4.34}$$

### 4.4.2 Non flip cross section for the magnetic part only

Now we calculate the NON FLIP functions $\Gamma^\nu_{\uparrow\uparrow}$ for the magnetic part only:

**$\mathbf{P} = \mathbf{P_x}$**

$$\begin{aligned}
(\gamma\mu_N)^2\Gamma^x_{\uparrow\uparrow}(\mathbf{r},\omega) &= \sum_{\lambda\lambda'} p_\lambda | < \lambda' \overset{x}{\uparrow} | \mu_x(M_x\sin^2\alpha \\
&\quad -M_y\sin\alpha\cos\alpha) | \lambda \overset{x}{\uparrow} > |^2 \delta(\hbar\omega + E_\lambda - E_{\lambda'}) \qquad (4.35) \\
&= (\gamma\mu_N)^2\{\ll M_xM_x \gg \sin^4\alpha + \ll M_yM_y \gg \sin^2\alpha\cos^2\alpha \\
&\quad -(\ll M_xM_y \gg + \ll M_yM_x \gg)\sin^3\alpha\cos\alpha\} \qquad (4.36)
\end{aligned}$$

$\mathbf{P} = \mathbf{P_y}$

$$\begin{aligned}\Gamma^{y}_{\uparrow\uparrow}(\mathbf{r},\omega) &= \ll M_yM_y \gg \cos^4\alpha + \ll M_xM_x \gg \sin^2\alpha\cos^2\alpha \\ &\quad -(\ll M_yM_x \gg + \ll M_xM_y \gg)\sin\alpha\cos^3\alpha \end{aligned} \tag{4.37}$$

$\mathbf{P} = \mathbf{P_z}$

$$\Gamma^{z}_{\uparrow\uparrow}(\mathbf{r},\omega) = \ll M_zM_z \gg \tag{4.38}$$

These results for $\Gamma^{\nu}_{ss'}$ can be combined in the following matrix equations for the phase shifted and non phase shifted parts: For the non phase shifted part one obtains

$$\begin{pmatrix} \Gamma^{x}_{\uparrow\downarrow}(\mathbf{r},\omega) \\ \Gamma^{y}_{\uparrow\downarrow}(\mathbf{r},\omega) \\ \Gamma^{z}_{\uparrow\downarrow}(\mathbf{r},\omega) \\ \Gamma^{x}_{\uparrow\uparrow}(\mathbf{r},\omega) \\ \Gamma^{y}_{\uparrow\uparrow}(\mathbf{r},\omega) \\ \Gamma^{z}_{\uparrow\uparrow}(\mathbf{r},\omega) \end{pmatrix} = \begin{pmatrix} \sin^2\alpha\cos^2\alpha & \cos^4\alpha & 1 & -\sin\alpha\cos^3\alpha \\ \sin^4\alpha & \sin^2\alpha\cos^2\alpha & 1 & -\sin^3\alpha\cos\alpha \\ \sin^2\alpha & \cos^2\alpha & 0 & -\sin\alpha\cos\alpha \\ \sin^4\alpha & \sin^2\alpha\cos^2\alpha & 0 & -\sin^3\alpha\cos\alpha \\ \sin^2\alpha\cos^2\alpha & \cos^4\alpha & 0 & -\sin\alpha\cos^3\alpha \\ 0 & 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} M_{xx}(\mathbf{r},\omega) \\ M_{yy}(\mathbf{r},\omega) \\ M_{zz}(\mathbf{r},\omega) \\ M_{xy}(\mathbf{r},\omega) + M_{yx}(\mathbf{r},\omega) \end{pmatrix} \tag{4.39}$$

and for the phase shifted part

$$\begin{pmatrix} \Gamma^{x}_{\uparrow\downarrow}(\mathbf{r},\omega) \\ \Gamma^{x}_{\downarrow\uparrow}(\mathbf{r},\omega) \\ \Gamma^{y}_{\uparrow\downarrow}(\mathbf{r},\omega) \\ \Gamma^{y}_{\downarrow\uparrow}(\mathbf{r},\omega) \end{pmatrix} = \begin{pmatrix} -\sin\alpha\cos\alpha & -\cos^2\alpha \\ \sin\alpha\cos\alpha & \cos^2\alpha \\ \sin^2\alpha & -\cos\alpha\sin\alpha \\ -\sin^2\alpha & \cos\alpha\sin\alpha \end{pmatrix} \begin{pmatrix} M_{zx}(\mathbf{r},\omega) - M_{xz}(\mathbf{r},\omega) \\ M_{zy}(\mathbf{r},\omega) - M_{yz}(\mathbf{r},\omega) \end{pmatrix} \tag{4.40}$$

For the elastic case these equations, combined with equation (8), correspond to the following equation given for the special case of $\mathbf{P} \parallel \boldsymbol{\kappa}$ for spin flip scattering by Moon, Riste, Koehler [8]:

$$\frac{d\sigma^{\pm\mp}}{d\Omega} = \sum_{i,j} p_i p_j^* e^{i\mathbf{K}\cdot(\mathbf{r_i}-\mathbf{r_j})}[\mathbf{S}_{\perp\mathbf{i}} \cdot \mathbf{S}_{\perp\mathbf{j}} \mp i\hat{z}\cdot(\mathbf{S}_{\perp\mathbf{i}} \times \mathbf{S}^*_{\perp\mathbf{j}}] \tag{4.41}$$

However, 4.39 and 4.40 are also applicable to inelastic scattering and for the geometry of the three orthogonal directions x,y,z, with x and y in the scattering plane as this is needed for the application of a multidetector with time of flight analysis.

## 4.5 Application to a powder measurement

For a powder with a collinear magnetization the correlation functions $\ll M_xM_x \gg = \ll M_yM_y \gg = \ll M_zM_z \gg$. All mixed ones as $\ll M_xM_z \gg$, $\ll M_xM_y \gg$,$\ll M_zM_y \gg$ are zero. Then magnetic cross sections become much simpler: the phase shifted parts (equ.(4.40)) are all zero and in matrix (4.39) only the first three columns remain for describing the spinflip and the non spin flip part of the respective magnetic cross sections. We now define

$$\frac{\partial^2\sigma^{\nu}_{ss'}}{\partial\Omega\partial\omega} = \frac{k'}{k}\left(\frac{r_0\gamma}{2}\right)^2 f^2(\boldsymbol{\kappa})\hat{S}^{\nu}_{ss'}(\boldsymbol{\kappa},\omega) \tag{4.42}$$

etc. corresponding to (4.25)-(4.26), with $\hat{S}^{\nu}_{ss'}(\boldsymbol{\kappa},\omega)$ being the space Fourier transform of the functions $\Gamma^{\nu}_{ss'}(\mathbf{r},\omega)$ and $\nu$=x,y,z; s,s'=$|\overset{\nu}{\uparrow}>$ or $|\overset{\nu}{\downarrow}>$. From eq.(4.39), and

$$\frac{\partial^2\sigma_{param}}{\partial\Omega\partial\omega} = \frac{k'}{k}\frac{2}{3}\left(\frac{r_0\gamma}{2}\right)^2 f^2(\boldsymbol{\kappa})M(\boldsymbol{\kappa},\omega) \tag{4.43}$$

$$\frac{\partial^2\sigma^{spin}_{incoh}}{\partial\Omega\partial\omega} = \frac{k'}{k}B^2 S_{incoh}(\boldsymbol{\kappa},\omega) \tag{4.44}$$

$$\frac{\partial^2\sigma_{coh}}{\partial\Omega\partial\omega} = \frac{k'}{k}b^2 S_{coh}(\boldsymbol{\kappa},\omega) \tag{4.45}$$

Then we gather all contributions for the respective scattering and obtain six cross sections each measured with the three polarisation directions in x, y and z direction, with and without neutron spin flip respectively. These include all kinds of scattering i.e. coherent, spin incoherent, isotope incoherent and magnetic scattering.

These cross sections read

$$\frac{\partial^2\sigma^{x}_{\uparrow\downarrow}}{\partial\Omega\partial\omega} = \frac{1}{2}\frac{\partial^2\sigma_{param}}{\partial\Omega\partial\omega}(\cos^2\alpha+1) + \frac{2}{3}\frac{\partial^2\sigma^{spin}_{incoh}}{\partial\Omega\partial\omega} \tag{4.46}$$

$$\frac{\partial^2\sigma^{y}_{\uparrow\downarrow}}{\partial\Omega\partial\omega} = \frac{1}{2}\frac{\partial^2\sigma_{param}}{\partial\Omega\partial\omega}(\sin^2\alpha+1) + \frac{2}{3}\frac{\partial^2\sigma^{spin}_{incoh}}{\partial\Omega\partial\omega} \tag{4.47}$$

$$\frac{\partial^2\sigma^{z}_{\uparrow\downarrow}}{\partial\Omega\partial\omega} = \frac{1}{2}\frac{\partial^2\sigma_{param}}{\partial\Omega\partial\omega} + \frac{2}{3}\frac{\partial^2\sigma^{spin}_{incoh}}{\partial\Omega\partial\omega} \tag{4.48}$$

$$\frac{\partial^2\sigma^{x}_{\uparrow\uparrow}}{\partial\Omega\partial\omega} = \frac{1}{2}\frac{\partial^2\sigma_{param}}{\partial\Omega\partial\omega}\sin^2\alpha + \frac{1}{3}\frac{\partial^2\sigma^{spin}_{incoh}}{\partial\Omega\partial\omega} + \frac{\partial^2\sigma_{coh}}{\partial\Omega\partial\omega} + \frac{\partial^2\sigma^{isotop}_{incoh}}{\partial\Omega\partial\omega} \tag{4.49}$$

$$\frac{\partial^2\sigma^{y}_{\uparrow\uparrow}}{\partial\Omega\partial\omega} = \frac{1}{2}\frac{\partial^2\sigma_{param}}{\partial\Omega\partial\omega}\cos^2\alpha + \frac{1}{3}\frac{\partial^2\sigma^{spin}_{incoh}}{\partial\Omega\partial\omega} + \frac{\partial^2\sigma_{coh}}{\partial\Omega\partial\omega} + \frac{\partial^2\sigma^{isotop}_{incoh}}{\partial\Omega\partial\omega} \tag{4.50}$$

$$\frac{\partial^2\sigma^{z}_{\uparrow\uparrow}}{\partial\Omega\partial\omega} = \frac{1}{2}\frac{\partial^2\sigma_{param}}{\partial\Omega\partial\omega} + \frac{1}{3}\frac{\partial^2\sigma^{spin}_{incoh}}{\partial\Omega\partial\omega} + \frac{\partial^2\sigma_{coh}}{\partial\Omega\partial\omega} + \frac{\partial^2\sigma^{isotop}_{incoh}}{\partial\Omega\partial\omega} \tag{4.51}$$

