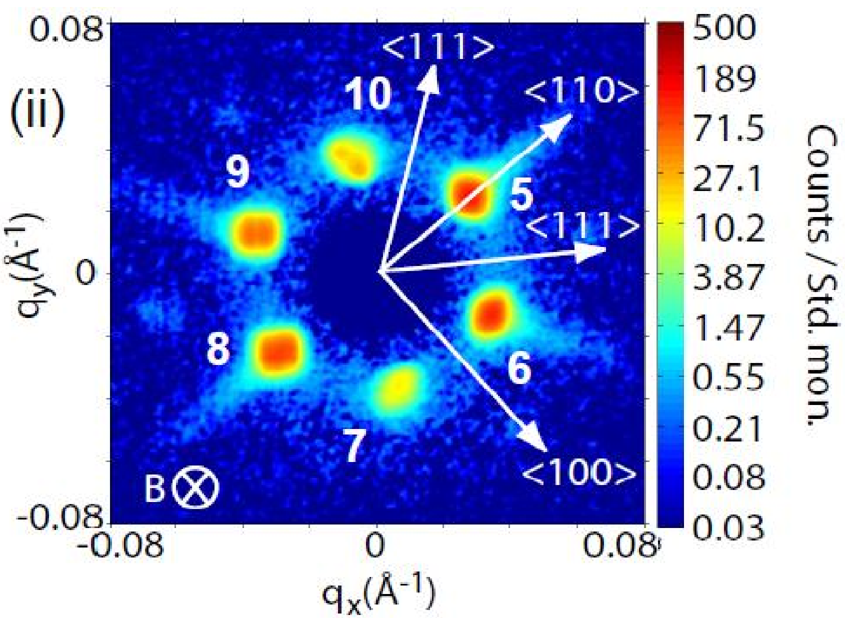
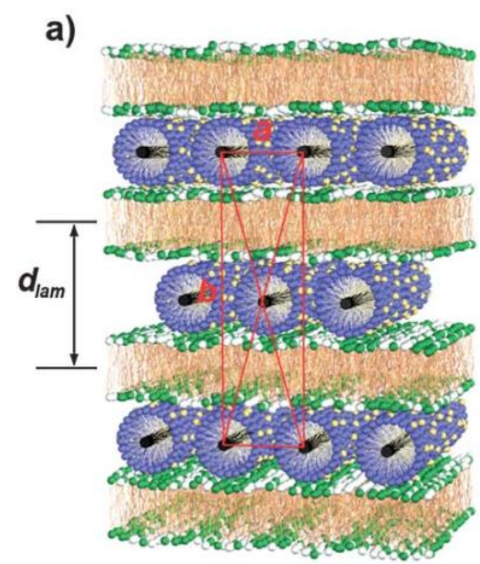
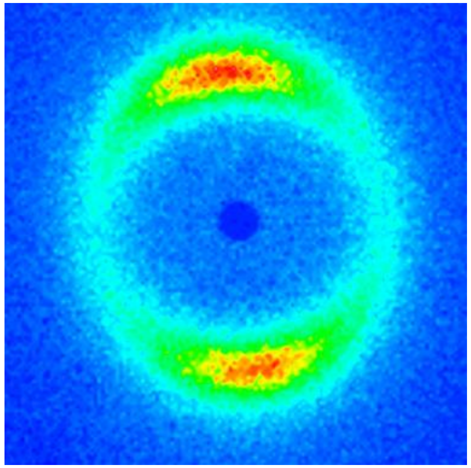
Physics with Neutrons II, SS 2016







Lecture 8, 20.6.2016

MLZ is a cooperation between:

JÜLICH
FORSCHUNGSZENTRUM

Helmholtz-Zentrum
Geesthacht
Zentrum für Material- und Küstenforschung

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: Inelastic scattering on magnetism
- VL10: 4.7.2016 (8:30!!) Phase transitions and critical phenomena as seen by neutrons
- VL11: Spin echo spectrocopy

Exam: Please register until 30.6.2016

Reminder:

- Cross section for magnetic neutron scattering
- Magnetic structures

Magnetic neutron scattering

Master formula

$$\left(\frac{d^2\sigma}{d\Omega dE'}\right) = (\gamma r_0)^2 \frac{k'}{k} F^2(\vec{Q}) e^{-2W(\vec{Q})} \sum_{\alpha,\beta} (\delta_{\alpha,\beta} - \frac{Q_\alpha Q_\beta}{Q^2}) S^{\alpha\beta}(Q,\omega)$$

$$S^{\alpha\beta}(Q,\omega) = \sum_{j,j'} e^{i\vec{Q}(R_j - R_{j'})} \sum_{\lambda,\lambda'} p_\lambda \langle\lambda|S^\alpha_{j'}|\lambda'\rangle\langle\lambda|S^\beta_j|\lambda'\rangle\delta(\hbar\omega + E_\lambda - E_{\lambda'})$$

Dipole-dipole interaction: Angular dependence

Neutron polarization factor $(\delta_{\alpha,\beta} - \frac{Q_\alpha Q_\beta}{Q^2})$

Only moments perpendicular to Q contribute to magnetic scattering

Don't confuse with polarized neutrons!

Magnetic neutron scattering

Master formula

$$\left(\frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega\mathrm{d}E'}\right) = (\gamma r_0)^2 \frac{k'}{k} \underline{F^2(\vec{Q})} e^{-2W(\vec{Q})} \sum_{\alpha,\beta} (\delta_{\alpha,\beta} - \frac{Q_\alpha Q_\beta}{Q^2}) S^{\alpha\beta}(Q,\omega)$$

