

This presentation might differ from the one which really  
will be presented

## Outline

- Basics
- Magnetic scattering
- Spin manipulation
- Instruments

## Basics

Reminder: The scattering cross section:

$$\frac{d\sigma}{d\Omega} = \sum_{i,j} b_i b_j \exp\left(i \vec{q} \cdot (\vec{R}_i - \vec{R}_j)\right)$$

Suppose that at position  $R_i$  we can have different scattering length with a certain probability distribution

$$\langle b_i b_j \rangle = \langle b_i \rangle \langle b_j \rangle + \delta_{ij} \left( \langle b_i^2 \rangle - \langle b_i \rangle^2 \right)$$

$$\frac{d\sigma}{d\Omega} = \sum_{i,j} \langle b_i \rangle \langle b_j \rangle \exp\left(i \vec{q} \cdot (\vec{R}_i - \vec{R}_j)\right) + \sum_i \left( \langle b_i^2 \rangle - \langle b_i \rangle^2 \right)$$

$$I_{coherent}(\vec{q}) + I_{incoherent}(\vec{q})$$

$b_i$  can have a distribution because:

- different isotopes exist
- the nucleus has a spin  $I \Rightarrow$  with the neutron  $1/2$  spin it forms two possible states

$I+1/2 \Rightarrow 2(I+1/2)+1$  states with scattering length  $b_+$

$I-1/2 \Rightarrow 2(I-1/2)+1$  states with scattering length  $b_-$

Coherent

$$\langle b_i \rangle = b_+ \frac{I+1}{2I+1} + b_- \frac{I}{2I+1}$$

Incoherent

$$\left( \langle b_i^2 \rangle - \langle b_i \rangle^2 \right) = (b_+ - b_-)^2 \frac{I(I+1)}{(2I+1)^2}$$

the nuclear spin is usually randomly oriented EXCEPT very low T or very high B

Let's define the polarization of the beam as:  $\vec{P} = 2 \langle \vec{s} \rangle = \langle \vec{\sigma} \rangle$

In terms of Pauli matrices

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

Scattering length on a nucleus with spin I:

$$b = A + \frac{1}{2} B \hat{\sigma} \hat{I}$$
$$A = b_+ \frac{I+1}{2I+1} + b_- \frac{I}{2I+1} \quad B = \frac{2(b_+ - b_-)}{2I+1}$$

$\sigma_x$  and  $\sigma_y$  changes the spin state of the neutron  $\Rightarrow$  spin flip scattering

$\sigma_z$  does not  $\Rightarrow$  non spin flip scattering

If the nuclear spin I is randomly oriented in space each one has 1/3 probability thus:

**Spin Incoherent scattering 2/3 spin flip 1/3 non spin flip  $P \Rightarrow -1/3P$**

## Magnetic scattering

The neutron has a 1/2 spin => magnetic moment  $\mu_n = \gamma_n \mu_N$   
 $\mu_N$  nuclear Bohr magneton and  $\gamma_n = -1.913$

With a magnetic field the interaction potential Lovesey 1986:

$$V(\vec{R}) = -\vec{\mu}_n \vec{B} = \gamma_n \mu_N \left[ 2\mu_B \text{curl} \left( \frac{\vec{s} \times \vec{R}}{|R^3|} \right) - \frac{e}{2m_e c} \left( \vec{p}_e \frac{\vec{\sigma} \times \vec{R}}{|R^3|} + \frac{\vec{\sigma} \times \vec{R}}{|R^3|} \vec{p}_e \right) \right]$$

$\vec{s}$  = electron spin operator,  $\vec{p}_e$  = electron momentum operator

$\vec{\sigma}$  = neutron spin operator

The matrix element (scattering probability) becomes:

$$\langle k' | V_M | k \rangle = -r_0 \hat{\sigma} \hat{Q}_\perp \text{ with } r_0 = \frac{\gamma_n e^2}{m_e c^2}$$
$$\hat{Q}_\perp = \sum_i \exp(i \vec{q} \cdot \vec{r}_i) \left( \tilde{q} \times (\vec{s} \times \tilde{q}) - \frac{i}{\hbar |\vec{q}|} (\tilde{q} \times \vec{p}_i) \right) \text{ with } \tilde{q} = \frac{\vec{q}}{|\vec{q}|}$$

or in terms of the magnetization and changing to integral to account for the spatial extent of the electrons

$$\vec{Q} = -\frac{1}{2\mu_B} \int d\vec{r} \exp(i \vec{k} \cdot \vec{r}) \vec{M}(\vec{r}) \text{ and } \vec{Q}_\perp = \vec{Q} - \tilde{q} (\vec{Q} \tilde{q})$$

Of the sample spins (magnetization) ONLY THE COMPONENT PERPENDICULAR to q contributes !!This is fundamentally different from the nuclear spin!