By combining the measured cross sections one can separate the different contributions from one another. Thus the two following combinations yield the paramagnetic cross section with no additional assumption other than that of a powder sample, namely that the correlation functions $\ll M_i M_i \gg$ for i=x,y,z are all equal and all the mixed correlation functions are zero:

$$\frac{\partial^2\sigma_{param}}{\partial\Omega\partial\omega} = 2\left(\frac{\partial^2\sigma^{x}_{\uparrow\downarrow}}{\partial\Omega\partial\omega} + \frac{\partial^2\sigma^{y}_{\uparrow\downarrow}}{\partial\Omega\partial\omega} - 2\frac{\partial^2\sigma^{z}_{\uparrow\downarrow}}{\partial\Omega\partial\omega}\right) \tag{4.52}$$

$$\frac{\partial^2\sigma_{param}}{\partial\Omega\partial\omega} = 2\left(2\frac{\partial^2\sigma^{z}_{\uparrow\uparrow}}{\partial\Omega\partial\omega} - \frac{\partial^2\sigma^{x}_{\uparrow\uparrow}}{\partial\Omega\partial\omega} - \frac{\partial^2\sigma^{y}_{\uparrow\uparrow}}{\partial\Omega\partial\omega}\right) \tag{4.53}$$

Correspondingly one obtains the $\partial^2\sigma^{spin}_{incoh}/(\partial\Omega\partial\omega)$ by the following combination:

$$\frac{\partial^2\sigma^{spin}_{incoh}}{\partial\Omega\partial\omega} = \frac{3}{2}\left(3\frac{\partial^2\sigma^{z}_{\uparrow\downarrow}}{\partial\Omega\partial\omega} - \frac{\partial^2\sigma^{x}_{\uparrow\downarrow}}{\partial\Omega\partial\omega} - \frac{\partial^2\sigma^{y}_{\uparrow\downarrow}}{\partial\Omega\partial\omega}\right) \tag{4.54}$$

as can be checked by combining eq.(4.46),(4.47) and (4.48). The $\partial^2\sigma_{coh}/(\partial\Omega\partial\omega)$ can be obtained by subtracting the cross sections obtained in a similar manner using $\partial^2\sigma^{z}_{\uparrow\uparrow}/(\partial\Omega\partial\omega)$:

$$\frac{\partial^2\sigma_{coh}}{\partial\Omega\partial\omega} + \frac{\partial^2\sigma^{isotop}_{incoh}}{\partial\Omega\partial\omega} = \frac{\partial^2\sigma^{z}_{\uparrow\uparrow}}{\partial\Omega\partial\omega} - \frac{1}{2}\frac{\partial^2\sigma_{param}}{\partial\Omega\partial\omega} - \frac{1}{3}\frac{\partial^2\sigma^{spin}_{incoh}}{\partial\Omega\partial\omega} \tag{4.55}$$

Coherent scattering cannot be distinguished from isotope incoherent scattering. These relationships are given in [2, 9, 16, 20] without derivation.

## 4.6 Derivation and limits of validity of $\mathbf{P}' = -\hat{\kappa}(\hat{\kappa} \cdot \mathbf{P})$

With equation (4.39) we can now derive the equation, already given by Halpern and Johnson [11]:

$$\boldsymbol{P'} = -\frac{\boldsymbol{\kappa}}{\kappa}(\frac{\boldsymbol{\kappa}}{\kappa} \cdot \boldsymbol{P}) \tag{4.56}$$

with **P**=polarization of the incident beam and **P'**=polarization of the beam scattered by a paramagnetic sample. It is often cited [5, 14, 15] with more or less convincing or even misleading demonstrations. Its main content is: (i) the scattered beam is polarized in the direction of the scattering vector (but see [5]), (ii) the spin is flipped and (iii) the intensity decreases with the cosine squared of the angle of rotation of the analysis. This is analogous to the law of Malus in optics. With our method of demonstration we can see its range of validity. If $\frac{\boldsymbol{\kappa}}{\kappa} = (\cos\alpha, \sin\alpha, 0)$ and the incident polarization is $\mathbf{P} = (P_x, 0, 0)$ and one determines $\mathbf{P'} = \mathbf{P'}_x$ i.e. the polarization in x direction, application of (4.56) yields $P'_x = -\kappa_x\kappa_x P_x = -P_x \cos^2\alpha$ and correspondingly for $P_y$ (4.56) yields $P'_y = -P_y \sin^2\alpha$ and for $P_z$ always $P'_z = 0$.

Using eqs.(4.39) and (4.40) it is possible to determine this polarization of the beam scattered by a paramagnetic or antiferromagnetic sample with disappearing interference term . This is done using the definition of polarization i.e. the equation

$$P'_\nu = \frac{\Gamma^\nu_{\uparrow\uparrow} - \Gamma^\nu_{\uparrow\downarrow}}{\Gamma^\nu_{\uparrow\uparrow} + \Gamma^\nu_{\uparrow\downarrow}} P_\nu \tag{4.57}$$

For non-collinear structures one cannot expect eq.(4.56) to be valid, as this can even give rise to two different results for $\uparrow\downarrow$ or $\downarrow\uparrow$ flips. For collinear structures one obtains for the general case

$$\begin{aligned}
P'_x &= P_x \frac{(1-2\cos^2\alpha)(M_{xx}\sin^2\alpha + M_{yy}\cos^2\alpha - (M_{xy}+M_{yx})\sin\alpha\cos\alpha) - M_{zz}}{M_{xx}\sin^2\alpha + M_{yy}\cos^2\alpha - (M_{xy}+M_{yx})\sin\alpha\cos\alpha + M_{zz}} \\
P'_y &= P_y \frac{(1-2\sin^2\alpha)(M_{xx}\sin^2\alpha + M_{yy}\cos^2\alpha - (M_{xy}+M_{yx})\sin\alpha\cos\alpha) - M_{zz}}{M_{xx}\sin^2\alpha + M_{yy}\cos^2\alpha - (M_{xy}+M_{yx})\sin\alpha\cos\alpha + M_{zz}} \\
P'_z &= P_z \frac{M_{zz} - M_{xx}\sin^2\alpha - M_{yy}\cos^2\alpha + (M_{xy}+M_{yx})\sin\alpha\cos\alpha}{M_{zz} + M_{xx}\sin^2\alpha + M_{yy}\cos^2\alpha - (M_{xy}+M_{yx})\sin\alpha\cos\alpha}
\end{aligned} \tag{4.58}$$

These equations are also valid for a single crystal, but they are more general than eq.(4.56). If for example the magnetization of the single crystal is in the z-direction, eq.(4.58) yields $P'_z = P_z$, $P'_x = -P_x$, $P'_y = -P_y$ independent of $\alpha$. Eq.(4.56) cannot comprise this result. Eq.(4.56) is only valid for a collinear powder if $M_{xx} = M_{yy} = M_{zz}$ and without interference term . For this case we obtain from (4.58)

$$P'_x = -P_x\cos^2\alpha \qquad P'_y = -P_y\sin^2\alpha \qquad P'_z = 0 \tag{4.59}$$

These are exactly the results of eq.(4.56).

For the case of paramagnetic and antiferromagnetic powder samples eq.(4.56) is very useful. Its content is, that the polarization of the beam scattered by a paramagnetic or antiferromagnetic sample has the direction of the scattering vector. In this case the direction of the polarization is very easy to determine experimentally from the three components of the xyz method using $\tan^2\alpha = (\Gamma^y_{\uparrow\downarrow} - \Gamma^z_{\uparrow\downarrow})/(\Gamma^x_{\uparrow\downarrow} - \Gamma^z_{\uparrow\downarrow})$ with $\Gamma^\nu_{\uparrow\downarrow}$ given in eq.(4.39) and it is proportional to the respective scattered intensity. This can then immediately indicate whether or not the scattering vector has the direction of an elastic scattering vector or that of an inelastic one. This can be done using an integral measurement without time of flight analysis. This was first shown by Maleev [12] and used by Mezei [13].

## 4.7 Instrumental

Fig.4.2 gives a perspective view of a multidetector instrument adapted to the xyz-difference method of polarization analysis for three different wavelengths $\lambda$=0.31 nm, 0.48 nm or 0.57 nm. The different chapters of this book describe the different possibilities of the instrument and so together result in a general description of the instrument. In this chapter we are interested in that part of the instrument which is necessary to guarantee the working of the rotation of the polarization into the x, y and z directions for these wavelengths. This comprises essentially everything that may influence the field direction. Different sample environments such as cryostats or furnaces have to avoid fields at the sample position by bifilar heater winding. The chopper disks for the time of flight have to avoid rotating metallic parts in the polarized beam, which would depolarize the beam by eddy currents. In the disks of the chopper the aluminium in the windows therefore has to be removed, and not only the absorbing gadolinium layer.

