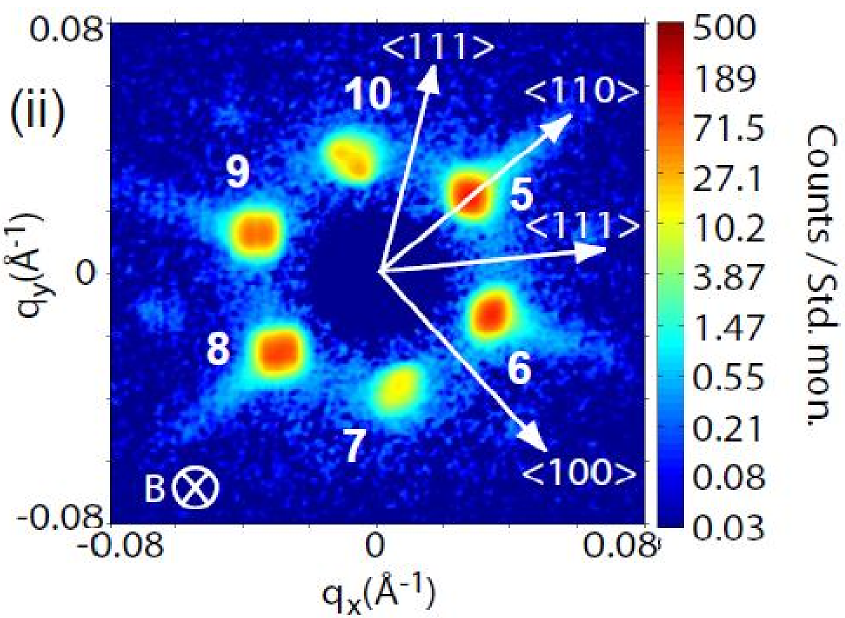
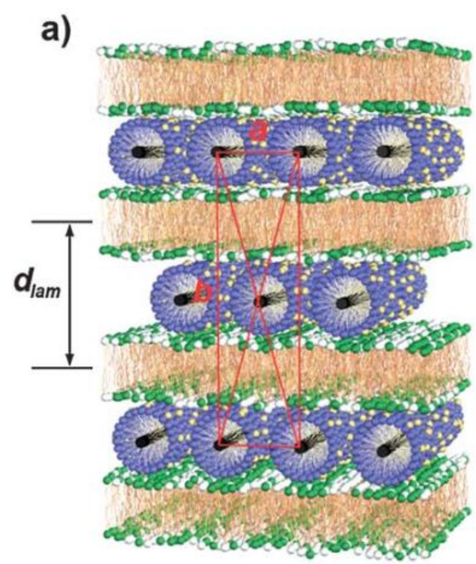
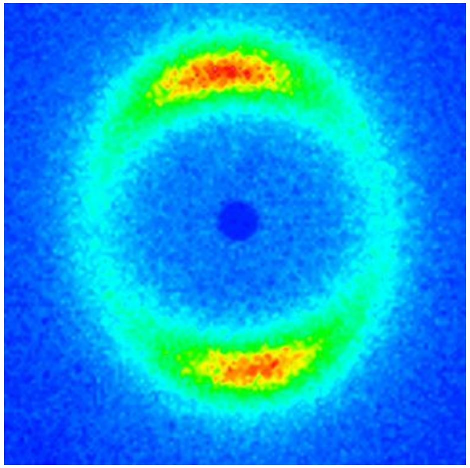
FRM II
Forschungs-Neutronenquelle
Heinz Maier-Leibnitz

MLZ
Heinz Maier-Leibnitz Zentrum

Physics with Neutrons II, SS 2016







Lecture 9, 27.6.2016

MLZ is a cooperation between:

JÜLICH FORSCHUNGSZENTRUM
Helmholtz-Zentrum Geesthacht
Zentrum für Material- und Küstenforschung
TUM Technische Universität München

Plan for SS 2016

- VL1: Repetition of winter term, basic neutron scattering theory
- VL2: SANS, theory and applications
- VL3: Neutron optics
- VL4: Reflectometry and dynamical scattering theory
- VL5: Diffuse neutron scattering
- VL6: Magnetic scattering cross section
- VL7: Magnetic structures and structure analysis
- VL8: Polarized neutrons
- VL9: 3D polarimetry, spin waves
- VL10: 4.7.2016 (8:30!!) Spin waves (continued), Phase transitions and critical phenomena as seen by neutrons
- VL11: Spin echo spectrocopy (C. Franz)

Exam: Please register until 30.6.2016

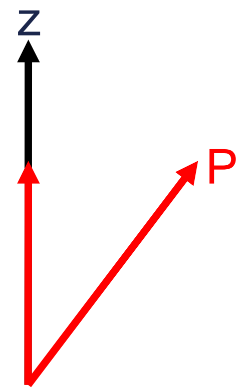
Polarized Neutrons
-
continued

Definition of Polarization

Magnetic moment of the neutron expressed in terms of the Pauli spin operator $\hat{\sigma}$

Spin states $|+\rangle$ $|-\rangle$ with eigenvalues +1, -1 for the operator $\hat{\sigma}_z$

Choose z axis as the polarization and quantization axis



Definition of polarization: Fraction f of a neutron beam in the $|+\rangle$ state

$$|P| = 2f - 1 \qquad |P| = \frac{n_- - n_-}{n_+ + n_-} \qquad f = \frac{n_+}{n_+ + n_-}$$

Cross section splits up into four terms:

$|+\rangle \Rightarrow |+\rangle$
$|-\rangle \Rightarrow |-\rangle$
Non-spin flip channels

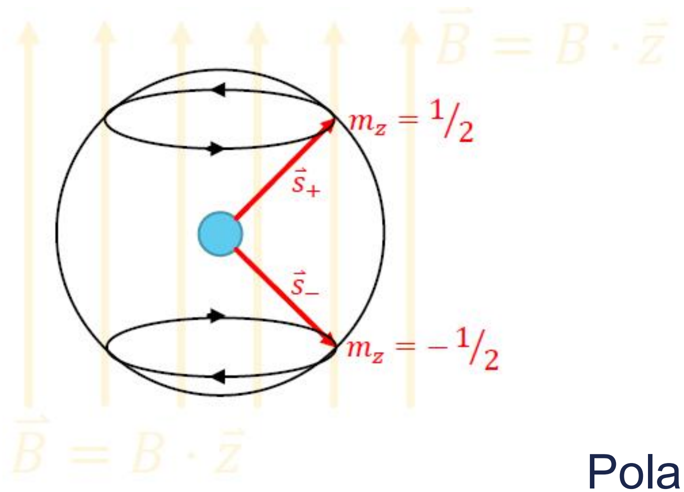
$|+\rangle \Rightarrow |-\rangle$
$|-\rangle \Rightarrow |+\rangle$
Spin flip channels

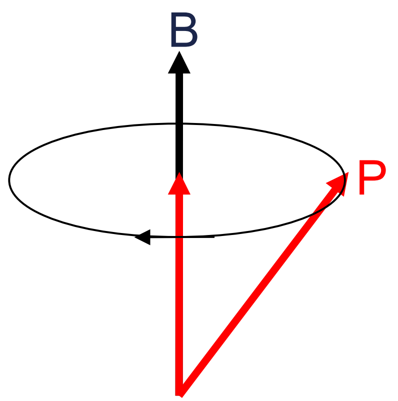
Lamor precession

Magnetic moment μ of the neutron in a magnetic field B

Precession around the field axis with Larmor frequency $f_{Larmor} = \frac{\gamma}{2\pi} B$