# Polarized Neutrons

The scattered intensity is the Fourier transform of the self correlation function of the scattering length density

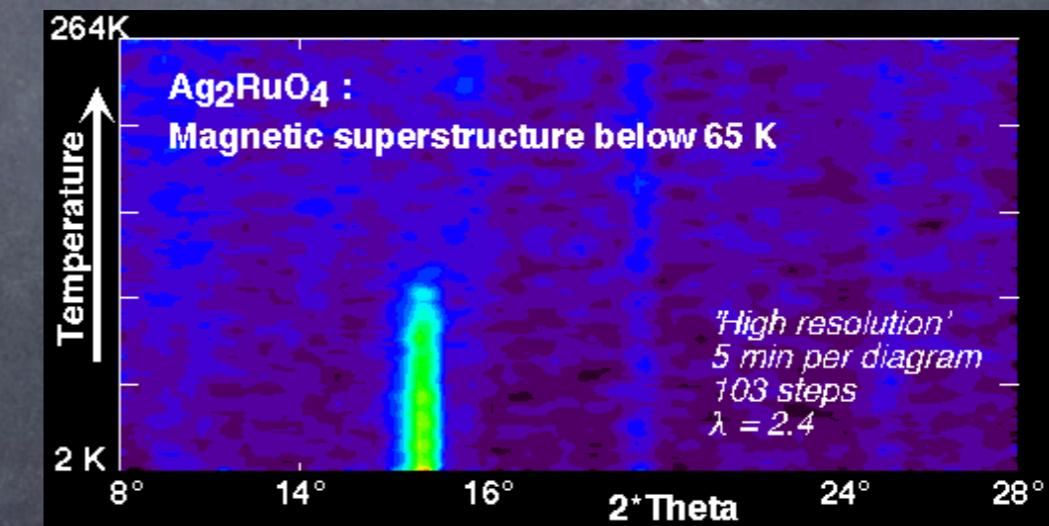
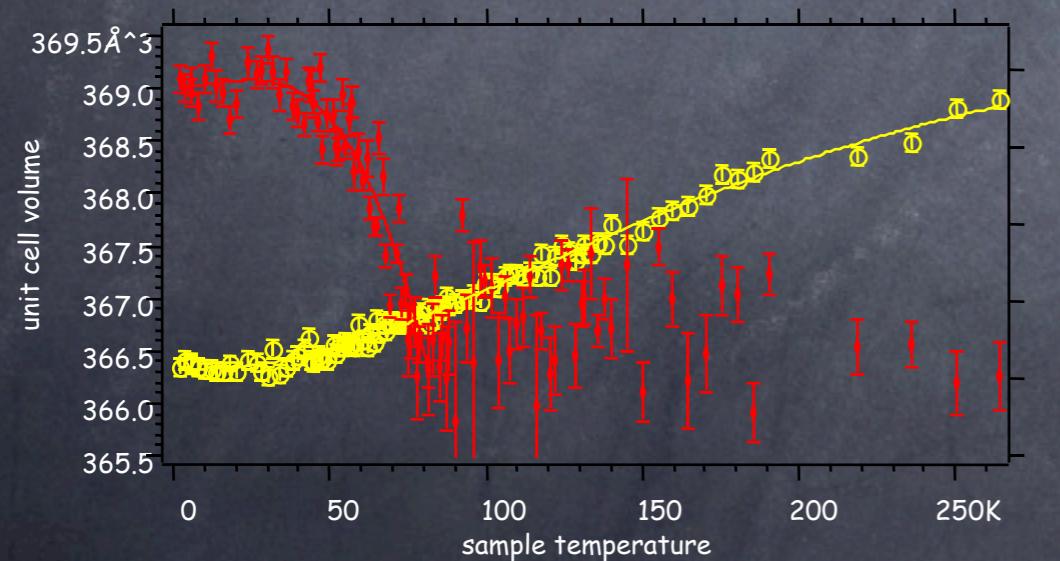
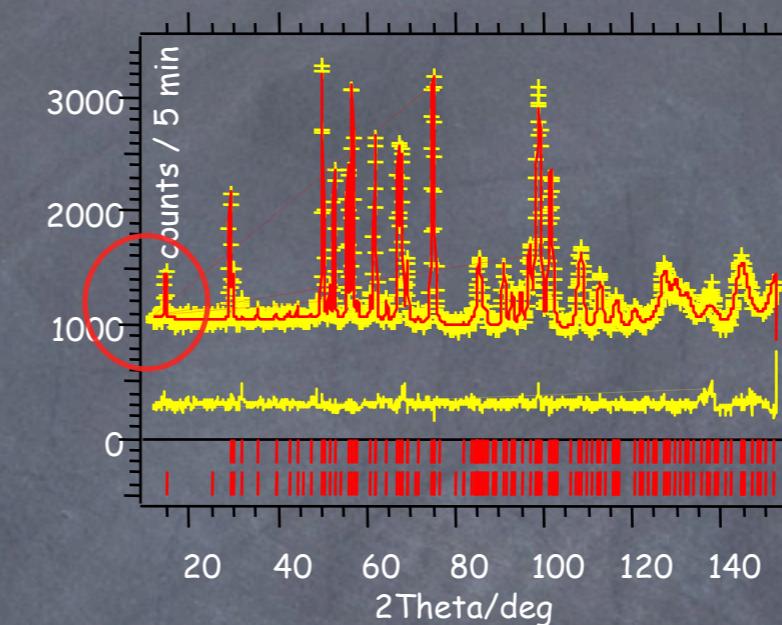
Alternatively if the Fourier transform of the scattering length density is  $F(q)$