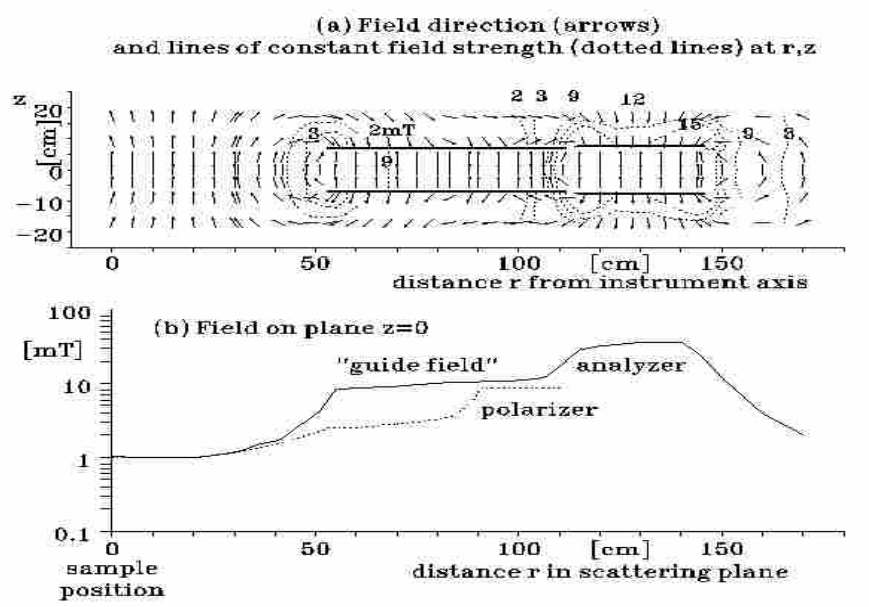



Figure 4.3: (a) Field pattern of one detector bank in a vertical section. Some lines (dotted) of constant field strength are given near the points where the field changes considerably. The arrows show the field direction in the centre point of the arrow line (zero of vertical scale: plane of scattering, zero of horizontal scale: instrument axis). (b) Field strength in the scattering plane on the way from the sample centre to the centre of the detector without current in the spin turn coil.

Fig.4.3a shows a vertical section through one detector bank. The detectors are located on banks, each with 16 $^3$He-detectors of 10 cm in height and 5 cm in diameter, with 2 atm gas pressure, and at a distance of r=150 cm away from the sample. Fig.4.3b shows the field in the scattering plane on the way from the polarizer to the sample (dotted) and from the sample to the analyzer (solid). If all analyzers are in the measuring position, then the field direction in the scattering plane is everywhere perpendicular to this plane and has the same direction. The magnetic backwards flux necessary to achieve div $\mathbf{B} = 0$ is always located inside the permanent magnets only. In the guide field in front of the polarizer a Mezei flipper with a Brookhaven correction coil around it [8] serves as flipper. A monitor behind the sample and the chopper together with an analyzer serves for monitoring the flipping ratio and the sample transmission.

The instrument comprises 4 such banks of 16 detectors each. Every second detector, i.e. 32

detectors, is equipped with a supermirror analyzer of 5 cm x 10 cm cross section as described in [3, 4] where the alignment and the achieved transmission and flipping ratios are also described as a function of wavelength. Fig.4.4 shows the contours of constant field strength in the scattering plane in the surroundings of one bank with 16 detectors and the associated guide fields.

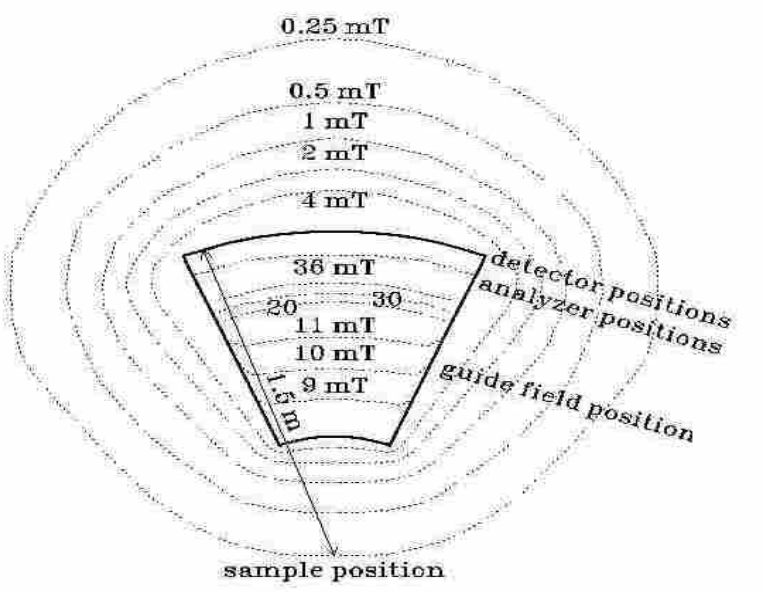



Figure 4.4: Magnetic field of one bank in the scattering plane. The field direction is perpendicular to the figure plane. The dotted lines are lines of constant field strength. The solid lines describe the lay-out of the guide field set-up, as given in fig.4.3 in a vertical cut.

Behind the chopper and centred at the sample position there is a spin rotator. This consists of a cube of three coil pairs to define the polarization direction of the beam at the sample position. The field strength is large enough to enable an adiabatic rotation of the polarization direction into either the x,y or z direction [6, 7] but not too strong, so that the field at the sample does not change the sample magnetization essentially. Fig.4.5 shows the field of this coil in the scattering plane in the absence of other sources of magnetization. This field should show rotational symmetry around the coil axis.

With four detector banks in the instrument the fields of these four banks are linearly superposed so that for example in the centre of the instrument there is a region of $4 \times 0.25$ mT $= 1.0$ mT resulting from all four banks (see figs.4.3 and 4.4). Therefore for polarization analysis measurements that do not need spin rotation there is no need for an additional guide field at the sample position, and one can even remove the xyz-spin-turner coil cube to increase the accessible angular range. For the case of the xyz-difference measurement, and for measurements with the polarization in x or y direction, one has to adjust the z-coil-current to compensate this z-field in the instrument. Otherwise the field would have also a component in the z-direction and consequently would not point exactly in the x- or the y-direction. All these conditions have to be kept under surveillance, because they can change with time, e.g. by changing the environment of the instrument, which is now kept as iron-free as possible.

This spin rotation has to take place on the flight path from the polarizer guide fields to the sample, and from the sample to the analyzer guide fields. For the scattering process in the sample which we call the xyz-difference method and which was treated theoretically in the first part of this paper, we need at the sample position three different, well defined polarization directions

$P_x$, $P_y$, $P_z$. After the scattering process and on the way to the analyzers there is again a spin reorientation process which rotates the component of the neutron spin, which was brought into the x or y direction for the scattering process, respectively, back to the z direction. This component is than transmitted by the analyzers. No rotation is required for the z component.

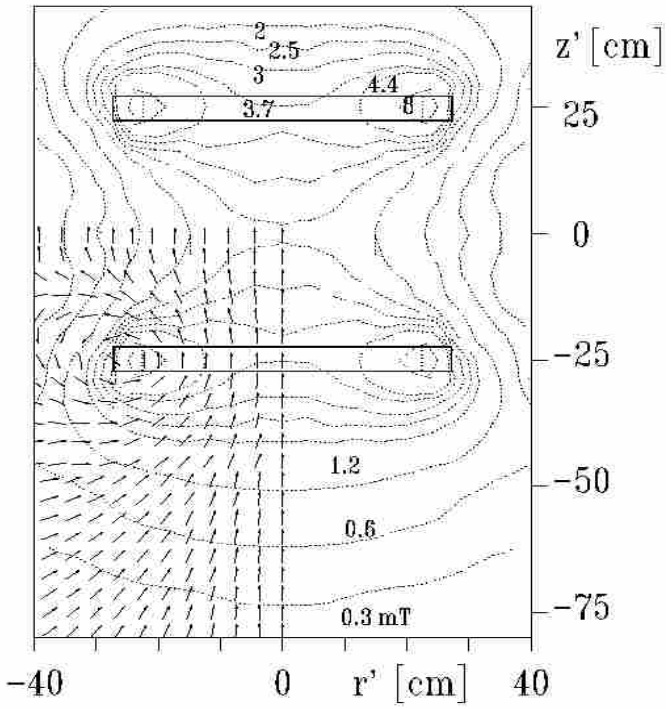



Figure 4.5: Field in and around the spin turn coil. The dotted lines are lines of constant field strength in mT for a current of 7.7 Ampère. The arrows in the lower left quarter show the field direction in this part of the plane at the center of the arrows. Solid thick lines: position of two circular coils with the coil axis z' in the figure plane through the zero point of the abscissa.