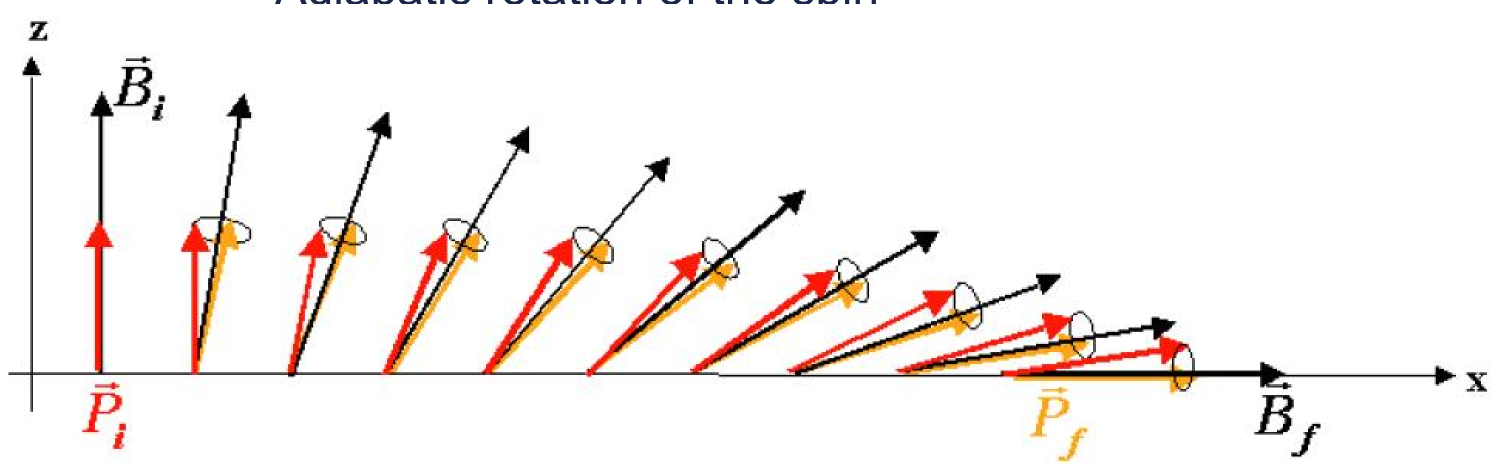
Lamor frequency f= 2.92kHz *B[G]   ΔΦ=2.654° * λ[Å] * B[G] * l[cm]





Polarization: Projection of P on B (z axis)

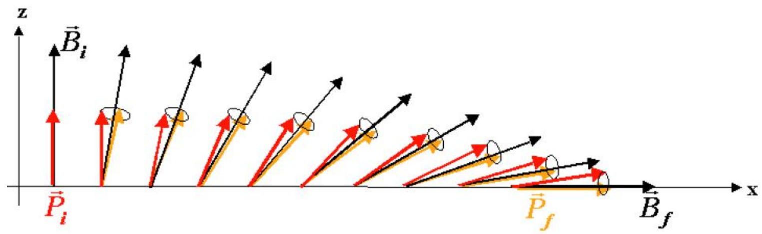
Adiabatic rotation of the spin

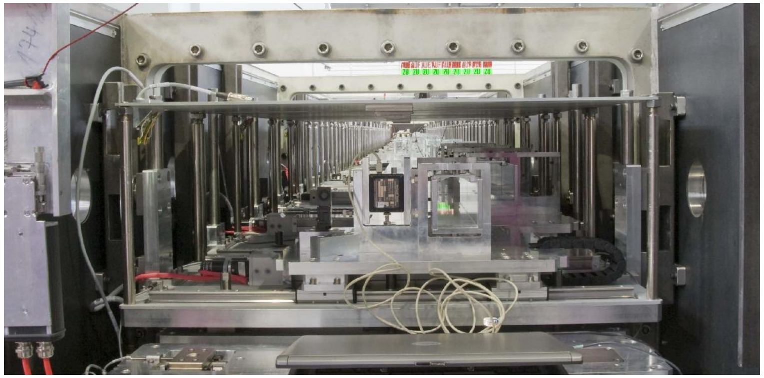


Lamor precession

How to transport polarized neutrons: Guide field (few mT)

Adiabatic rotation





How to manipulate the polarization direction: Non adiabatic rotation, new quatization axis

Mezei flipper

π-flip, static field

Shield stray field

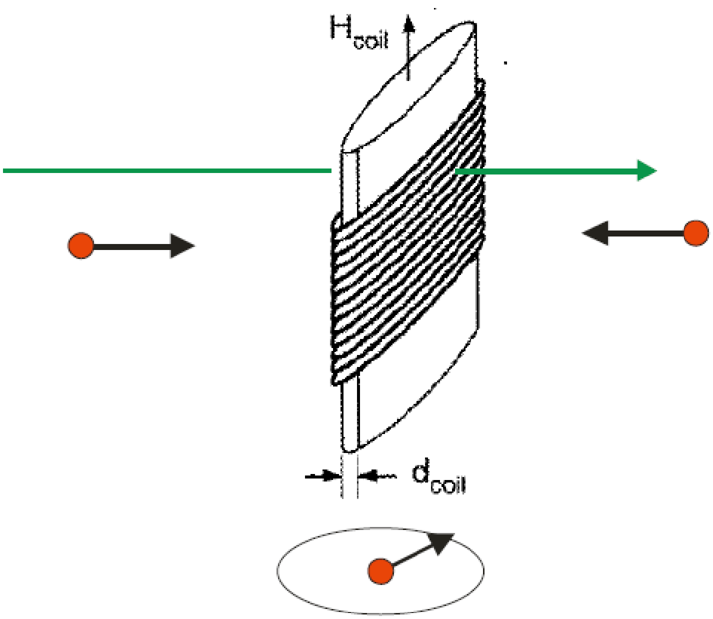
Wavelength dependent

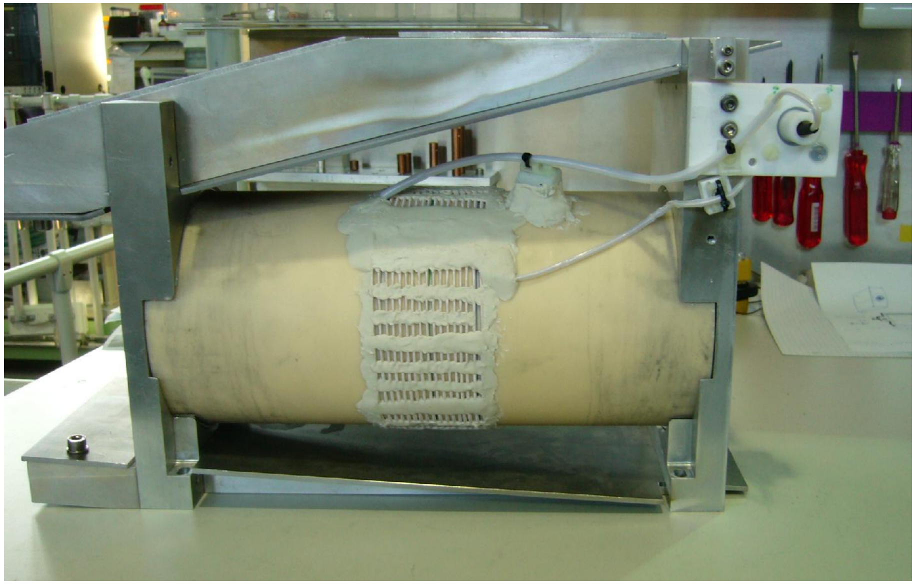
RF flipper

Static field + RF field

π-flip in rotating reference frame

Independent of wavelngth





Polarization effects

Modify the interaction operator taking the polarization into account

Matrix element $\langle \hat{k}'\hat{\sigma}'\hat{\lambda}'|\hat{U}|\hat{k}\hat{\sigma}\hat{\lambda}\rangle$

Interaction $\hat{U} = \hat{b} + A\vec{I}\hat{\sigma} + B\vec{M}\hat{\sigma}$

Nuclear interaction

Interaction due to nuclear spins

Magnetic moments of the electrons

Spin states and momentum of neutron are orthogonal

$$\langle \hat{k}'\hat{\sigma}'\hat{\lambda}'|\hat{U}|\hat{k}\hat{\sigma}\hat{\lambda}\rangle = \langle \hat{k}'\hat{\lambda}'|\hat{U}|\hat{k}\hat{\lambda}\rangle\langle \hat{\sigma}'|\hat{U}|\hat{\sigma}\rangle$$