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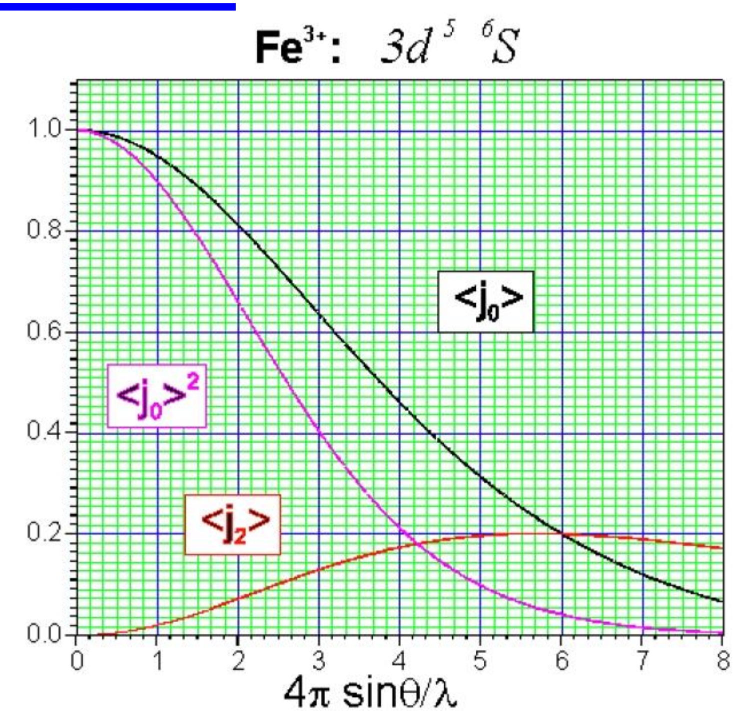
Dipole-dipole interaction: Magnetic form factor

- Fourier transform of electron cloud
- Useful to discriminate magnetic/nuclear scattering
- Check the tables for each ion!



Magnetic neutron scattering

Magnetic scattering function

$$S^{\alpha\beta}(Q,\omega) = \sum_{j,j'} e^{i\vec{Q}(R_j - R_{j'})} \underline{\langle S_{j'}^{\alpha}(0)\; S_{j'}^{\beta}(t)\rangle} e^{-i\omega t} \mathrm{d}t$$

<u>Spin correlation funtion:</u>

Correlation of magnetic moment at site j, time t=0
and site j', time t=t

⇨ <u>Fourier transform measured with neutrons!</u>

Paramagnets

By defition no correlation between spins $\langle \hat{S}_0^\alpha \rangle \langle \hat{S}_l^\beta \rangle = 0$

Consider only l=0 (self correlation) ⇨ Incoherent scattering

$$\langle \hat{S}_0^\alpha \rangle \langle \hat{S}_0^\beta \rangle = \delta_{\alpha\beta} \langle \hat{S}_0^\alpha \rangle \langle \hat{S}_0^\beta \rangle = \delta_{\alpha\beta} \langle (\hat{S}_0^\alpha)^2 \rangle = \frac{1}{3} \delta_{\alpha\beta} \langle \hat{\boldsymbol{S}} \rangle^2 = \frac{1}{3} \delta_{\alpha\beta} S(S+1)$$

Non-zero only for α=β

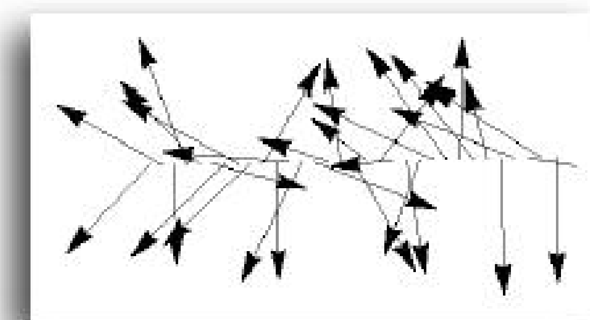
$$\sum_{\alpha,\beta} \left(\delta_{\alpha\beta} - \frac{Q_\alpha Q_\beta}{Q^2} \right) = \sum_\alpha \left(1 - \left(\frac{Q_\alpha}{Q} \right)^2 \right) = 2$$

Paramagnetic scattering (isotropic in Q)

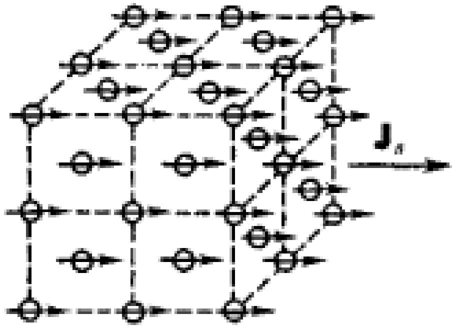
$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \frac{2}{3} N (\gamma r_0)^2 e^{-2W(\boldsymbol{Q})} F^2(\boldsymbol{Q}) S(S+1)$$

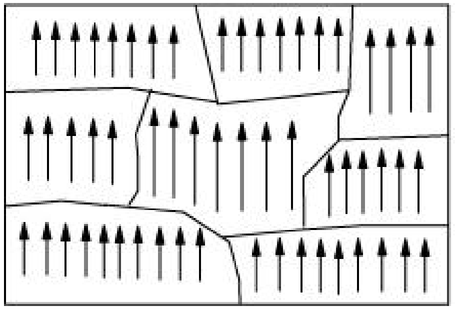
Scales with S(S+1), S^2

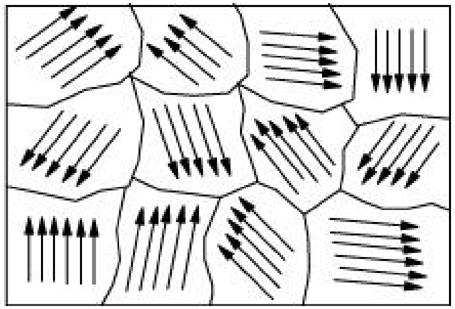
Scales with magnetic form factor F(Q)

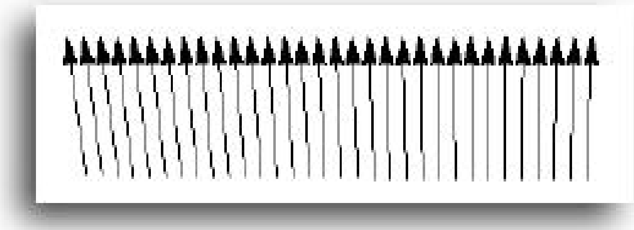


Ferromagnets









$$\frac{d\sigma}{d\Omega} = N\frac{(2\pi)^3}{v_0}(\gamma r_0)^2 e^{-2W(\boldsymbol{Q})} F^2(\boldsymbol{Q})\langle\hat{S}^z\rangle^2 \sum_{\boldsymbol{\tau}}\langle 1 - \left(\frac{\boldsymbol{\tau}\cdot\boldsymbol{e}}{\tau}\right)^2\rangle\,\delta(\boldsymbol{Q}-\boldsymbol{\tau})$$

- Scattering appears at reciprocal lattice vectors
- Scattering proportional to square of the magn. moment
- Strong temperature dependence close to transition temp.
- Intensity folows magn. Form factor F(Q)
- Depends on relative direction of S and Q

Alignment with field ⇨ vary polarization factor!