In the spin turner coils the spin of the neutrons has to follow the field direction. At the polarizer and the analyzer the guide fields are always high, roughly 10 mT at the polarizer and 40 mT at the analyzer with the fields being oriented along the vertical direction (z-direction). If the spin turner coils are excited for the horizontal x or y direction, then the vertical field in front of the bank decreases with the distance from the bank and is exactly compensated at the sample position by the z-coils. This combines with the field in the x direction, field strength of which behaves as shown in the contour plots of fig.4.5. This figure indicates the field direction (arrows) and the lines of constant field strength (dotted) of one coil pair of the spin turn coils for a current of 7.7 Ampère. (0,0) is the centre of the sample on the scattering plane and on the axis of the instrument. As the coils are circular the figure is valid for the whole space. It can be applied for all three coil pairs and can be used to describe the total resulting field of all three coil pairs just by linear superposition of the figure with z' in x or y or z direction respectively. From the field patterns in figs.4.3 to 4.5 one can obtain the exact rotation of the guide field as a function of the distance from the centre of the spin turner coil for each detector. Examples of this are given in fig.4.6 for a neutron path through the centre of a spin turner coil and for a neutron path just behind the edge of such a coil. In order to allow the neutron spin orientation to follow the field direction one has to fulfil the condition of adiabaticity i.e. the change of the field direction has to be slow enough. Fig.4.6 shows that the field direction is changing by $62^0 = 1.082$ rad on the way from the centre to the entrance into the

guide field for the analyzer in the range of r = 25 cm to 45 cm. Fig.4.6b shows that the rotation is indeed homogeneous over this distance of 20 cm and is not taking place over the whole path. The neutron with a velocity v(m/s)=3956/$\lambda$(Å) feels this as a rotation of $|\omega| = \frac{1.082 \cdot v}{s}$. The condition of adiabaticity requires $|\omega| \ll |\omega_L|$ with $\omega_L = -\gamma H$ being the Larmor frequency. It is known [6, 7] that the maximum deviation of the neutron spin direction from the magnetic field direction is given by the angle $2\delta = 2 \arctan \frac{\omega}{\omega_L}$. In our case $\omega_L = -2\pi \cdot 29164 \frac{H}{mT} = 183242.8 \frac{H}{mT}$ $[s^{-1}]$ and for $\lambda = 4.8$ Å we have $\omega = 1.081 \frac{3956}{0.2 \cdot 4.8} = 4459.2$ $[s^{-1}]$. This corresponds to $2\delta = 2.22^0$ for a field of 1.255 mT as rotating guide field, which is the minimum field in the region of the rotation of fig.4.6 b. On the way from the polarizer to the sample one gets exactly the same deviation. For the wavelength of 5.7 Å this deviation is $1.87^0$ and for 3.1 Å it is $3.4^0$. On the way through the corner of the coil the behaviour is a little more complicated as seen in fig.4.6 c) and d). There one can observe two rotations of the field, one in $\varphi$ and one in $\vartheta$. With the same sort of estimate one finds there a maximum deviation for a wavelength of 4.8 Å of $2.2^0$ for the $\varphi$– rotation and $0.74^0$ for the $\vartheta$–rotation. The behaviour of the neutron spin in a conically rotating guide field is treated further in chapter 2 and in [19].

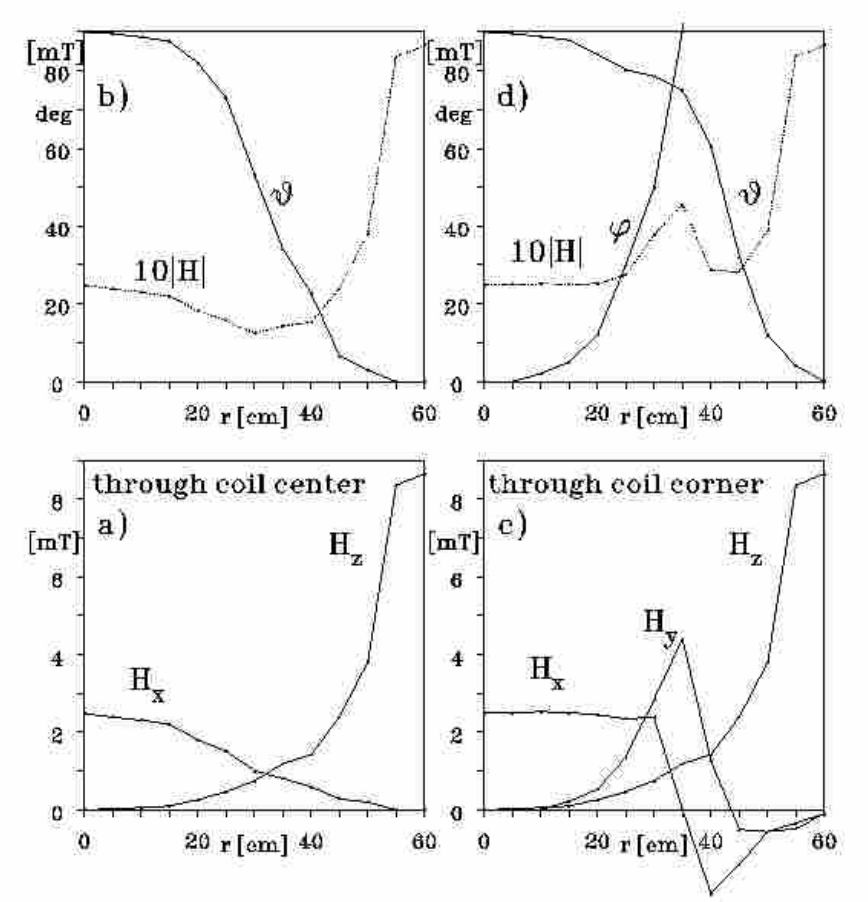



Figure 4.6: a) and c) rectangular, b) and d) spherical field components of the guide field on the way of the neutron for two characteristic neutron pathes, a) and b) through the center of the coils, c) and d) near the corner of the coils. In b) and d) the ordinate scale is mT for the field $|H|$ and degree for the angles $\vartheta$, $\varphi$.

The error introduced into the measured magnetic cross section by such a deviation of the

neutron spin direction can be estimated by using the law derived above of the polarization direction for paramagnetic scattering (eq.(4.56)). From this one obtains a maximum error of 0.15% for the measured intensities corresponding to the deviation of $2.2^0$ at the sample position and another 0.15% for the deviation of $2.2^0$ on the way from sample to analyzers. By analogy to the law of Malus for optical polarization the intensities are proportional to $\cos^2(2\delta)$ with $2\delta$ being the angle of rotation of the polarization. Because of this small maximum error and also due to the size of the detectors of 10 cm on a radius of 1.5 m the angle $\vartheta$ is only determined to within $3.8^0$. It is not practical to try to diminish this angle of $2\delta = 2.2^0$.

A quantitative test is described in chapter 10 and in [20] of cross section measurements using this instrument and a sample whose cross section can be calculated exactly for different $\boldsymbol{\kappa}$ and $\omega$. As this test cross section is only slightly dependent on the scattering vector this measurement represents another test for the fulfilment of the adiabaticity condition for all the neutron flight paths through the fields of the spin rotation coils.

A remark is in order concerning the difference of $\uparrow\downarrow$ and $\downarrow\uparrow$ flip measurements, which play a role only in $P_x$ or $P_y$ or $P_\parallel$ measurements with spin flip. For the instrument described above this can be measured by inverting the current in the x or y coils. This process inverts the initial spin on the sample from $\uparrow$ to $\downarrow$ and if the sample flips the set-up of the instrument is able to measure the $\uparrow\downarrow$ and the $\downarrow\uparrow$ flip cross sections separately.

Finally the procedure of the xyz-method corresponds to part of a measurement which constitutes a generalization of the neutron polarization analysis [18]. Here, however, only the main diagonal elements of the general matrix, namely $P_{xx}$, $P_{yy}$, $P_{zz}$ i.e. the scattering with polarization in x direction and analyzed in x direction ($P_{xx}$) is measured and similarly with y and z components. The full generalised polarization analysis would also measure all other components, i.e. it would be able to measure 9 components of the scattered polarization with and without spin flip, which needs correspondingly more measuring time. This would only increase the information about the sample in cases where it has a noncentrosymmetric structure or more generally if there is no parity conservation and no time inversion symmetry, as we have seen in 3.2.3 on page 33. The instrument D7 can handle such questions for as many detectors as can be equipped with a unit like in fig.2.5 on page 22 (see 2.2.2 on page 21). The present instrument is equipped with 32 analyzers, it can handle large samples and simultaneously afford time of flight analysis of energy changes of the scattered beams in the range of up to 30 meV energy gain [17]. To combine these possibilities with at least some features of the generalized polarization analysis is a very interesting and challenging task, especially for a multidetector instrument. For symmetry determinations in complicated magnetic structures it may be necessary to measure all components as J.Brown et al. has shown in many interesting papers. Derivation of the respective formulae will show which minimal possibility will be sufficient to provide the maximum possible information. D7 is already a very complicated instrument, if one wishes to use all its possibilities. These can certainly still be enhanced, for example by including this generalization of the spin analysis. Another possible improvement would be spin echo, but this would only be worthwhile if the instrument is moved to an end position of a guide where it could gain a factor ten in intensity.

# Bibliography


[1] K.R.A.Ziebeck and P.J.Brown, J.Phys.F **10**, 2015 (1980)

[2] O.Schaerpf, Proceedings Series: Neutron Scattering in the Nineties, Int.Atomic Energy Agency Vienna, 85(1985)

[3] O.Schaerpf, Physica B **156&157**, 631 (1989)

[4] O.Schaerpf, Physica B **156&157**, 639 (1989)

[5] W.G.Williams, Polarized Neutrons, Clarendon Press, Oxford 1988

[6] Ch.Schwink, O.Schärpf, Z.Phys.B **21**, 305 (1975)

[7] O.Schaerpf, in "Neutron Spin Echo" ed.F.Mezei, p.32, Lecture Notes in Physics vol.128, Springer-Verlag, Berlin 1980

[8] R.Pynn, Rev. Sci. Instrum. **55**, 837 (1984)

[9] O.Schaerpf, H.Capellmann, Th.Brueckel, A.Comberg and H.Pasing Z.Phys.B **78**, 345 (1990)

[10] R.M.Moon, T.Riste and W.C.Koehler, Phys.Rev. **181**, 920 (1969)

[11] O.Halpern, M.H.Johnson, Phys.Rev. **55**, 898 (1939)

[12] S.V.Maleev, Sov.Phys. JETP Lett. **2**, 338 (1966)

[13] F.Mezei, A.P.Murani, J.Magn.Magn.Mat. **14**, 211 (1979)

[14] Y.A.Izyumov, R.P.Ozerov, Magnetic Neutron Diffraction, Plenum Press, New York 1970, p.175

[15] S.W.Lovesey, Theory of Neutron Scattering from Condensed Matter, vol.2, p.167, Clarendon Press, Oxford 1986

[16] O.Schärpf and H.Capellmann, Z.Phys.B **80**, 253 (1990)

[17] O.Schärpf, Physica B in press. (1992)

[18] M.Blume, Phys.Rev. **130**, 1670 (1963)

[19] O.Schärpf, J.Appl.Cryst. **11**, 631 (1978)

[20] O.Schärpf, T.Chattopadhyay, H.W.Weber, O.B.Huyn, D.K. Finnemore, phys.stat.sol.(b) in press.