Result for the four channels

$$\langle +|\hat{U}|+\rangle = b + AI_z + BM_z$$

$$\langle -|\hat{U}|-\rangle = b - AI_z - BM_z$$

$$\langle +|\hat{U}|-\rangle = A(I_x + iI_y) + B(M_x + iM_y)$$

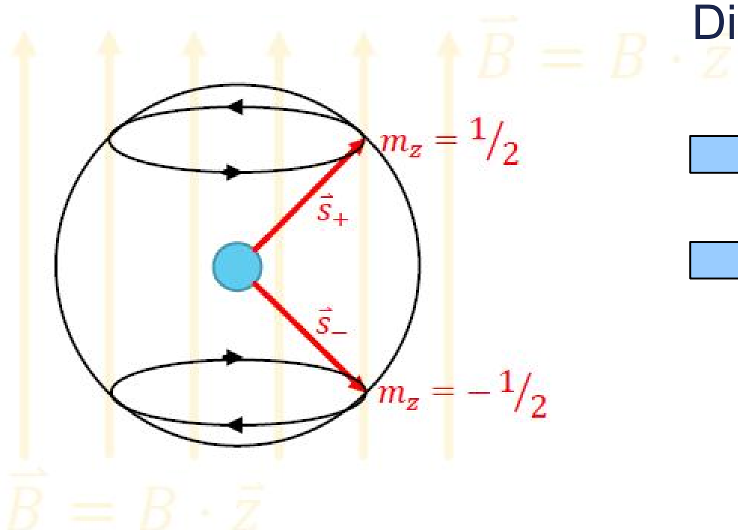
$$\langle -|\hat{U}|+\rangle = A(I_x - iI_y) + B(M_x - iM_y)$$

Polarization effects

Result for the four channels

$$\left.\begin{aligned}\langle +|\hat{U}|+\rangle &= b + AI_z + BM_z \\ \langle -|\hat{U}|-\rangle &= b - AI_z - BM_z\end{aligned}\right\} \text{Non spin flip}$$

$$\left.\begin{aligned}\langle +|\hat{U}|-\rangle &= A(I_x + iI_y) + B(M_x + iM_y) \\ \langle -|\hat{U}|+\rangle &= A(I_x - iI_y) + B(M_x - iM_y)\end{aligned}\right\} \text{Spin flip}$$



Direct consequences (remember, P along z):

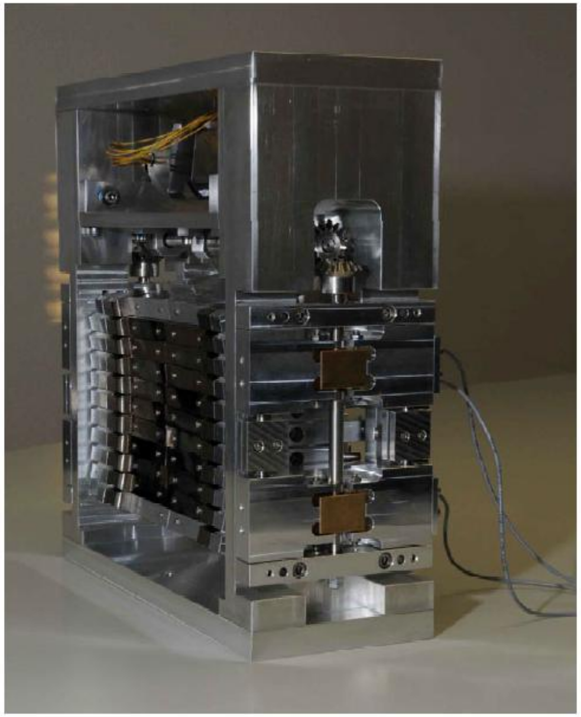
- Spin flip only for for M_x and M_y
- No slip only for for M_z

- Remember flipper coil!

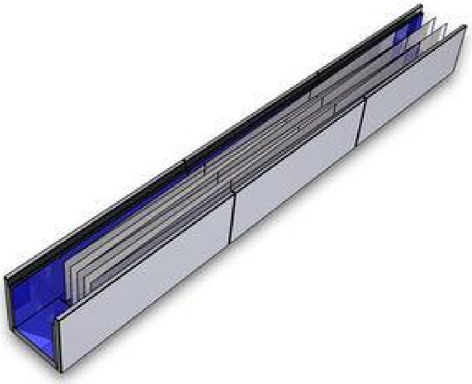
How to polarize?

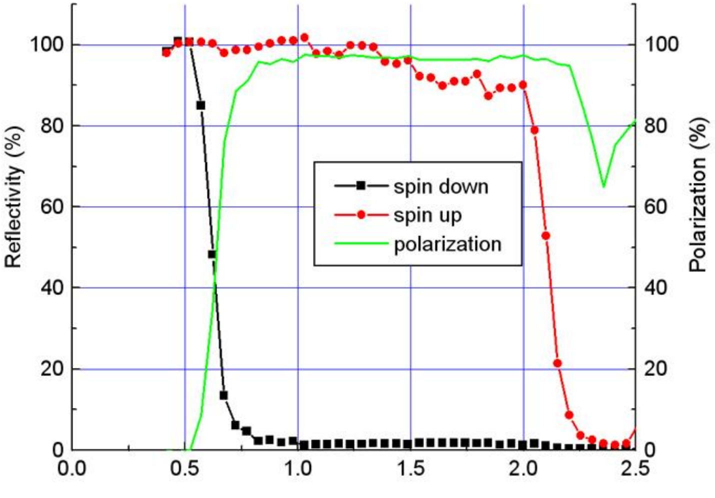
Polarizing monochromators

- Materials:
  - Fe, Co alloys
  - Cu_2MnAl (111)
  Heusler alloy- 95% polarization
- Need to maintain single ferro domain in entire monochromator
- Low reflectivity