Antiferromagnets

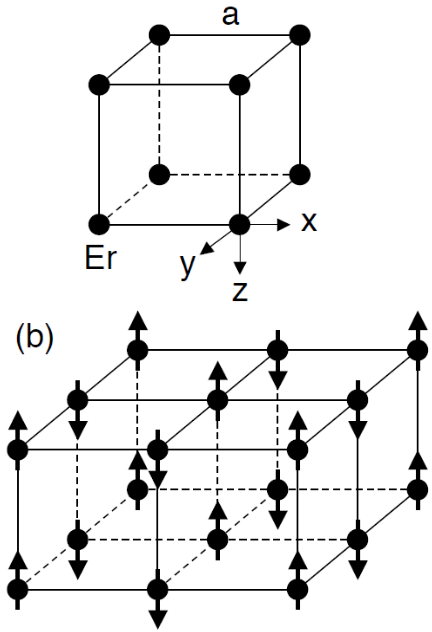
Antiferromagnet

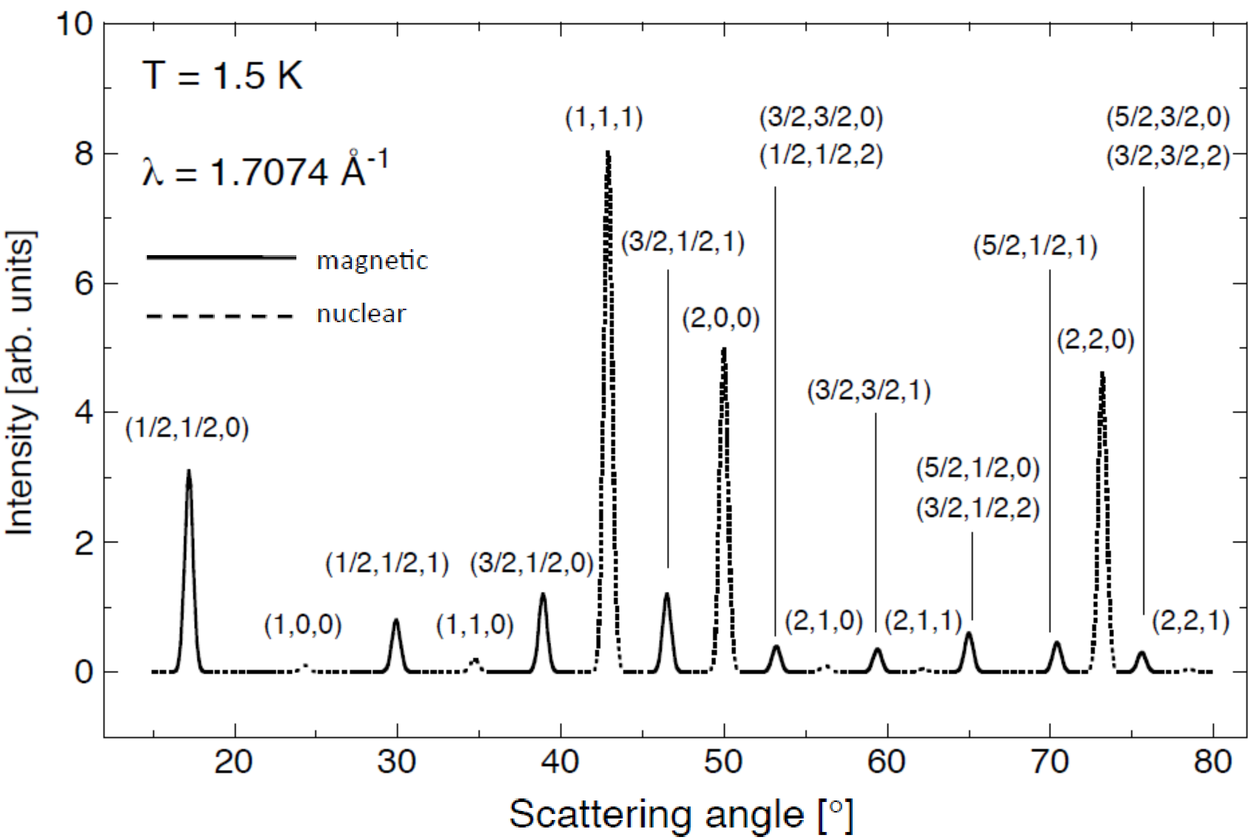
$$\frac{d\sigma}{d\Omega} = N_m \frac{(2\pi)^3}{v_{0m}} (\gamma r_0)^2 e^{-2W(\boldsymbol{Q})} \times \sum_{\boldsymbol{\tau}_m} |S_m(\boldsymbol{\tau}_m)|^2 \langle 1 - \left(\frac{\boldsymbol{\tau}_m \cdot \boldsymbol{e}}{\boldsymbol{\tau}_m}\right)^2 \rangle \delta(\boldsymbol{Q} - \boldsymbol{\tau}_m)$$

$$S_m(\boldsymbol{\tau}_m) = \langle S^z \rangle F(\boldsymbol{\tau}_m) \sum_{\boldsymbol{d}} \sigma_{\boldsymbol{d}} e^{\imath \boldsymbol{\tau}_m \cdot \boldsymbol{d}}$$