# Chapter 5

# Density matrix formalism to treat magnetic scattering more completely

The study of magnetic structures by neutrons shows a very rich world of possible moment arrangements and can not be treated here. To enter deeper into this question one should study such books like [1] or [2]. There are not only ferromagnetic and antiferromagnetic types of ordering, but also ferrimagnetic ones. These are known as collinear structures. There exist many kinds of noncollinear structures. Another group is treated under the name of weak ferromagnetism. There are also magnetic structures which cannot be described by means of a unit cell: the helicoidal structures. In this chapter we want to apply the density matrix method

1. to see that it is much simpler and simultaneously more powerful than the transition probability method
2. to learn how to get from its formulas the intensities, which we need to get scattering cross sections
3. to include then also the nuclear magnetic interference terms
4. to include also the spin orbit interaction.
5. to discuss in a more general way the possibilities of the general results which one gets by the formulas first derived by Maleev [3] and by Blume [4, 5] .

## 5.1 General formulas for magnetic scattering only

The thermal and quantum mechanical average can here be included by the density matrix formalism. One could again formulate the whole process as functions of $\vec{r}$ and t or $\omega$ as in the last chapter to get the most general form also useful for inelastic scattering. But to show the essential process it is also here clearer to avoid to write all the variables necessary to show the full process which results in the correlation functions. We use eq.(4.8 on page 44) and 4.9 on page 45 for the interaction potentials for magnetic scattering. This we know from 4.12 on page 45 can be written

$$\mu_n\vec{\sigma}_n \cdot \vec{Q}_\perp = \mu_n\vec{Q} \cdot (\vec{\sigma}_n - \vec{e}(\vec{e} \cdot \vec{\sigma}_n)) = \mu_n\vec{\sigma}_n(\vec{Q} - \vec{e}(\vec{e} \cdot \vec{Q})) \quad \text{with} \quad \vec{e} = \vec{\kappa}/\kappa \text{ and } \vec{Q} = \vec{M}_e \tag{5.1}$$

So the magnetic interaction is described by an expression of the form $\vec{\sigma} \cdot \vec{Q}_\perp$ which includes the magnetic form factors of the different magnetic atoms and is a function of $\vec{r}$ and $\omega$. We want first

to derive the magnetic part only. With the form 5.1 we can use the more sophisticated rules of 3.24 on page 33 with

$$\begin{aligned} L_1 &= \vec{Q}^\dagger \cdot (\vec{\sigma} - \vec{e}(\vec{\sigma}\cdot\vec{e})) && (5.2)\\ L_2 &= \vec{Q} \cdot (\vec{\sigma} - \vec{e}(\vec{\sigma}\cdot\vec{e})) && (5.3)\\ \vec{M}_1 &= \vec{Q}^\dagger - \vec{e}(\vec{Q}^\dagger\cdot\vec{e}) = \vec{Q}^\dagger_\perp && (5.4)\\ \vec{M}_2 &= \vec{Q} - \vec{e}(\vec{Q}\cdot\vec{e}) = \vec{Q}_\perp && (5.5) \end{aligned}$$

### 5.1.1 $I^{\uparrow\uparrow} + I^{\uparrow\downarrow}$

For the total scattered intensity $I^{\uparrow\uparrow} + I^{\uparrow\downarrow}$ we get:

$$\begin{aligned} \frac{d\sigma}{d\Omega} &= \mathrm{Tr}_\sigma(\rho(\vec{\sigma}\cdot\vec{Q}^\dagger_\perp)(\vec{\sigma}\cdot\vec{Q}_\perp)) = \mathrm{Tr}_\sigma(\rho L_1 L_2) = \frac{1}{2}\mathrm{Tr}_\sigma(\underline{1} + \vec{P}\cdot\vec{\sigma})(L_1 L_2) && (5.6)\\ &= (\vec{Q}^\dagger_\perp \cdot \vec{Q}_\perp) + i\vec{P}\cdot(\vec{Q}^\dagger_\perp \times \vec{Q}_\perp) && (5.7) \end{aligned}$$

### 5.1.2 $I^{\uparrow\uparrow} - I^{\uparrow\downarrow}$

For the polarization of the scattered beam we get:

$$\begin{aligned} \vec{P}^{out}_\gamma \frac{d\sigma}{d\Omega} &= I^{\uparrow\uparrow}_\gamma - I^{\uparrow\downarrow}_\gamma && (5.8)\\ &= \mathrm{Tr}_\sigma[\rho(\vec{\sigma}\cdot\vec{Q}^\dagger_\perp)\vec{\sigma}(\vec{\sigma}\cdot\vec{Q}_\perp)] = \mathrm{Tr}_\sigma[\rho L_1 \sigma L_2] = \frac{1}{2}\mathrm{Tr}_\sigma[(\underline{1} + (\vec{\sigma}\cdot\vec{P}))_1 \vec{\sigma} L_2] && (5.9)\\ &= -i(\vec{Q}^\dagger_\perp \times \vec{Q}_\perp)_\gamma + [\vec{Q}^\dagger_{\perp\gamma}(Q_\perp\cdot\vec{P}) + (\vec{Q}^\dagger_\perp\cdot\vec{P})Q_{\perp\gamma} - (\vec{Q}^\dagger_\perp\cdot\vec{Q}_\perp)P_\gamma && (5.10) \end{aligned}$$

### 5.1.3 Express $\vec{Q}_\perp$ by $(M_x, M_y, M_z)$ and $\alpha$

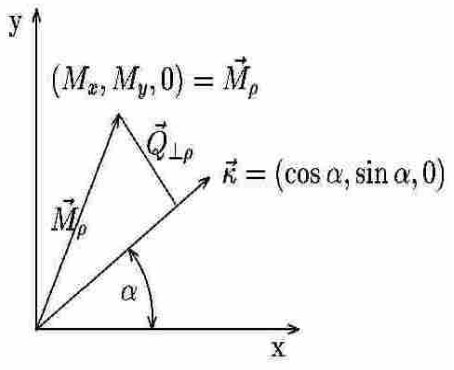



Figure 5.1: The geometry of the scattering vector and the magnetization vector to express $\vec{Q}_\perp$ by the components of $\vec{M}$ and $\alpha$. With the projection of $\vec{M}$ into the xy plane $\vec{M}_\rho = (M_x, M_y, 0)$ we get $\sqrt{M_x^2 + M_y^2}\cos(\vec{\kappa}, \vec{M}_\rho) = M_x\cos\alpha + M_y\sin\alpha$. A unit vector normal to $\vec{\kappa}$ is $(\sin\alpha, -\cos\alpha, 0)$. It is $Q_\perp^2 = M_x^2 + M_y^2 + M_z^2 - (M_x\cos\alpha + M_y\sin\alpha)^2 = (M_x\sin\alpha - M_y\cos\alpha)^2 + M_z^2$.

Fig.5.1 gives the geometry of the scattering vector and the function $\vec{Q}_\perp$ in relation to the adiabatic spinturner coils x, y, and z. With the help of this figure one finds that

$$\vec{Q}_\perp = (0, 0, M_z) + (M_x\sin\alpha - M_y\cos\alpha)(\sin\alpha, -\cos\alpha, 0) = (A\sin\alpha, -A\cos\alpha, M_z) \qquad (5.11)$$

### 5.1.4 Derivation of the correlation functions $\Gamma^{\nu}_{ss'}(\vec{r},\omega)$

To obtain the scattering and polarization for the three components $P_x^{out}$, $P_y^{out}$, and $P_z^{out}$ as scattering with and without flip with $\vec{P}^{in}=(1,0,0)$, $\vec{P}^{in}=(0,1,0)$ and $\vec{P}^{in}=(0,0,1)$ we insert these and $\vec{Q}_\perp=(M_x\sin^2\alpha - M_y\sin\alpha\cos\alpha, -M_x\sin\alpha\cos\alpha + M_y\cos^2\alpha, M_z)$ in eqs.(5.7,5.10). We must remember that products of components of $\vec{Q}_\perp$ in these equations correspond to correlation functions, if one includes all variables summations and transforms in the case, which includes inelastic scattering. If we forget this and insert $\vec{Q}_\perp$ and the corresponding incident polarizations, we obtain the equations for elastic scattering.

First we evaluate the vector product $\vec{Q}^\dagger_\perp \times \vec{Q}_\perp$. With

$$\begin{aligned} A &= M_x\sin\alpha - M_y\cos\alpha && (5.12)\\ \vec{Q}_\perp &= (A\sin\alpha, -A\cos\alpha, M_z) && (5.13)\end{aligned}$$

and assuming that A and $M_z$ can be complex, we get

$$\begin{aligned} i(\vec{Q}^\dagger_\perp \times \vec{Q}_\perp) &= \begin{vmatrix} \vec{e}_1 & \vec{e}_2 & \vec{e}_3 \\ A^*\sin\alpha & -A^*\cos\alpha & M_z^* \\ A\sin\alpha & -A\cos\alpha & M_z \end{vmatrix} && (5.14)\\ &= i((-A^*M_z + M_z^*A)\cos\alpha, -(A^*M_z - M_z^*A)\sin\alpha, (-A^*A + A^*A)\sin\alpha\cos\alpha) && (5.15)\\ &= -(2\cos\alpha\Im(AM_z^*), 2\sin\alpha\Im(AM_z^*), 0) && (5.16)\\ &= -2\Im(AM_z^*)(\cos\alpha,\sin\alpha,0) && (5.17)\\ &= -2\Im(M_xM_z^*\sin\alpha - M_yM_z^*\cos\alpha)(\cos\alpha,\sin\alpha,0) && (5.18)\end{aligned}$$

$\Im(M_xM_z^*)$ and $\Im(M_yM_z^*)$ can only contribute something if $M_x$ or $M_y$ or $M_z$ or all are complex and the real and imaginary part do not have the same direction.