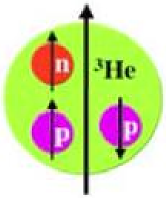


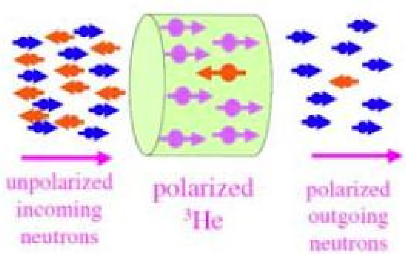
Polarizing supermirrors

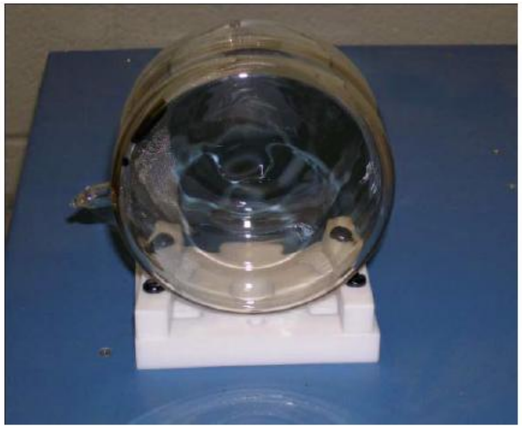




^{3}He spin filters







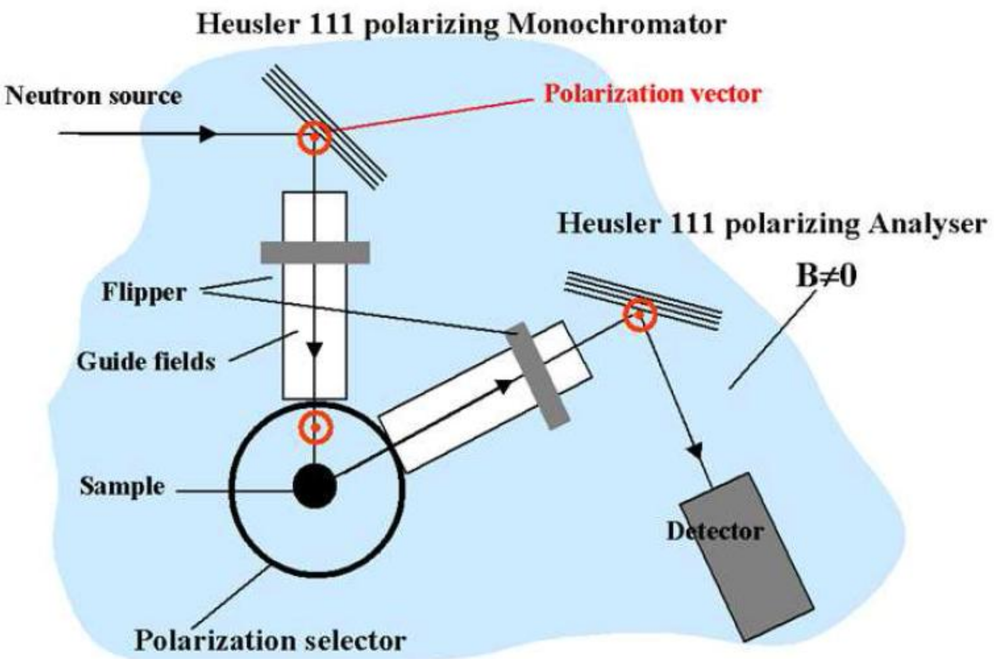
Pol. effects: Summary

	Non spin flip	Spin flip	Polarization dependent
Nuclear coherent	1	0	no
Nuclear incoherent spin (single isotope)	1/3	2/3	no
Nuclear incoherent isotope (I=0)	1	0	no
Paramagnetic scattering	$1/2(1-Q^2)$	$1/2(1-Q^2)$	no
FM, collinear, P perp. to Q, M ||Q	1 nuclear coh. + magnetic (b+p vs. b-p)	0 nuclear incoh.	yes
FM, non-collinear, P perp. to Q	<1 nuclear coh. + magnetic	>0 nuclear incoh. + magnetic	yes
FM, collinear, P||Q, M perp. to Q	Useless configuration, external field problem, No magnetic signal nuclear coh.	0 nuclear incoh.	no
AF, collinear, P||Q M perp. to Q	Only nuclear for P perp. to M	<1	yes
AF, non-collinar	<1	>0	yes

Typical Setup

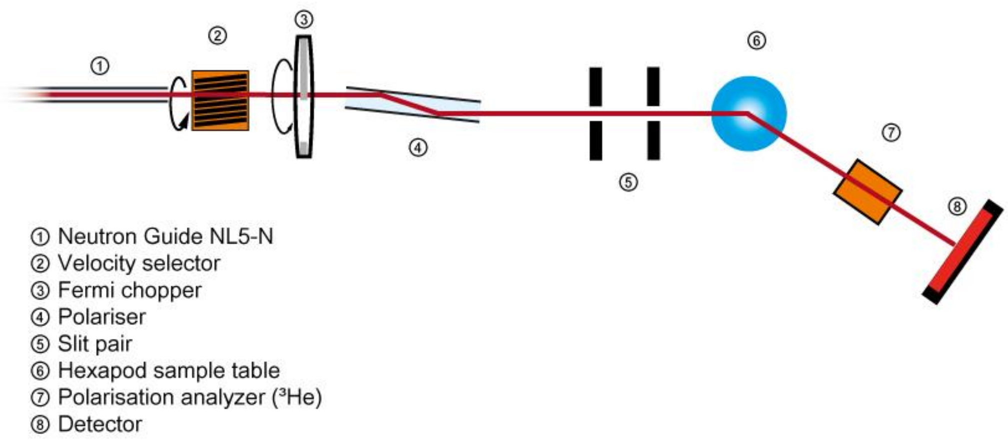
- Polarization option for a TAS:

Heusler mono
Mezei flipper
Uniaxial setup
Heusler analyzer
(3D polarimetry as add on)



- Polarization on a reflectometer (or SANS):

Polarizing cavity (mirror)
RF flipper
^{3}He analyzer
(3D polarimetry as add on)



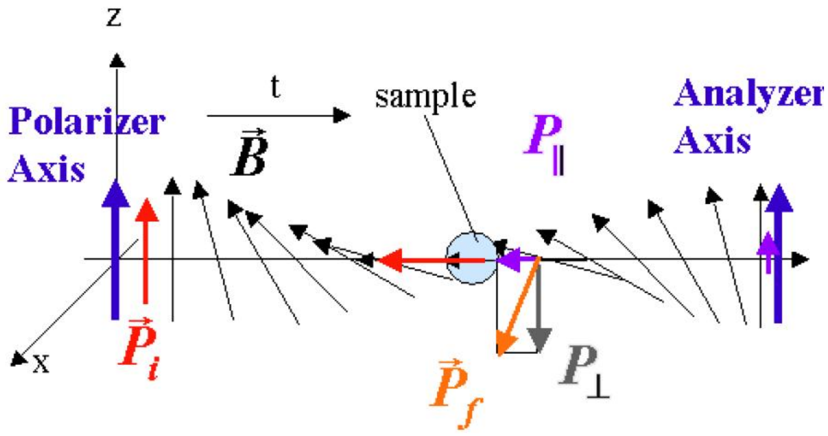
Neutron polarization: Things to consider

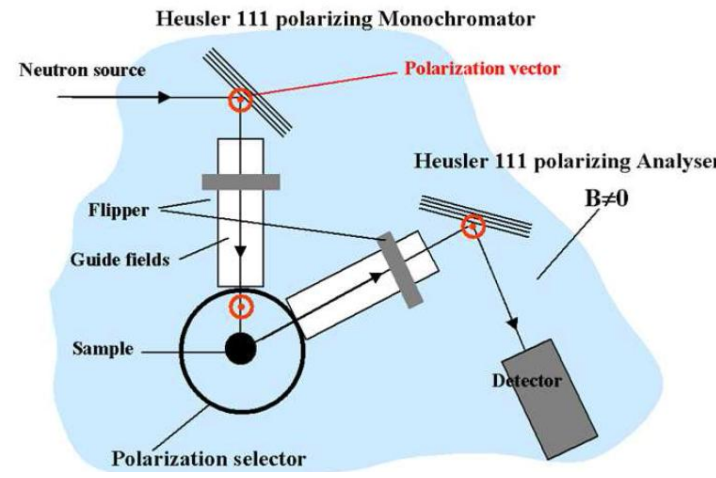
Uni-axial polarization analysis

- Reflectivity of polarizing monochromators is weak (have to be kept single domain). The polarized intensity typically amounts 20-30% of the unpolarized beam.
- Guide field necessary, difficulties with magnetic field at the sample region
- All flippers / polarizers /analyzers have finite efficiency! Corrections needed, difficult for small signals due to leakage from one channel to the other. ^{3}He analyzers are time-dependent.
- Four channels instead of one need to be measured!
- Only the projection of the polarization on the quantization axis (z-axis, guide field) can be measured

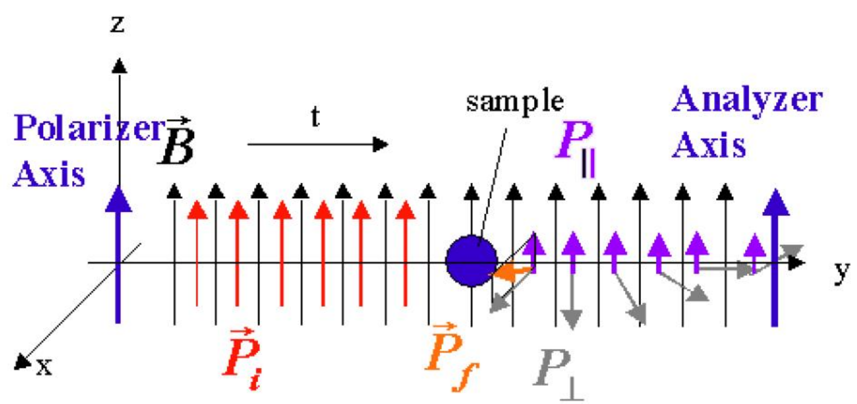
Uniaxial polarization analysis

Adiabatic rotation of polarization allows to measure three components (x,y,z)





Assume that scattering process at the sample rotates the polarization



- Spin precesses in guide field
- Only component parallel to z is measured

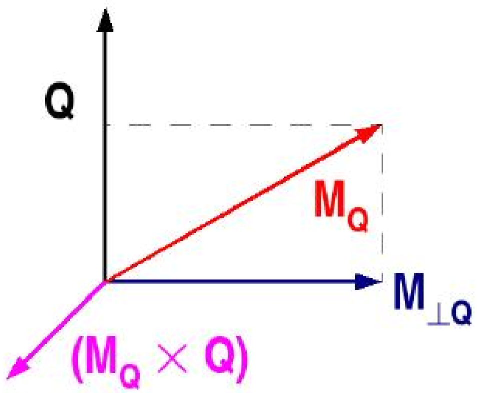
Information is lost!