Magnetic structure factor

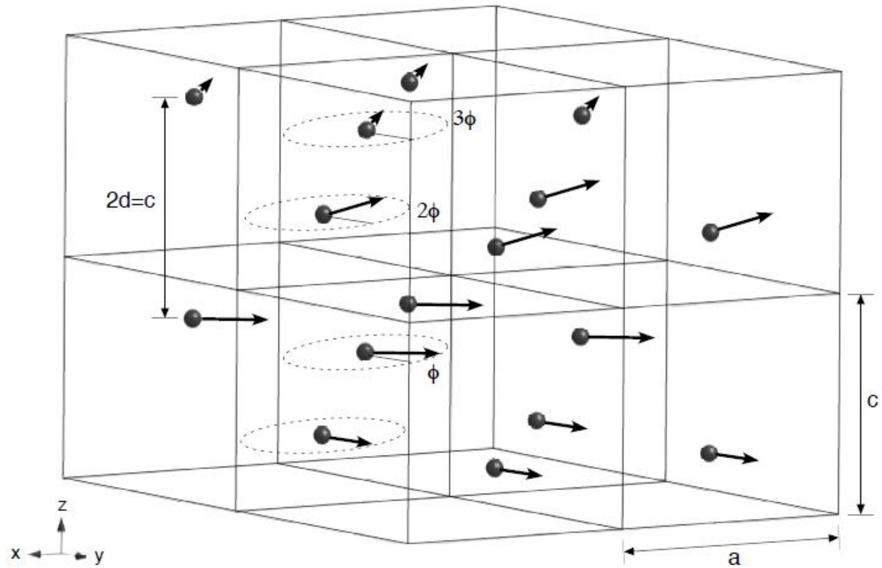
Example $ErPd_3$





→ Magnetic Bragg peaks at half integer position

Spiral Magnetic Structures



$$\langle \hat{S}_l^x \rangle = \langle \hat{S} \rangle \cos(\boldsymbol{P}^* \cdot \boldsymbol{l})$$

$$\langle \hat{S}_l^y \rangle = \langle \hat{S} \rangle \sin(\boldsymbol{P}^* \cdot \boldsymbol{l})$$

$$\langle \hat{S}_l^z \rangle = 0$$

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = (\gamma r_0)^2 e^{-2W(\boldsymbol{Q})} F^2(\boldsymbol{Q}) \sum_{\boldsymbol{l}} e^{\imath \boldsymbol{Q}\cdot\boldsymbol{l}} \langle \hat{S} \rangle^2 \times \left[\left(1 - \left(\frac{Q_x}{Q} \right)^2 \right) \cos(\boldsymbol{P}^* \cdot \boldsymbol{l}) - \frac{Q_x Q_y}{Q^2} \sin(\boldsymbol{P}^* \cdot \boldsymbol{l}) \right]$$

Rewrite cos as exp. function

vanishes

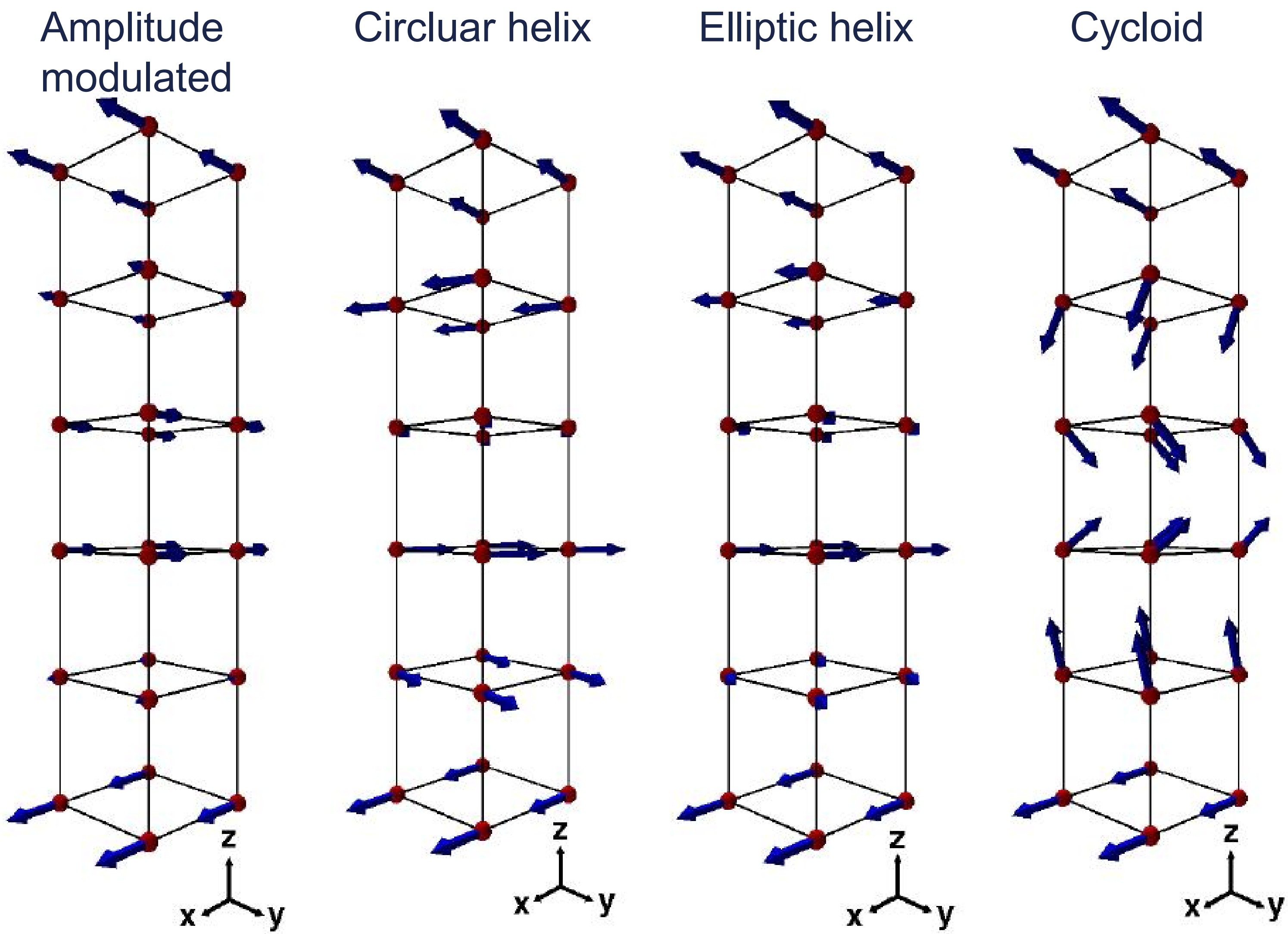
Use lattice sum identity

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \frac{N}{2} \frac{(2\pi)^3}{v_0} (\gamma r_0)^2 e^{-2W(\boldsymbol{Q})} F^2(\boldsymbol{Q}) \langle \hat{S} \rangle^2 \left(1 - \left(\frac{Q_x}{Q} \right)^2 \right) \times \sum_{\boldsymbol{\tau}} \left(\delta(\boldsymbol{Q} + \boldsymbol{P}^* - \boldsymbol{\tau}) + \delta(\boldsymbol{Q} - \boldsymbol{P}^* - \boldsymbol{\tau}) \right)$$