With this and eq.(5.7) we obtain for the elastic scattering:

$$\begin{aligned} \frac{d\sigma}{d\Omega} &= I^{\uparrow\uparrow} + I^{\uparrow\downarrow} && (5.19)\\ &= \vec{Q}^\dagger_\perp\cdot\vec{Q}\perp + i\vec{P}(\vec{Q}\,\dagger_\perp \times \vec{Q}_\perp) && (5.20)\\ &= |A|^2 + |M_z|^2 - 2\Im(M_xM_z^*\sin\alpha - M_yM_z^*\cos\alpha)(P_x\cos\alpha + P_y\sin\alpha) && (5.21)\\ &= |M_x|^2\sin^2\alpha + |M_y|^2\cos^2\alpha - 2\Re(M_x^*M_y)\sin\alpha\cos\alpha + |M_z|^2 \\ &\quad -2\Im(M_xM_z^*\sin\alpha - M_yM_z^*\cos\alpha)(P_x\cos\alpha + P_y\sin\alpha) && (5.22)\end{aligned}$$

Using eq.(5.10) and $P_\nu^{out}\|P_\nu^{in}$ we get

$$\begin{aligned} P_\nu^{out}\frac{d\sigma}{d\Omega} &= I_\nu^{\uparrow\uparrow} - I_\nu^{\uparrow\downarrow} && (5.23)\\ &= -i(\vec{Q}^\dagger_\perp \times \vec{Q}_\perp)_\nu + Q_{\perp\nu}Q^\dagger_{\perp\nu} + Q^\dagger_{\perp\nu}Q_{\perp\nu} - (Q^\dagger_{\perp x}Q_{\perp x} + Q^\dagger_{\perp y}Q_{\perp y} + Q^\dagger_{\perp z}Q_{\perp z}) && (5.24)\\ P_x^{out}\frac{d\sigma}{d\Omega} &= 2\Im(M_xM_z^*\sin\alpha\cos\alpha - M_yM_z^*\cos^2\alpha) + \\ &\quad +2AA^*\sin^2\alpha - (AA^*\sin^2\alpha + AA^*\cos^2\alpha + M_zM_z^*) && (5.25)\\ &= 2\Im(M_xM_z^*\cos\alpha\sin\alpha - M_yM_z^*\cos^2\alpha) + |A|^2(\sin^2\alpha - \cos^2\alpha) - |M_z|^2 && (5.26)\\ P_y^{out}\frac{d\sigma}{d\Omega} &= 2\Im(M_xM_z^*\sin^2\alpha - M_yM_z^*\cos\alpha\sin\alpha) - |A|^2(\sin^2\alpha - \cos^2\alpha) - |M_z|^2 && (5.27)\end{aligned}$$

$$P_z^{out}\frac{d\sigma}{d\Omega} = M_z M_z^* + M_z^* M_z - (AA^*\sin^2\alpha + AA^*\cos^2\alpha + M_z M_z^*) \quad (5.28)$$
$$= |M_z|^2 - |A|^2 \quad (5.29)$$

with

$$|A|^2 = |M_x\sin\alpha - M_y\cos\alpha|^2 = |M_x|^2\sin^2\alpha + |M_y|^2\cos^2\alpha - 2\Re(M_x^* M_y)\sin\alpha\cos\alpha \quad (5.30)$$

Combining these results to get $I_x^{\uparrow\uparrow}$, $I_y^{\uparrow\uparrow}$,$I_z^{\uparrow\uparrow}$, $I_x^{\uparrow\downarrow}$,$I_y^{\uparrow\downarrow}$, $I_z^{\uparrow\downarrow}$ gives

$$I_x^{\uparrow\uparrow} = |A|^2\sin^2\alpha \quad (5.31)$$
$$= M_x^* M_x\sin^4\alpha + M_y^* M_y\cos^2\alpha\sin^2\alpha - 2ReM_x^* M_y\sin^3\alpha\cos\alpha \quad (5.32)$$
$$I_y^{\uparrow\uparrow} = |A|^2\cos^2\alpha \quad (5.33)$$
$$= |M_x|^2\sin^2\alpha\cos^2\alpha + |M_y|^2\cos^4\alpha - 2\Re M_x^* M_y\sin\alpha\cos^3\alpha \quad (5.34)$$
$$I_z^{\uparrow\uparrow} = |M_z|^2 \quad (5.35)$$
$$I_x^{\uparrow\downarrow} = |A|^2\cos^2\alpha + |M_z|^2 - 2\Im(M_x^* M_z\sin\alpha - M_y^* M_z\cos\alpha)\cos\alpha \quad (5.36)$$
$$= |M_x|^2\sin^2\alpha\cos^2\alpha + |M_y|^2\cos^4\alpha - 2\Re M_x^* M_y\sin\alpha\cos^3\alpha + |M_z|^2 \quad (5.37)$$
$$-2\Im M_x^* M_z\sin\alpha\cos\alpha + M_y^* M_z\cos^2\alpha \quad (5.38)$$
$$I_y^{\uparrow\downarrow} = |A|^2\sin^2\alpha + |M_z|^2 - 2\Im(M_x^* M_z\sin\alpha - M_y^* M_z\cos\alpha)\sin\alpha \quad (5.39)$$
$$= |M_x|^2\sin^4\alpha + |M_y|^2\cos^2\alpha\sin^2\alpha - 2\Re M_x^* M_y\sin^3\alpha\cos\alpha + |M_z|^2 \quad (5.40)$$
$$-2\Im M_x^* M_z\sin^2\alpha + M_y^* M_z\cos\alpha\sin\alpha \quad (5.41)$$
$$I_z^{\uparrow\downarrow} = 0 \quad (5.42)$$

This corresponds to what we found in eqs.(4.39 on page 51) and (4.40 on page 51). The result eq.(5.31) can immediately be seen by adding 5.21 to 5.26, the result eq.(5.36) by subtracting 5.26 from 5.21 with $P_x = 1$ and the others respectively.

## 5.2 Nuclear-magnetic interference terms

We have investigated the nuclear scattering resulting from $\hat{N}$ (see 3.3 on page 35) and the magnetic scattering resulting from $\vec{\sigma}\cdot\vec{Q}_\perp$ (see 5.1 on page 61). If both are present then we have to investigate the scattering matrix resulting from $(N+\vec{\sigma}\cdot\vec{Q}_\perp)(N^\dagger+\vec{\sigma}\cdot\vec{Q}_\perp)$. We have then still to calculate the traces of the interference terms

$$N\vec{\sigma}\cdot\vec{Q}_\perp^\dagger + \vec{\sigma}\cdot\vec{Q}_\perp N^\dagger \quad (5.43)$$

We get for the total scattering from the nuclear magnetic interference term

$$\frac{d\sigma}{d\Omega} = \mathrm{Tr}_\sigma[\rho(N\vec{\sigma}\cdot\vec{Q}_\perp^\dagger + \vec{\sigma}\cdot\vec{Q}_\perp N^\dagger)] \quad (5.44)$$
$$= \frac{1}{2}\mathrm{Tr}_\sigma[(\underline{1}+\vec{\sigma}\cdot\vec{P})(N\vec{\sigma}\cdot\vec{Q}_\perp^\dagger + N^\dagger\vec{\sigma}\cdot\vec{Q}_\perp)]$$
$$= \frac{1}{2}\mathrm{Tr}_\sigma[N\sigma_\alpha Q_{\perp\alpha}^\dagger + N^\dagger\sigma_\alpha Q_{\perp\alpha} + N\sigma_\alpha P_\alpha\sigma_\beta Q_{\perp\beta} + N^\dagger\sigma_\alpha P_\alpha\sigma_\beta Q_{\perp\beta}] \quad (5.45)$$
$$= \frac{1}{2}[2\delta_{\alpha\beta}NQ_{\perp\beta}^\dagger + 2\delta_{\alpha\beta}N^\dagger P_\alpha Q_{\perp\beta}] \quad (5.46)$$
$$= NP_\alpha Q_{\perp\alpha}^\dagger + N^\dagger P_\alpha Q_{\perp\alpha} \quad (5.47)$$
$$= 2\Re(N\vec{P}\cdot\vec{Q}_\perp^\dagger) \quad (5.48)$$

and for the polarization

$$\begin{aligned}
P_\nu^{out}\frac{d\sigma}{d\Omega} &= \frac{1}{2}\mathrm{Tr}_\sigma[(\underline{1}+\vec{\sigma}\cdot\vec{P})(N\sigma_\nu(\vec{\sigma}\cdot\vec{Q}_\perp^\dagger)+N^\dagger\sigma_\nu(\vec{\sigma}\cdot\vec{Q}_\perp^\dagger))] && (5.49)\\
&= \frac{1}{2}[N\sigma_\nu\sigma_\alpha Q_{\perp\alpha}^\dagger + N^\dagger\sigma_\nu\sigma_\alpha Q_{\perp\alpha} + \sigma_\alpha P_\alpha N\sigma_\nu\sigma_\beta Q_{\perp\beta}^\dagger + \sigma_\alpha P_\alpha N^\dagger\sigma_\nu\sigma_\beta Q_{\perp\beta}]\\
&= \frac{1}{2}(2\delta_{\nu\alpha}Q_{\perp\alpha}^\dagger N + 2\delta_{\nu\alpha}N^\dagger Q_{\perp\alpha} + 2i\epsilon^{\alpha\nu\beta}P_\alpha Q_{\perp\beta}^\dagger N + 2iN^\dagger\epsilon^{\alpha\nu\beta}P_\alpha Q_{\perp\beta}) && (5.50)\\
&= Q_{\perp\nu}^\dagger N + Q_{\perp\nu}N^\dagger + iN(\vec{P}\times\vec{Q}_\perp^\dagger)_\nu - iN^\dagger(\vec{P}\times\vec{Q}_\perp)_\nu && (5.51)\\
&= 2\Re(Q_{\perp\nu}^\dagger N) - 2\Im(N^\dagger\cdot(\vec{P}\times\vec{Q}_\perp)_\nu) && (5.52)
\end{aligned}$$