3D polarimetry: Theory

Full treatment: Blume Maleyev equations:

$$
\begin{aligned}
\frac{d^2\sigma}{d\Omega dE'} = \; & \frac{k_f}{k_i}\frac{1}{2\pi\hbar}\int dt \Big\{ \\
& \langle N_{\boldsymbol{Q}} N^{\dagger}_{\boldsymbol{Q}} \rangle + && \text{pure nuclear contribution} \\
& +(\gamma r_0)^2 \langle \boldsymbol{M}_{\perp \boldsymbol{Q}} \boldsymbol{M}^{\dagger}_{\perp \boldsymbol{Q}} \rangle + && \text{pure magnetic contribution} \\
& +(\gamma r_0)\boldsymbol{P}_0 \left[\langle N^{\dagger}_{\boldsymbol{Q}} \boldsymbol{M}_{\perp \boldsymbol{Q}} \rangle + \langle \boldsymbol{M}^{\dagger}_{\perp \boldsymbol{Q}} N_{\boldsymbol{Q}} \rangle \right] - && \text{nuclear-magnetic interference} \\
& -i(\gamma r_0)\boldsymbol{P}_0 \langle \boldsymbol{M}_{\perp \boldsymbol{Q}} \times \boldsymbol{M}^{\dagger}_{\perp \boldsymbol{Q}} \rangle && \text{chiral magnetic contribution} \\
& \Big\} \exp(-i\omega t),
\end{aligned}
$$

$M_{\perp Q}$ is the magnetic interaction vector (component perp. to Q)



Notation:

$$
\begin{array}{lll l}
x & \parallel & \boldsymbol{Q} & \\
y & \perp & \boldsymbol{Q} & \text{in the scattering plane} \\
z & \perp & \boldsymbol{Q} & \text{out of the scattering plane}
\end{array}
$$

3D polarimetry: Theory

Blume Maleyev equations for the final polarization:

$$\begin{aligned}
\boldsymbol{P}'\frac{d^2\sigma}{d\Omega dE'} &= \frac{k_f}{k_i}\frac{1}{2\pi\hbar}\int dt\Big\{\boldsymbol{P}_0\langle N_{\boldsymbol{Q}}N^\dagger_{\boldsymbol{Q}}(t)\rangle - (\gamma r_0)^2\boldsymbol{P}_0\langle \boldsymbol{M}_{\perp\boldsymbol{Q}}\boldsymbol{M}^\dagger_{\perp\boldsymbol{Q}}(t)\rangle + \\
&+ (\gamma r_0)^2\langle(\boldsymbol{P}_0\boldsymbol{M}^\dagger_{\perp\boldsymbol{Q}}(t))\boldsymbol{M}_{\perp\boldsymbol{Q}}\rangle + (\gamma r_0)^2\langle \boldsymbol{M}^\dagger_{\perp\boldsymbol{Q}}(t)(\boldsymbol{P}_0\boldsymbol{M}_{\perp\boldsymbol{Q}})\rangle + \\
&+ (\gamma r_0)\Big(\langle N^\dagger_{\boldsymbol{Q}}\boldsymbol{M}_{\perp\boldsymbol{Q}}(t)\rangle + \langle \boldsymbol{M}^\dagger_{\perp\boldsymbol{Q}}N_{\boldsymbol{Q}}(t)\rangle\Big) + \\
&+ i(\gamma r_0)\boldsymbol{P}_0\times\Big(\langle \boldsymbol{M}^\dagger_{\perp\boldsymbol{Q}}N_{\boldsymbol{Q}}(t)\rangle - \langle N^\dagger_{\boldsymbol{Q}}\boldsymbol{M}_{\perp\boldsymbol{Q}}(t)\rangle\Big) + \\
&+ i(\gamma r_0)^2\langle \boldsymbol{M}_{\perp\boldsymbol{Q}}\times\boldsymbol{M}^\dagger_{\perp\boldsymbol{Q}}(t)\rangle\Big\}\exp(-i\omega t).
\end{aligned}$$

Polarization is a vector that may turn at the scattering process!

Rewrite as tensor! $\boldsymbol{P}' = \tilde{P}\boldsymbol{P}_0 + \boldsymbol{P}''$

Final polarization — Rotation of polarization — Generation of polarization

$$\sigma\tilde{\boldsymbol{P}} = \begin{pmatrix} (N-M^y-M^z) & iI^z & -iI^y \\ -iI^z & (N+M^y-M^z) & M_{mix} \\ iI^y & M_{mix} & (N-M^y+M^z) \end{pmatrix} \qquad \sigma\boldsymbol{P}'' = \begin{pmatrix} C \\ R^y \\ R^z \end{pmatrix}$$

3D polarimetry: Theory

Polarization is a vector that may turn at the scattering process!

Rewrite as tensor! $\boldsymbol{P}' = \tilde{P}\boldsymbol{P}_0 + \boldsymbol{P}''$

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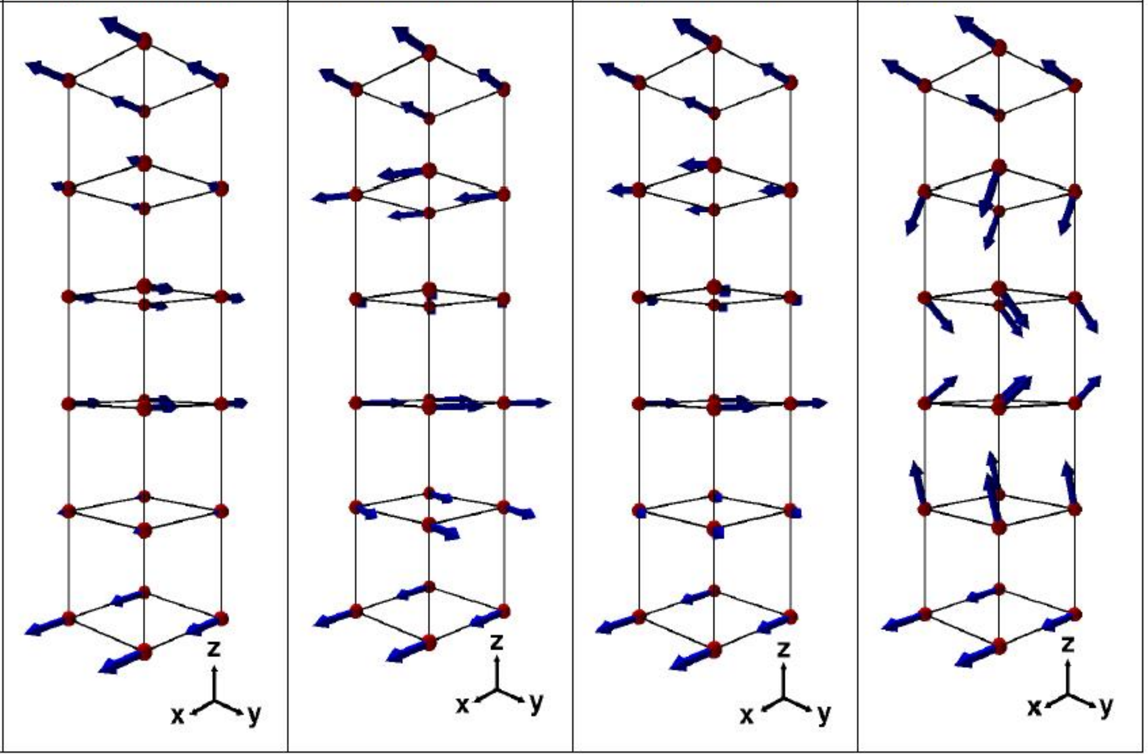
$$\sigma \tilde{\boldsymbol{P}} = \begin{pmatrix} (N-M^y-M^z) & iI^z & -iI^y \\ -iI^z & (N+M^y-M^z) & M_{mix} \\ iI^y & M_{mix} & (N-M^y+M^z) \end{pmatrix} \qquad \sigma \boldsymbol{P}'' = \begin{pmatrix} C \\ R^y \\ R^z \end{pmatrix}$$