Intensity at (in)commensurate peaks which flank the nucear Bragg peak

Spiral Magnetic Structures

There is a zoo of incommensurate structures:



- And of course the corresponding AF representation of each
- Typically generated by frustration or Dzyaloshinsky-Moriya interaction

Zero Field Magnetization

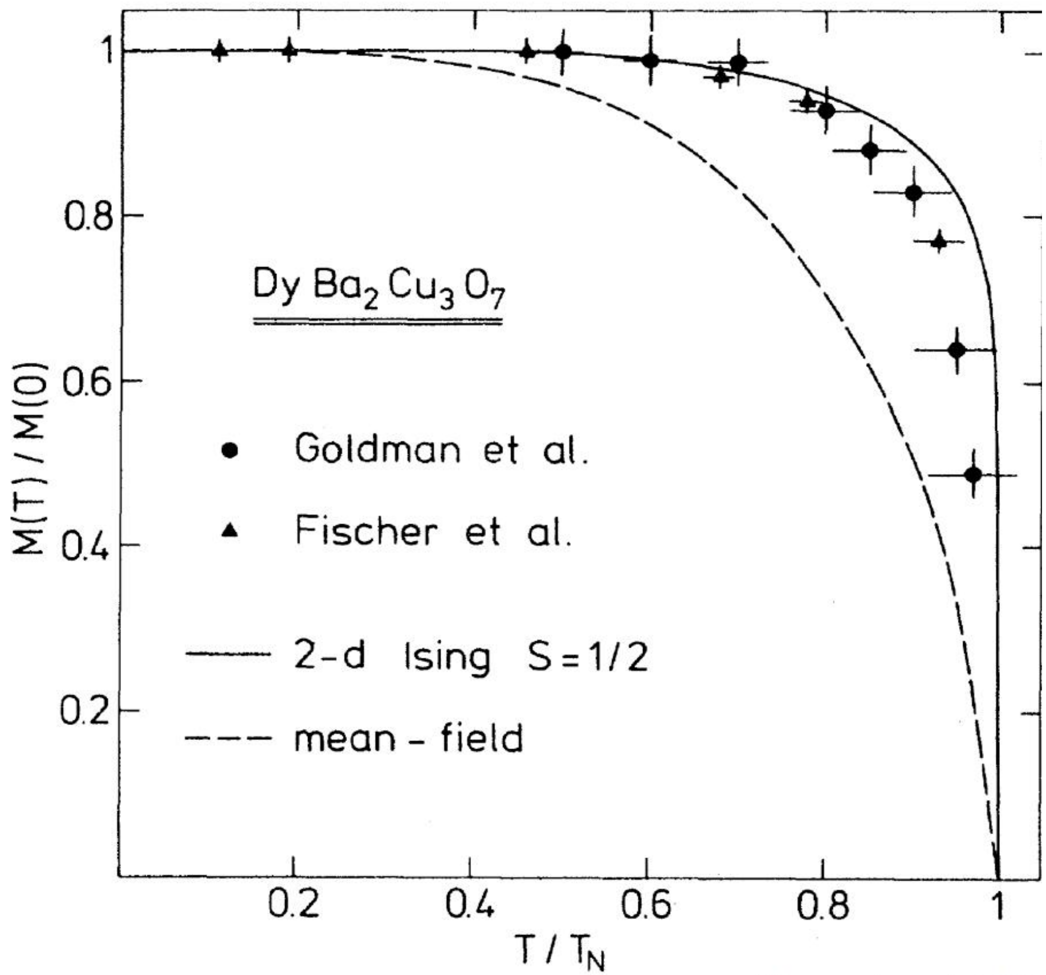
Magnetic intensity proportional to square of expectation value of spin operator $\langle \hat{\boldsymbol{S}}^2 \rangle$

Magnetic neutron diffraction probes moments perpendicular to Q

Related to magnetic moment

$$\Rightarrow \boldsymbol{\mu} = g\mu_B \langle \hat{\boldsymbol{S}} \rangle$$

Magnetic neutron diffraction probes the absolute moment and its direction



Allenspach et al., 1989

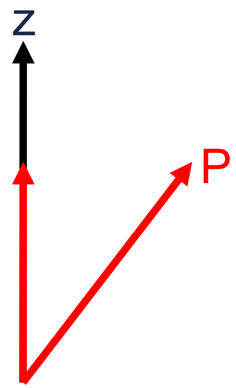
Polarized Neutrons

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

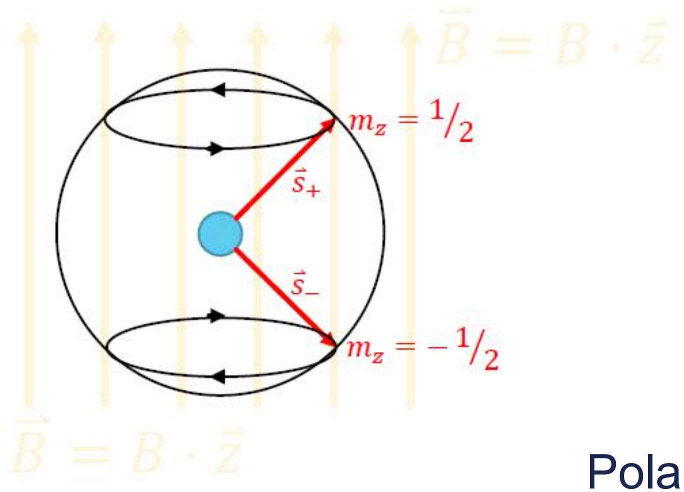
$|+\rangle \Rightarrow |-\rangle$
$|-\rangle \Rightarrow |+\rangle$
Spin flip channels