One can use this again as above to determine the intensities of the scattering without spin flip and with spin flip for the incident and analyzed polarization in x, y, z direction:

$$\begin{aligned}
I_{\uparrow\uparrow}^{(x)} &= 2\Re(NA^*)\sin\alpha && (5.53)\\
I_{\uparrow\uparrow}^{(y)} &= -2\Re(NA^*)\cos\alpha && (5.54)\\
I_{\uparrow\uparrow}^{(z)} &= 2\Re(NM_z^*) && (5.55)\\
I_{\uparrow\downarrow}^{(x)} &= 0 && (5.56)\\
I_{\uparrow\downarrow}^{(y)} &= 0 && (5.57)\\
I_{\uparrow\downarrow}^{(z)} &= 0 && (5.58)
\end{aligned}$$

This only gives a contribution if there is a resulting magnetic operator $\mathbf{Q}_\perp$, which does not average to zero or for magnetic Bragg peaks coinciding with nuclear ones. In the case of ferro- or ferri- magnetism one can force this by an applied magnetic field. For antiferromagnetism this term averages to zero if there are equal numbers of spins with one direction and of the opposite direction in the same lattice plane. If this is not the case this term does not average to zero. For none centro symmetric structures these terms are often very helpful to determining the magnetic symmetry. They can also produce none diagonal contributions to the polarization vector.

The nuclear-magnetic interference term is the term that makes possible the form factor determination, the use of polarizing crystals i.e. a large field of applications not treated here. If the incident beam is not polarized a magnetic field applied to order the magnetic moments can give a polarization in the direction of $\vec{Q}_\perp$ but in general not completely polarized as it is on top of a not polarized intensity. To see this we use the above derived equations and exclude non centro symmetric terms. We obtain then

$$\begin{aligned}
I^{\uparrow\uparrow}+I^{\uparrow\downarrow} &= N^\dagger N + (\vec{P}^{(in)}\cdot\vec{Q}_\perp^\dagger)N + (\vec{P}^{(in)}\cdot\vec{Q}_\perp)N^\dagger + \vec{Q}_\perp^\dagger\cdot\vec{Q}_\perp && (5.59)\\
I^{\uparrow\uparrow}-I^{\uparrow\downarrow} &= \vec{P}^{(in)}N^\dagger N + N\vec{Q}_\perp^\dagger + N^\dagger\vec{Q}_\perp + (\vec{P}^{(in)}\cdot\vec{Q}_\perp^\dagger)\vec{Q}_\perp\\
&\quad +(\vec{P}^{(in)}\cdot\vec{Q}_\perp)\vec{Q}_\perp^\dagger - \vec{P}^{(in)}(\vec{Q}_\perp^\dagger\cdot\vec{Q}_\perp) && (5.60)
\end{aligned}$$

With unpolarized incident beam $\vec{P}^{(in)}=0$ these equations simplify strongly and one gets for the out going polarization

$$P^{(out)} = \frac{I^{\uparrow\uparrow}-I^{\uparrow\downarrow}}{I^{\uparrow\uparrow}+I^{\uparrow\downarrow}} = \frac{NQ^\dagger+N^\dagger Q}{N^\dagger N+Q^\dagger Q} \qquad (5.61)$$

If for any direction $N=\pm Q_\perp$ then

$$P^{(out)} = \frac{N(\pm N^\dagger)+N^\dagger(\pm N)}{N^\dagger N+N^\dagger N} = \pm 1 \qquad (5.62)$$

If this is not the case then one has a polarization on top of an unpolarized background.

If the crystal is antiferromagnetic the domains may hinder that this condition is fulfilled in the whole crystal. The same is valid if one would like to polarize with the helical structure.

The reader interested in these topics (form factor determination) should consult [6] or [7].

## 5.3 Visualization of the full formalism of the density matrix method for the 3d PA

Taking together all results of the scattering of polarized neutrons described by the density matrix method in chapter 3.3 on page 35, 3.3.3 on page 38, 5.1 on page 61 we get the following equations:

$$\begin{aligned}\frac{d\sigma}{d\Omega} &= N^\dagger N + (\vec{P}^{(in)}\cdot\vec{Q}_\perp^\dagger)N + (\vec{P}^{(in)}\cdot\vec{Q}_\perp)N^\dagger + \vec{Q}_\perp^\dagger\cdot\vec{Q}_\perp \\ &\quad + i\vec{P}^{(in)}\cdot(\vec{Q}_\perp^\dagger\times\vec{Q}_\perp) + B^\dagger B[\vec{I}^\dagger\cdot\vec{I} + i\vec{P}^{(in)}\cdot(\vec{I}^\dagger\times\vec{I})] \qquad (5.63)\\ \vec{P}^{(out)}\frac{d\sigma}{d\Omega} &= \vec{P}^{(in)}N^\dagger N + N\vec{Q}_\perp^\dagger + N^\dagger\vec{Q}_\perp + iN(\vec{P}^{(in)}\times\vec{Q}_\perp^\dagger) - iN^\dagger(\vec{P}^{(in)}\times\vec{Q}_\perp) \\ &\quad + [(\vec{P}^{(in)}\cdot\vec{Q}_\perp^\dagger)\vec{Q}_\perp + (\vec{P}^{(in)}\cdot\vec{Q}_\perp)\vec{Q}_\perp^\dagger - \vec{P}^{(in)}(\vec{Q}_\perp^\dagger\cdot\vec{Q}_\perp)] - i(\vec{Q}_\perp^\dagger\times\vec{Q}_\perp) \\ &\quad + B^\dagger B[-i(\vec{I}^\dagger\times\vec{I}) + (\vec{P}^{(in)}\cdot\vec{I}^\dagger)\vec{I} + (\vec{P}^{(in)}\cdot\vec{I})\vec{I}^\dagger - \vec{P}^{(in)}\vec{I}^\dagger\cdot\vec{I}] \qquad (5.64)\end{aligned}$$

Now we remember (see 3.94 on page 39) that for the measurement of the polarization in $\nu$-direction (with $\nu = x, y, z$) of the scattered beam

$$\begin{aligned}\frac{d\sigma}{d\Omega} &= I_\nu^{\uparrow\uparrow} + I_\nu^{\uparrow\downarrow} \qquad (5.65)\\ P_\nu^{(out)}\frac{d\sigma}{d\Omega} &= I_\nu^{\uparrow\uparrow} - I_\nu^{\uparrow\downarrow} \qquad (5.66)\end{aligned}$$

and that for unpolarized nuclear spins the above equations simplify to

$$\begin{aligned}\frac{d\sigma}{d\Omega} &= N^\dagger N + (\vec{P}^{(in)}\cdot\vec{Q}_\perp^\dagger)N + (\vec{P}^{(in)}\cdot\vec{Q}_\perp)N^\dagger + \vec{Q}_\perp^\dagger\cdot\vec{Q}_\perp \\ &\quad + i\vec{P}^{(in)}\cdot(\vec{Q}_\perp^\dagger\times\vec{Q}_\perp) + B^\dagger BI(I+1) \qquad (5.67)\\ \vec{P}^{(out)}\frac{d\sigma}{d\Omega} &= \vec{P}^{(in)}N^\dagger N + N\vec{Q}_\perp^\dagger + N^\dagger\vec{Q}_\perp + iN(\vec{P}^{(in)}\times\vec{Q}_\perp^\dagger) - iN^\dagger(\vec{P}^{(in)}\times\vec{Q}_\perp) \\ &\quad + [(\vec{P}^{(in)}\cdot\vec{Q}_\perp^\dagger)\vec{Q}_\perp + (\vec{P}^{(in)}\cdot\vec{Q}_\perp)\vec{Q}_\perp^\dagger - \vec{P}^{(in)}(\vec{Q}_\perp^\dagger\cdot\vec{Q}_\perp)] \\ &\quad - i(\vec{Q}_\perp^\dagger\times\vec{Q}_\perp) - \frac{1}{3}B^\dagger B\vec{P}^{(in)}I(I+1) \qquad (5.68)\end{aligned}$$