Item	correlation functions	description
N	$\frac{k_f}{k_i}\langle N_{\boldsymbol{Q}} N_{\boldsymbol{Q}}^\dagger\rangle_\omega$	nuclear contribution
$M^{y/z}$	$(\gamma r_0)^2 \frac{k_f}{k_i}\langle M_{\perp\boldsymbol{Q}}^{y/z} M_{\perp\boldsymbol{Q}}^{\dagger y/z}\rangle_\omega$	y- and z-components of the magnetic contribution.
$R^{y/z}$	$(\gamma r_0)\frac{k_f}{k_i}\langle N_{\boldsymbol{Q}}^\dagger M_{\perp\boldsymbol{Q}}^{y/z}\rangle_\omega + \langle M_{\perp\boldsymbol{Q}}^{\dagger y/z} N_{\boldsymbol{Q}}\rangle_\omega$	real parts of the nuclear-magnetic interference term.
$I^{y/z}$	$(\gamma r_0)\frac{k_f}{k_i}\langle N_{\boldsymbol{Q}}^\dagger M_{\perp\boldsymbol{Q}}^{y/z}\rangle_\omega - \langle M_{\perp\boldsymbol{Q}}^{\dagger y/z} N_{\boldsymbol{Q}}\rangle_\omega$	imaginary parts of the nuclear-magnetic interference term.
C	$i(\gamma r_0)^2\frac{k_f}{k_i}(\langle M_{\perp\boldsymbol{Q}}^y M_{\perp\boldsymbol{Q}}^{\dagger z}\rangle_\omega - \langle M_{\perp\boldsymbol{Q}}^z M_{\perp\boldsymbol{Q}}^{\dagger y}\rangle_\omega)$	chiral contribution
M_{mix}	$(\gamma r_0)^2\frac{k_f}{k_i}(\langle M_{\perp\boldsymbol{Q}}^y M_{\perp\boldsymbol{Q}}^{\dagger z}\rangle_\omega + \langle M_{\perp\boldsymbol{Q}}^z M_{\perp\boldsymbol{Q}}^{\dagger y}\rangle_\omega)$	mixed magnetic contribution or magnetic-magnetic interference term

3D polarimetry: Example

Name	Ampl. modulated	Circular helix	Elliptical helix	Cycloid
Figure				

Different types of incommensurate spin "spirals"

⇨ Can be distinguished only using 3D polarimetry!

$\boldsymbol{Q}_+ = (0,0,1+k)$				
$\boldsymbol{S^k}$	$\frac{a\hat{e}_x}{2}$	$\frac{(a\hat{e}_x - ia\hat{e}_y)}{2}$	$\frac{(a\hat{e}_x - ib\hat{e}_y)}{2}$	$\frac{(a\hat{e}_x - ia\hat{e}_z)}{2}$
$\boldsymbol{M_{\perp Q}}$	$(0, \frac{a}{2}, 0)$	$(0, \frac{a}{2}, -\frac{ia}{2})$	$(0, \frac{a}{2}, -\frac{ib}{2})$	$(0, \frac{a}{2}, 0)$
M^y	$(\gamma r_0)^2 \frac{a^2}{4}$	$(\gamma r_0)^2 \frac{a^2}{4}$	$(\gamma r_0)^2 \frac{a^2}{4}$	$(\gamma r_0)^2 \frac{a^2}{4}$
M^z	0	$(\gamma r_0)^2 \frac{a^2}{4}$	$(\gamma r_0)^2 \frac{b^2}{4}$	0
M^{mix}	0	0	0	0
C	0	$-(\gamma r_0)^2 \frac{a^2}{2}$	$-(\gamma r_0)^2 \frac{ab}{2}$	0
$\frac{d\sigma}{d\Omega}$	$(\gamma r_0)^2 \frac{a^2}{4}$	$(\gamma r_0)^2 \frac{a^2}{2}(1 + P_0^x)$	$(\gamma r_0)^2 (\frac{a^2+b^2}{4} + P_0^x \frac{ab}{2})$	$(\gamma r_0)^2 \frac{a^2}{4}$
P_{ij}	$\begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 & 0 \\ -1 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix}$	pol. tensor provided in table 2.3	$\begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$

	$\boldsymbol{Q}_- = (0,0,1+k)$
P_{ij}	$\begin{pmatrix} \frac{-(\alpha^2+1)P_0^x - 2\alpha}{\alpha^2+1+2\alpha P_0^x} & 0 & 0 \\ -\frac{2\alpha}{\alpha^2+1} & \frac{\alpha^2-1}{\alpha^2+1} & 0 \\ -\frac{2\alpha}{\alpha^2+1} & 0 & \frac{1-\alpha^2}{\alpha^2+1} \end{pmatrix}$

3D polarimetry: Setup

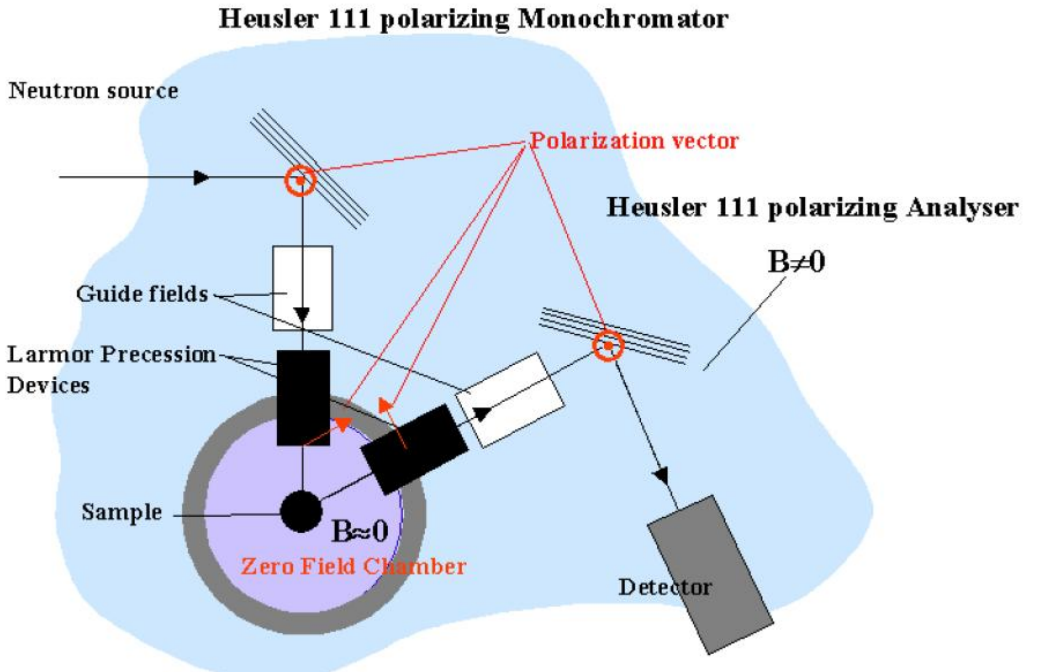
Mu-pad of Cryopad:

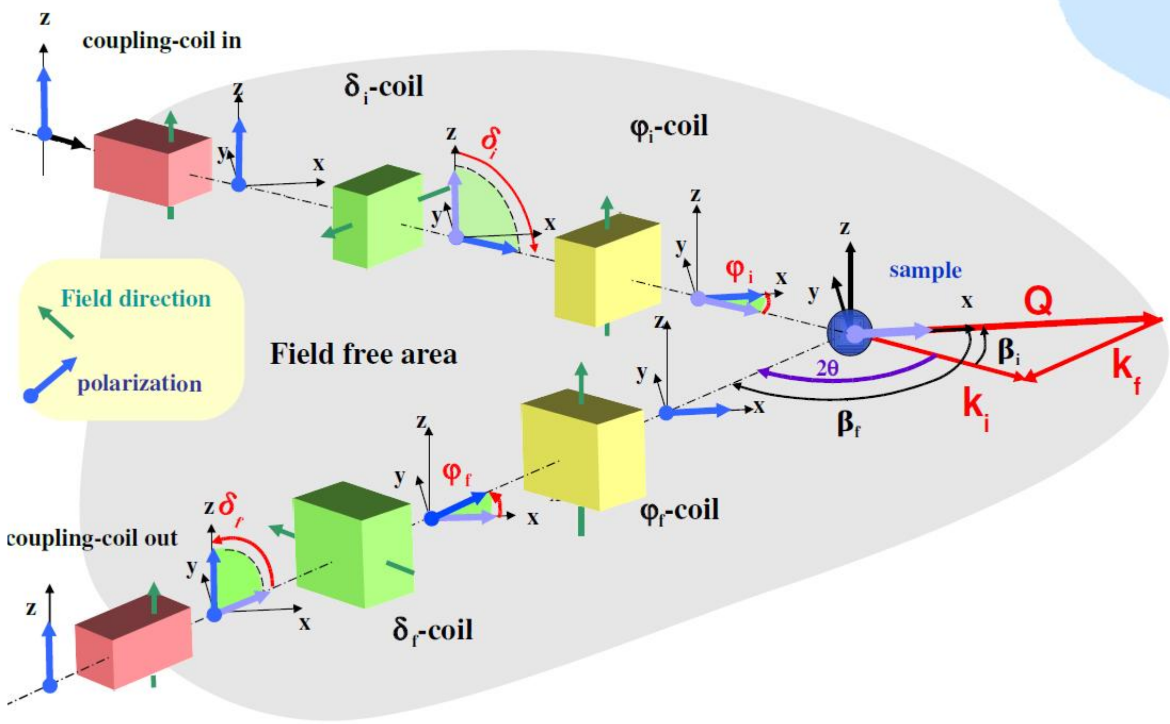
Mu-metal or Meissner shield:

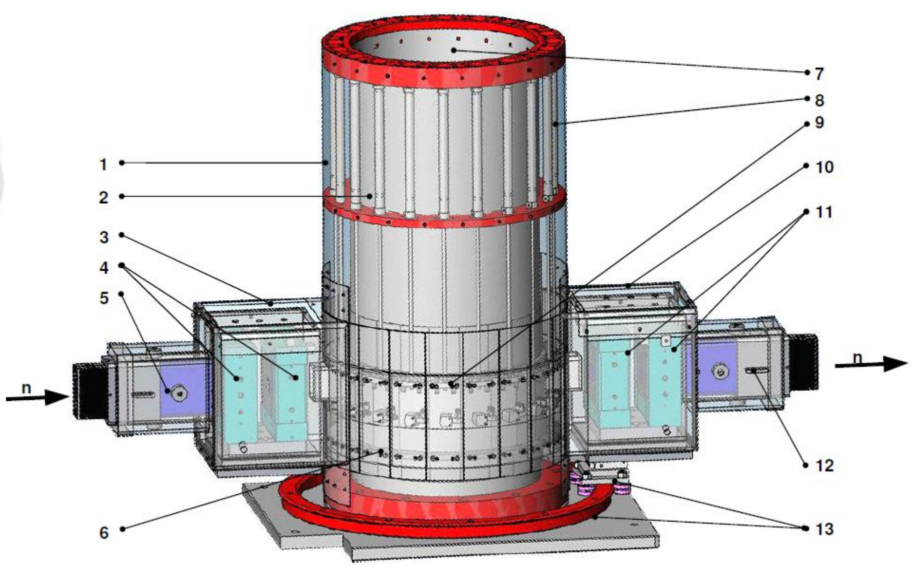
- Zero field chamber to maintain spin direction

Spin precession devices:

- Turn the spin adiabatically to the desired direction and back to the analyzer axis.







3D polarimetry: Summary

Uni-axial polarization analysis vs. 3D polarimetry

Uni-axial polarization analysis

$$\check{P} = \begin{pmatrix} \check{P}_{xx} & & \\ & \check{P}_{yy} & \\ & & \check{P}_{zz} \end{pmatrix}$$

Measurement of the diagonal terms only

- Slow, but helps solving <u>most</u> typical magnetic structures
- Magnetic field at the sample is possible
- Complicated due to leakage caused by finite efficiencies of flipper and analyzer

⟺

3D polarimetry

$$\mathrm{P}_{ij} = (P_{i0}\tilde{P}_{ji} + P_j'')/|\boldsymbol{P}_0|$$

Measurement of the 9 elements of the polarization matrix

- Even slower, but helps solving <u>almost all</u> magnetic structures
- Complicated for FM samples
- Complicated due to leakage caused by finite efficiencies of flipper and analyzer
- No magnetic field at the sample allowed
- This is the last measurement to be done!

Magnetic diffraction

Measurement strategy for magnetic diffraction

Identification of magnetic peaks:

- Strong temperature dependence close to T_c
- Polarization factor
- Q-dependence (form factor)

Solving the magnetic structure

- Use symmetry arguments and crystal symmetry!
- Use field to align domains/magnetization, use different polarization factors

If more than one structure remains

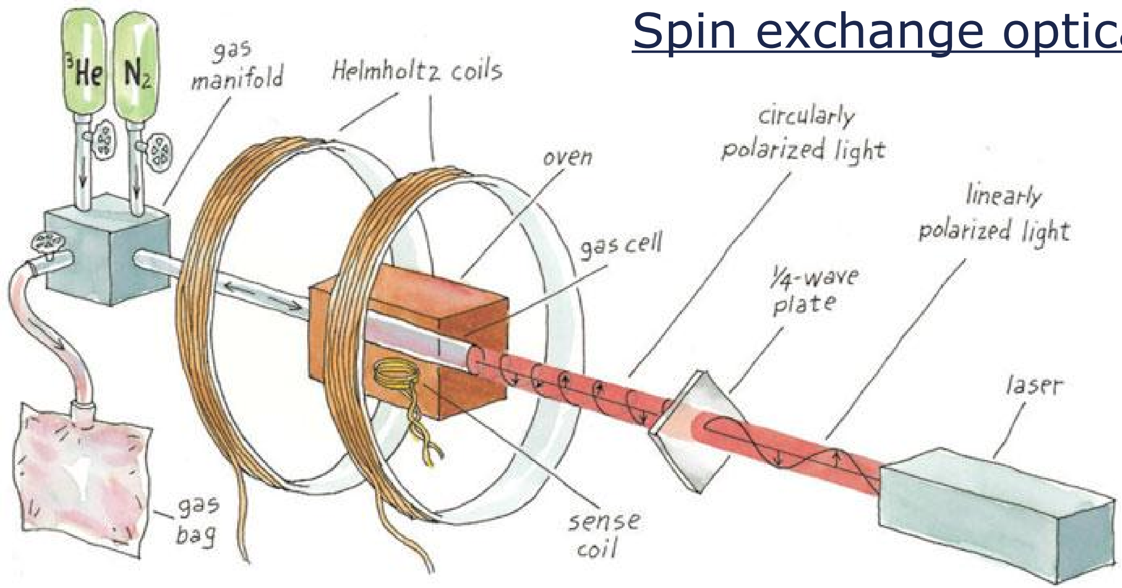
- Use classical uniaxial polarization analysis, measure flipping ratio $(b+p)^2$, $(b-p)^2$,