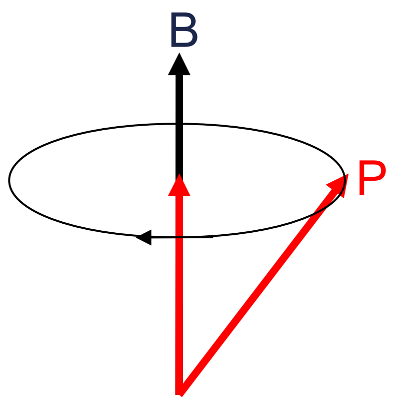
Lamor precession

Magnetic moment μ of the neutron in a magnetic field B

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

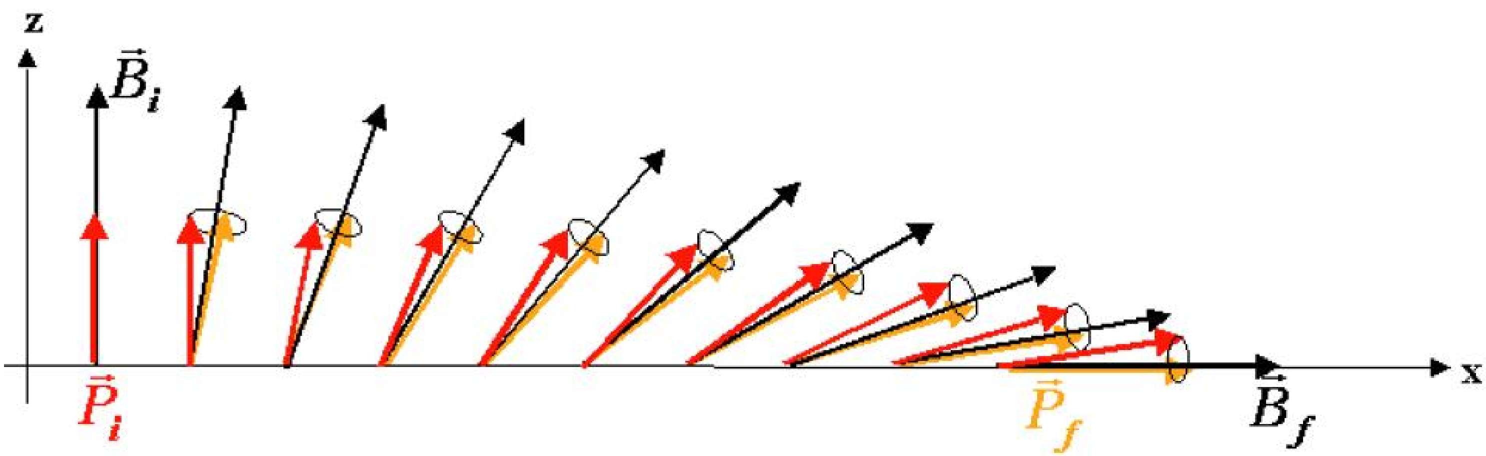
Lamor frequency f= 2.92kHz *B[G]   ΔΦ=2.654° * λ[Å] * B[G] * l[cm]





Polarization: Projection of P on B (z axis)