This allows us to determine the scattered intensity with polarization of the incident beam in $\nu$ direction and analyzed with the polarization in the same $\nu$ direction with $\nu = x, y, z$. This gives

$$\begin{aligned}I_{xx}^{\uparrow\uparrow} &= N^\dagger N + NQ_{\perp x}^\dagger + N^\dagger Q_{\perp x} + Q_{\perp x}^\dagger Q_{\perp x} + \frac{1}{3}B^\dagger BI(I+1) \qquad (5.69)\\ I_{xx}^{\uparrow\downarrow} &= Q_{\perp y}^\dagger Q_{\perp y} + Q_{\perp z}^\dagger Q_{\perp z} + i(\vec{Q}_\perp^\dagger\times\vec{Q}_\perp)_x + \frac{2}{3}B^\dagger BI(I+1) \qquad (5.70)\\ I_{yy}^{\uparrow\uparrow} &= N^\dagger N + NQ_{\perp y}^\dagger + N^\dagger Q_{\perp y} + Q_{\perp y}^\dagger Q_{\perp y} + \frac{1}{3}B^\dagger BI(I+1) \qquad (5.71)\end{aligned}$$

$$I_{yy}^{\uparrow\downarrow} = Q_{\perp x}^{\dagger}Q_{\perp x} + Q_{\perp z}^{\dagger}Q_{\perp z} + i(\vec{Q}_{\perp}^{\dagger} \times \vec{Q}_{\perp})_y + \frac{2}{3}B^{\dagger}BI(I+1) \tag{5.72}$$

$$I_{zz}^{\uparrow\uparrow} = N^{\dagger}N + NQ_{\perp z}^{\dagger} + N^{\dagger}Q_{\perp z} + Q_{\perp z}^{\dagger}Q_{\perp z} + \frac{1}{3}B^{\dagger}BI(I+1) \tag{5.73}$$

$$I_{zz}^{\uparrow\downarrow} = Q_{\perp x}^{\dagger}Q_{\perp x} + Q_{\perp y}^{\dagger}Q_{\perp y} + i(\vec{Q}_{\perp}^{\dagger} \times \vec{Q}_{\perp})_z + \frac{2}{3}B^{\dagger}BI(I+1) \tag{5.74}$$

This shows again the already well known behaviour that only those components of $\vec{Q}_{\perp}$ which are perpendicular to the spin of the neutrons can contribute to the scattering with spin flip. And this is also the case for the nuclear spins. The term with the cross product give only a contribution if the $\Re(\vec{Q}_{\perp})$ has another direction than the $\Im(\vec{Q}_{\perp})$ and not the same size.

More about these things you can find in neutronpol.pdf section 4.4 on the same site.

## 5.4 Application to paramagnetic powder scattering

Here we want to give the density matrix method derivation of the equation $\vec{P}' = -\vec{\kappa}(\vec{\kappa} \cdot \vec{P})/\kappa^2$ and visualize what it says. Practically the latter is already done in chapter 3.7.

### 5.4.1 Determination of the polarization of paramagnetic scattering using the density matrix formalism

To determine the polarization of the paramagnetic scattering we use the fact that

$$\vec{M}_e \cdot \vec{\mu}_{n\perp} = \vec{\mu} \cdot \vec{M}_{e\perp} \tag{5.75}$$

already derived in 4.12 on page 45. With $\vec{S}_i$ the operator of the electron magnetization including all factors and sums as in eq.(4.10 on page 45), $\vec{M}_i = \vec{S}_i - (\vec{e} \cdot \vec{S}_i)\vec{e}$ 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 the polarization of the neutron beam scattered by $L_i$ is

$$\vec{P}^{out} = \frac{\mathrm{Tr}_{\sigma}(\rho L^{\dagger}\vec{\sigma}L)}{\mathrm{Tr}_{\sigma}(\rho L^{\dagger}L)} \tag{5.76}$$

$$= \frac{\frac{1}{2}\mathrm{Tr}_{\sigma}(L^{\dagger}\vec{\sigma}L + (\vec{P} \cdot \vec{\sigma})L^{\dagger}\vec{\sigma}L)}{\frac{1}{2}\mathrm{Tr}_{\sigma}(L^{\dagger}L + (\vec{P} \cdot \vec{\sigma})L^{\dagger}L)} \tag{5.77}$$

$$= \frac{-i(\vec{M}^{\dagger} \times \vec{M}) + \vec{M}^{\dagger}(\vec{M} \cdot \vec{P}) + (\vec{M}^{\dagger} \cdot \vec{P})\vec{M} - \vec{P}(\vec{M}^{\dagger} \cdot \vec{M})}{(\vec{M}^{\dagger} \cdot \vec{M}) + i(\vec{M}^{\dagger} \times \vec{M})\vec{P}} \tag{5.78}$$

the last line by applying the rules eq.(3.24 on page 33) seq.. For a paramagnet without helical structures i.e. without noncentrosymmetric structure the cross product in the nominator and denominator disappear and we get

$$\vec{P}^{out} = \frac{\vec{M}^{\dagger}(\vec{M} \cdot \vec{P}) + (\vec{M}^{\dagger} \cdot \vec{P})\vec{M} - \vec{P}(\vec{M}^{\dagger} \cdot \vec{M})}{(\vec{M}^{\dagger} \cdot \vec{M})} \tag{5.79}$$

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

$$\langle(\vec{S}^{\dagger} \cdot \vec{S})\rangle = S(S+1) \tag{5.80}$$

$$
\begin{aligned}
&= \langle S_x^\dagger S_x\rangle + \langle S_y^\dagger S_y\rangle + \langle S_z^\dagger S_z\rangle && (5.81)\\
\langle S_\nu^\dagger S_\nu\rangle &= \frac{1}{3}S(S+1) \text{ with } \nu\text{=x,y,z} && (5.82)\\
\langle S_x\rangle &= \langle S_y\rangle = \langle S_z\rangle = \langle S_\nu^\dagger\rangle = 0 && (5.83)
\end{aligned}
$$

With these the average of the first product is

$$
\begin{aligned}
\langle(\vec{S}^\dagger - (\vec{e}\cdot\vec{S}^\dagger)\vec{e})[(\vec{S}\cdot\vec{P}) - (\vec{e}\cdot\vec{S})(\vec{e}\cdot\vec{P})]\rangle &= \langle\vec{S}^\dagger(\vec{S}\cdot\vec{P})\rangle - \langle\vec{S}^\dagger(\vec{e}\cdot\vec{S})(\vec{e}\cdot\vec{P})\rangle\\
&\quad -\langle(\vec{e}\cdot\vec{S}^\dagger)\vec{e}(\vec{S}\cdot\vec{P})\rangle + \langle(\vec{e}\cdot\vec{S}^\dagger)\vec{e}(\vec{e}\cdot\vec{S})(\vec{e}\cdot\vec{P})\rangle\\
&= \frac{1}{3}S(S+1)[\vec{P} - (\vec{e}\cdot\vec{P})\vec{e} - (\vec{e}\cdot\vec{P})\vec{e} + (\vec{e}\cdot\vec{P})\vec{e}]\\
&= \frac{1}{3}S(S+1)[\vec{P} - (\vec{e}\cdot\vec{P})\vec{e}] && (5.84)
\end{aligned}
$$

We used for this

$$
\begin{aligned}
\langle\vec{S}^\dagger(\vec{S}\cdot\vec{P})\rangle &= \langle(S_x^\dagger, S_y^\dagger, S_z^\dagger)(S_xP_x + S_yP_y + S_zP_z)\rangle && (5.85)\\
&= \frac{1}{3}S(S+1)(P_x, P_y, P_z) && (5.86)\\
&= \langle(\vec{S}^\dagger\cdot\vec{P})\vec{S}\rangle && (5.87)\\
\langle\vec{S}^\dagger(\vec{e}\cdot\vec{S})\rangle &= \frac{1}{3}S(S+1)(e_x, e_y, e_z) && (5.88)\\
\langle(\vec{e}\cdot\vec{S}\dagger)(\vec{S}\cdot\vec{P})\rangle &= \frac{1}{3}S(S+1)(\vec{e}\cdot\vec{P}) && (5.89)\\
\langle(\vec{e}\cdot\vec{S}^\dagger)(\vec{e}\cdot\vec{S})\rangle &= \frac{1}{3}S(S+1) && (5.90)
\end{aligned}
$$

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

$$
\begin{aligned}
\langle(\vec{M}^\dagger\cdot\vec{M})\rangle &= \langle(\vec{S}^\dagger - (\vec{e}\cdot\vec{S}^\dagger)\vec{e})\cdot(\vec{S} - (\vec{e}\cdot\vec{S})\vec{e})\rangle\\
&= \langle(\vec{S}^\dagger\cdot\vec{S}) - (\vec{S}^\dagger\cdot\vec{e})(\vec{e}\cdot\vec{S}) - (\vec{e}\cdot\vec{S}^\dagger)(\vec{e}\cdot\vec{S}) + (\vec{e}\cdot\vec{S}^\dagger)(\vec{e}\cdot\vec{S})e^2\rangle\\
&= \langle(\vec{S}^\dagger\cdot\vec{S}) - (\vec{S}^\dagger\cdot\vec{e})(\vec{e}\cdot\vec{S})\rangle = S(S+1) - \frac{1}{3}S(S+1)\\
&= \frac{2}{3}S(S+1) && (5.91)
\end{aligned}
$$

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

$$
\vec{P}^{out}_{paramagnet} = \frac{\frac{1}{3}S(S+1)[P - (\vec{\vec{e}}\cdot\vec{P})\vec{e} + \vec{P} - (\vec{e}\cdot\vec{P})\vec{e} - 2\vec{P}]}{\frac{2}{3}S(S+1)} = -(\vec{e}\cdot\vec{P})\vec{e} \qquad (5.92)
$$

# Bibliography


[1] Yu.A. Izyumov, R.P. Ozerov, *Magnetic Neutron Diffraction* Plenum Press, New York (1970)

[2] A.P. Cracknell, *Magnetism in Crystalline Materials* Pergamon Press, Oxford, New York (1975)

[3] S.V.Maleev, *JETP* **13**, (1961), 860

[4] M.Blume, *Phys.Rev.* **130**, (1963), 1670 *Phys.Rev.* **133**, (1964), A1366

[5] R.I.Schermer, M.Blume *Phys. Rev.* **166**, (1968), 554

[6] J.Schweizer *Interpretation of magnetization densities* 501-519 *Interpretation of the spin densities in metals and alloys* 479-499 *Proceedings of the Nato Advanced Study Institute, editor P.Becker Summer School, Arles 1978* Plenum Press, New York **(1980)**

[7] P.J.Brown *Magnetic neutron scattering Proceedings of the Nato Advanced Study Institute, editor P.Becker Summer School, Arles 1978* Plenum Press, New York **(1980)** 255-285

# Index