If more than one structure remains

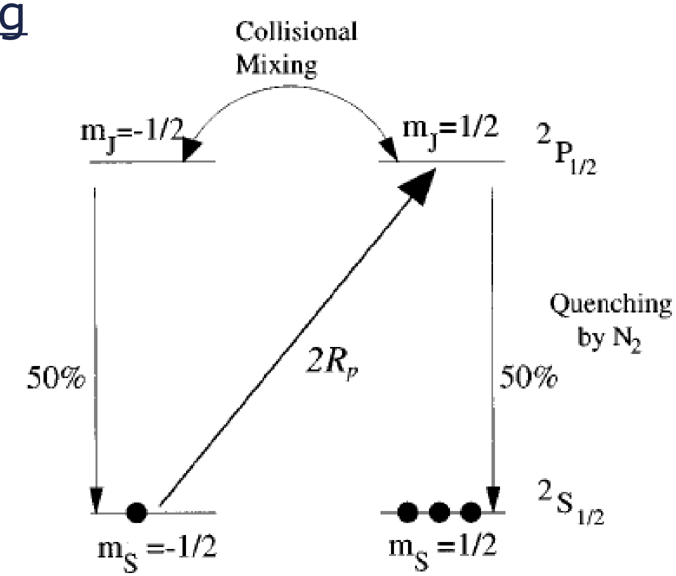
- Use 3-D polarimetry

^{3}He polarizer: SEOP

Spin exchange optical pumping



S. Kadlecek S. Am Sci 2002;90:540-549.

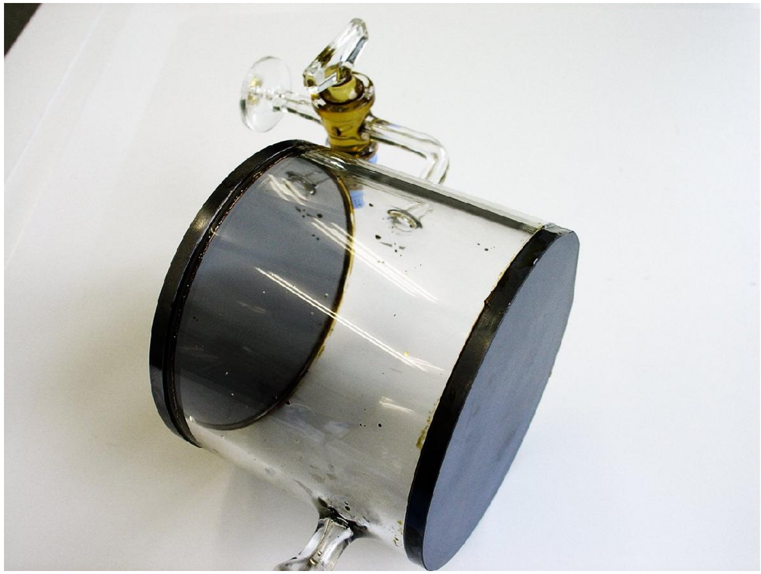


Circularly polarized light polarizes alkali metal electrons

Quenching gas (N2) supresses reradiation

Transfer of spin polarization to ^{3}He via binary collisions

Guide field necessary, sensitive to stray fields



⇨ Time dependent decay of ^{3}He (days)

⇨ No alternation of beam path

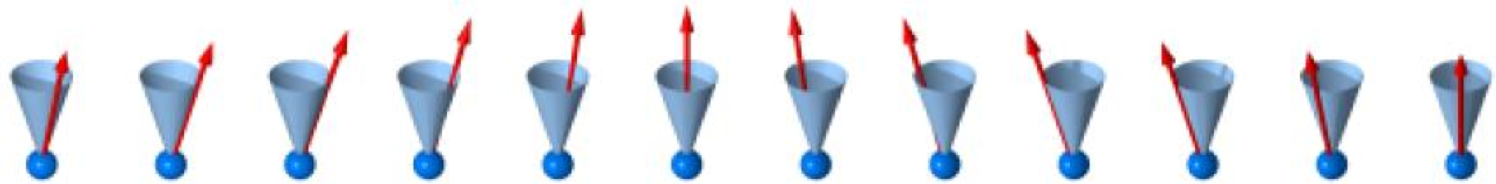
Spin waves: Magnetic excitations seen by neutrons

Spin waves

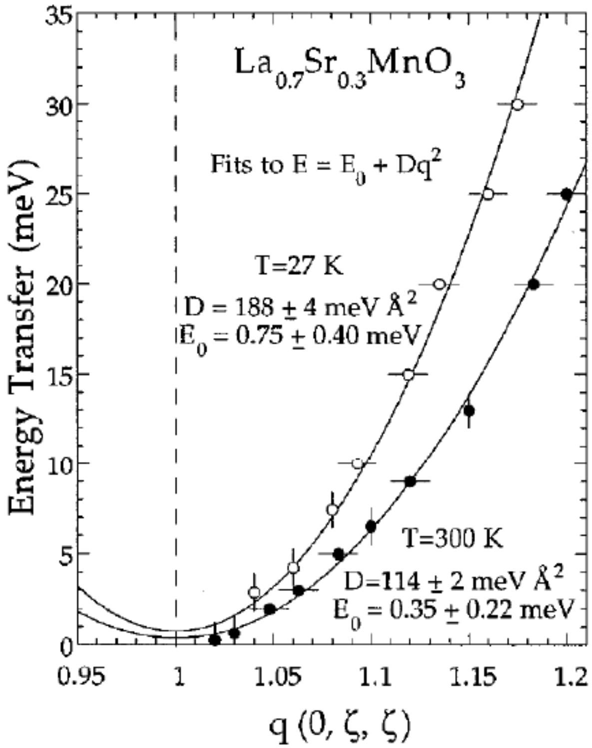
Spin waves (physical picture)

➡ Collective excitation of the order parameter

➡ Involves oscillation of spin components transverse to the ordered moment

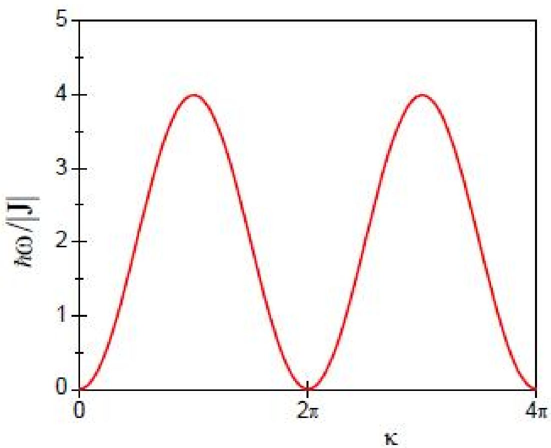


Dispersion ~q^2



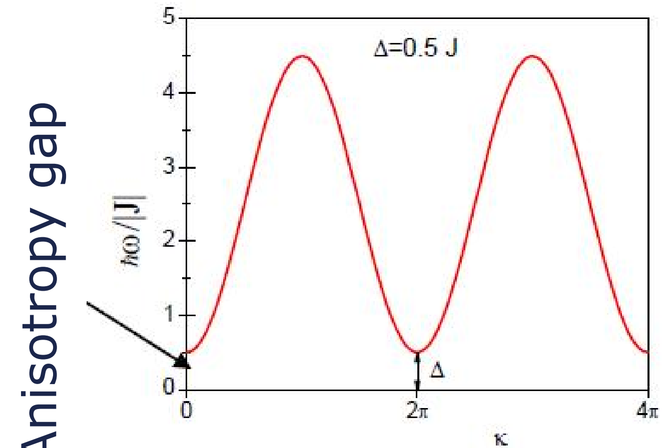
Martin et al 1996

Example: linear chain Heisenberg FM



$$\hat{H} = -|J| \sum_j \hat{\boldsymbol{S}}_j \hat{\boldsymbol{S}}_{j+1}$$

$$\hbar\omega = 2|J|S\left[1-\cos(\kappa a)\right]$$



$$\hat{H} = -|J| \sum_j \hat{\boldsymbol{S}}_j \hat{\boldsymbol{S}}_{j+1} - \Delta \sum_j \left(S_j^z\right)^2$$

$$\hbar\omega = 2|J|S\left[1-\cos(\kappa a)\right] + \Delta$$

Spin waves

Spin waves: seen by neutrons

- Similar to Phonons: Use QM picture with raising and lowering operator

- Bose-Einstein occupany $\langle n_{\boldsymbol{q}} \rangle = \left(\exp\left(\frac{\hbar\omega(\boldsymbol{q})}{k_B T} \right) - 1 \right)^{-1}$

Inelastic cross-sectrion for spin wave scattering

$$\boxed{\begin{aligned} \frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega\mathrm{d}\omega} = {} & (\gamma r_0)^2 \frac{(2\pi)^3 S}{2v_0} \frac{k'}{k} F^2(\boldsymbol{Q}) e^{-2W(\boldsymbol{Q})} \left[1 + \left(\frac{Q_z}{Q} \right)^2 \right] \\ & \times \sum_{\boldsymbol{\tau},\boldsymbol{q}} [\langle n_{\boldsymbol{q}} + 1 \rangle \delta(\boldsymbol{Q} - \boldsymbol{q} - \boldsymbol{\tau}) \delta(\hbar\omega(\boldsymbol{q}) - \hbar\omega) \\ & + \langle n_{\boldsymbol{q}} \rangle \delta(\boldsymbol{Q} + \boldsymbol{q} - \boldsymbol{\tau}) \delta(\hbar\omega(\boldsymbol{q}) + \hbar\omega)] \end{aligned}}$$