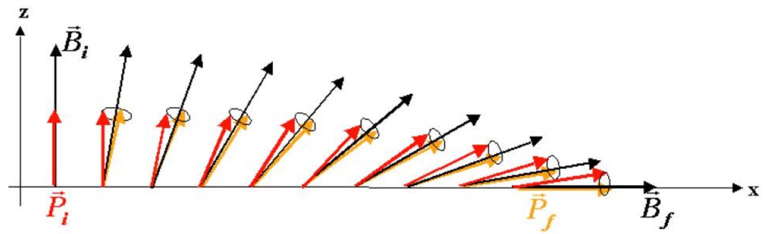
Adiabatic rotation of the spin

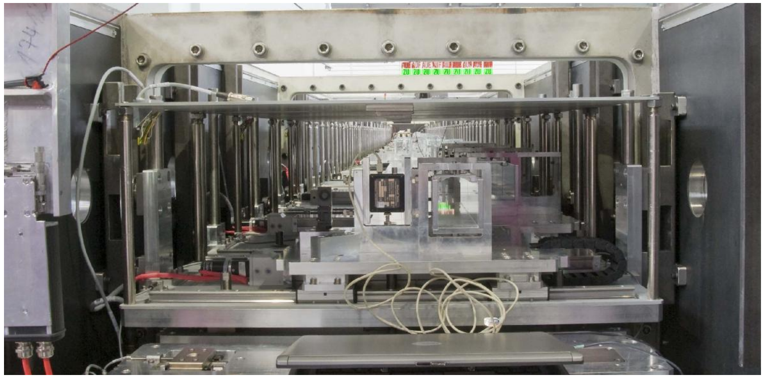


Lamor precession

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

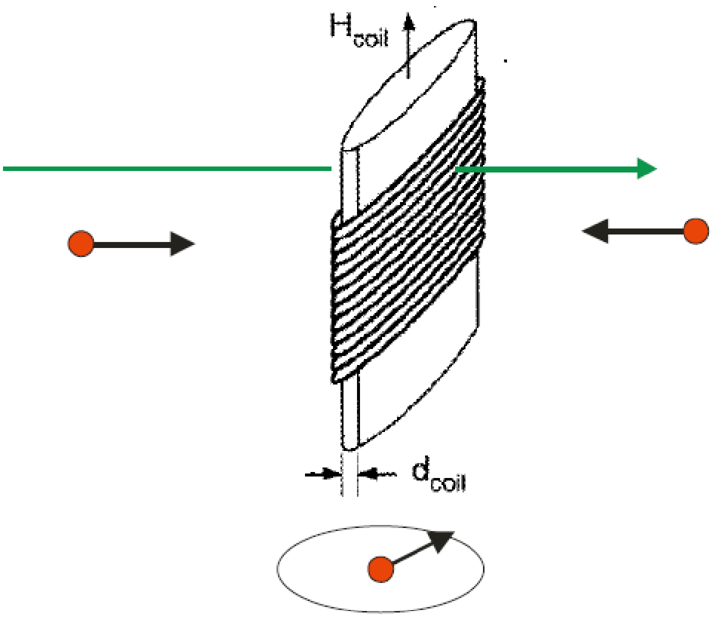
Wavelength dependent

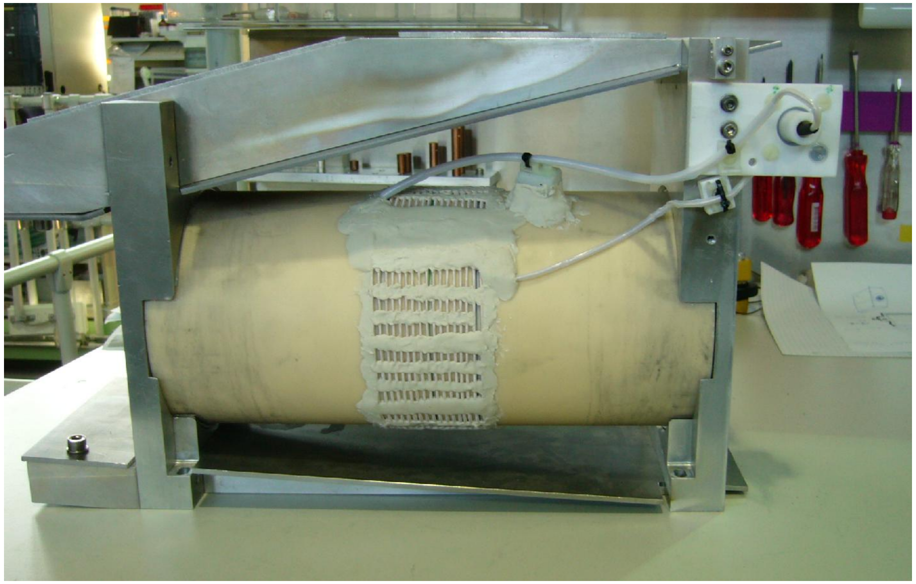
RF flipper

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

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

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

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

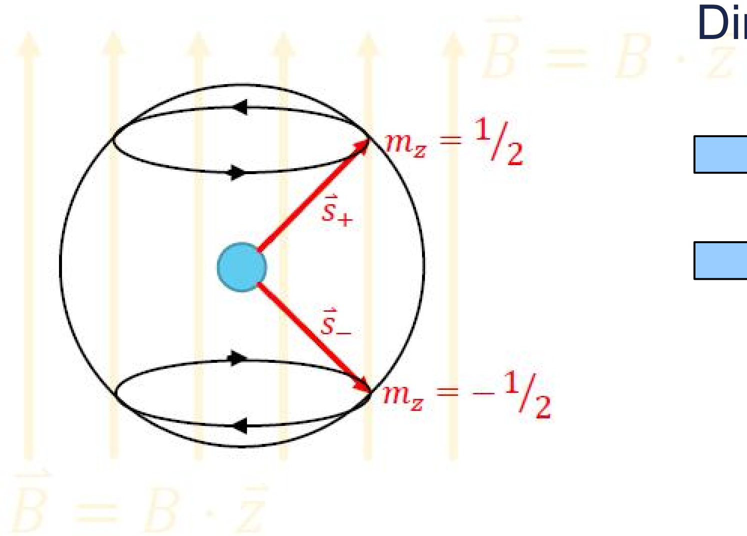
$$\langle -|\hat{U}|+\rangle = A(I_x - iI_y) + B(M_x - iM_y)$$

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

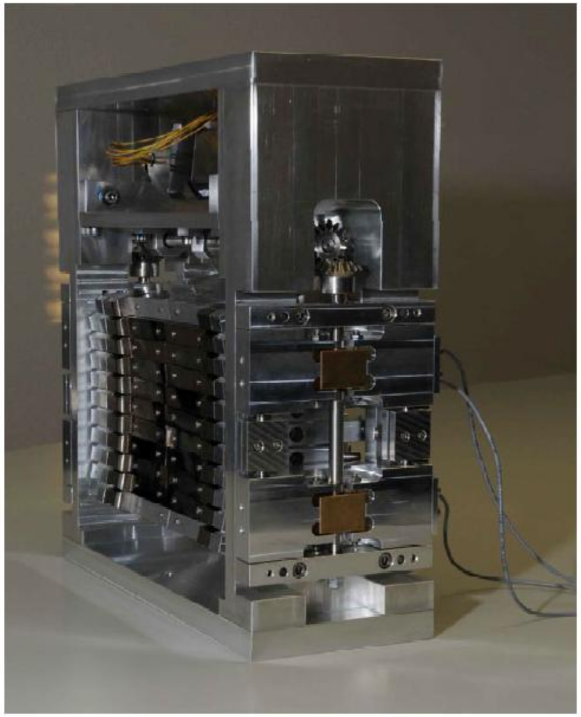
- Remember flipper coil!

How to polarize?

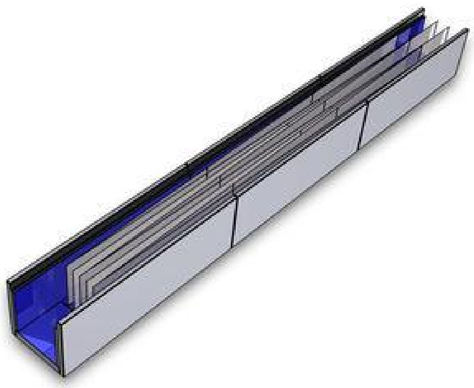
Polarizing monochromators

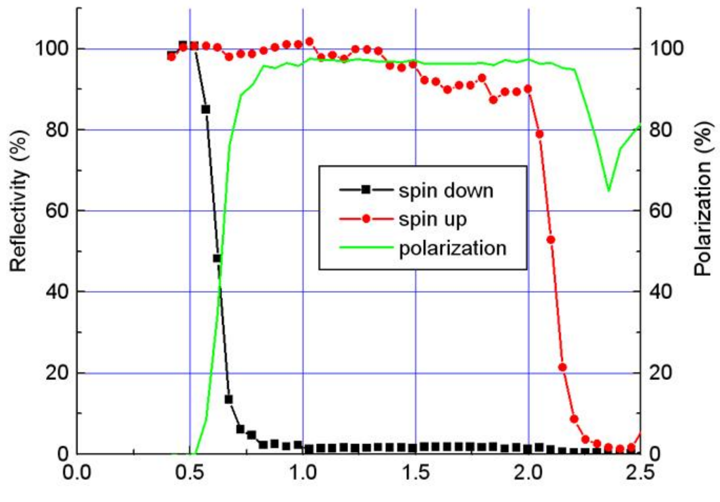
- Materials:
  - Fe, Co alloys
  - Cu_2MnAl (111)

  Heusler alloy- 95% polarization
- Need to maintain single ferro domain in entire monochromator
- Low reflectivity

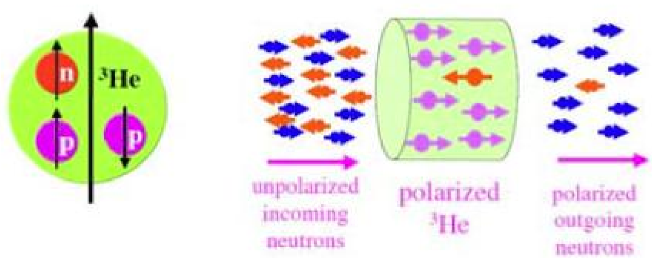


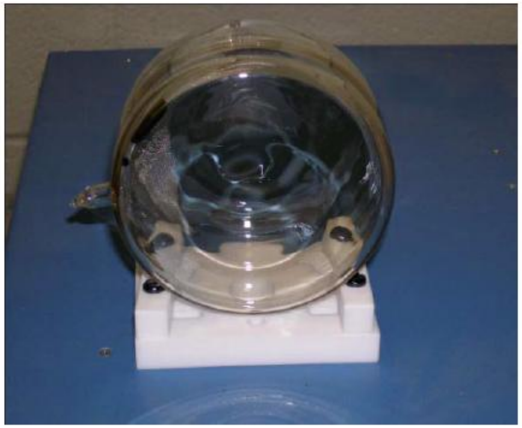
Polarizing supermirrors





^{3}He spin filters



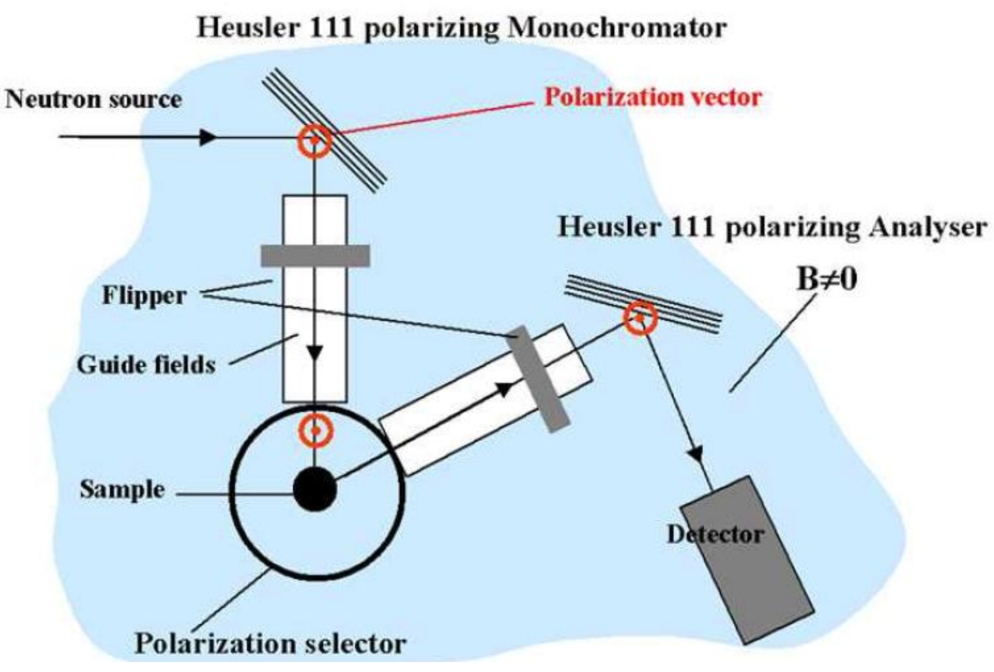


Polarization effects: Summary

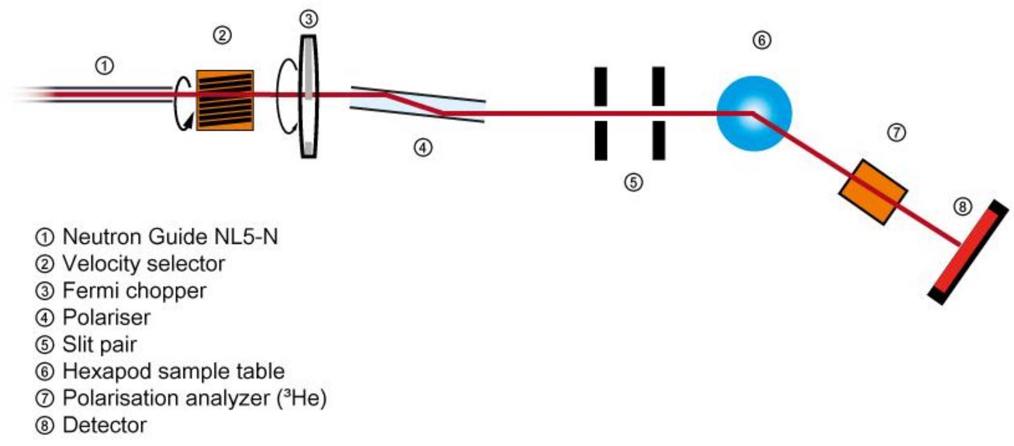
	Non spin flip	Spin flip	Polarization dependent
Nuclear coherent	1	0	no
Nuclear incoherent spin (single isotope)	1/3	2/3	no
Nuclear incoherent isotope (I=0)	1	0	no
Paramagnetic scattering	$1/2(1-Q^2)$	$1/2(1-Q^2)$	no
FM, collinear, P perp. to Q, M ||Q	1 nuclear coh. + magnetic (b+p vs. b-p)	0 nuclear 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:



Polarization on a reflectometer:



Neutron polarization: Things to consider

- 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!