$$S(q) = F(q)F^*(q)$$

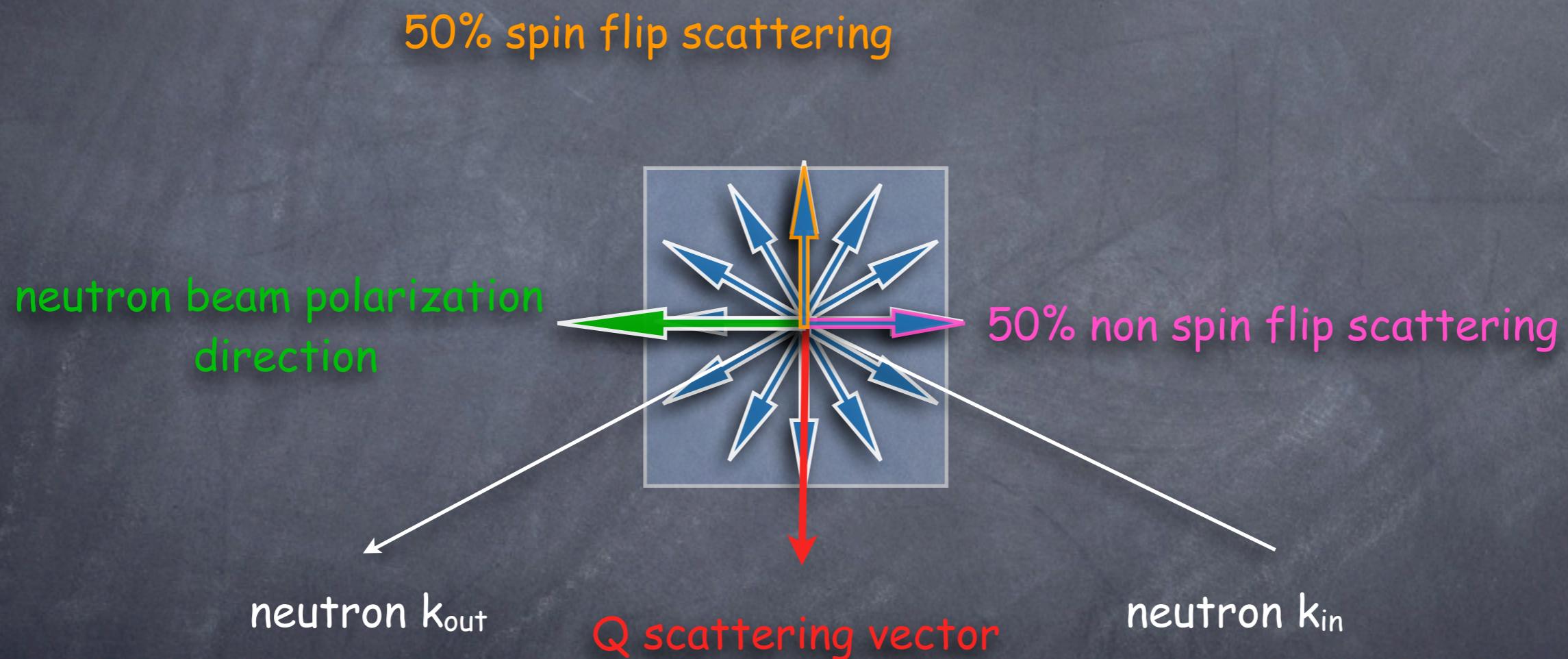
If  $F(q) = F_N(q) + F_M(q)$  in the most generic case there will be four terms:

- nuclear
- magnetic
- nuclear magnetic interference
- chiral

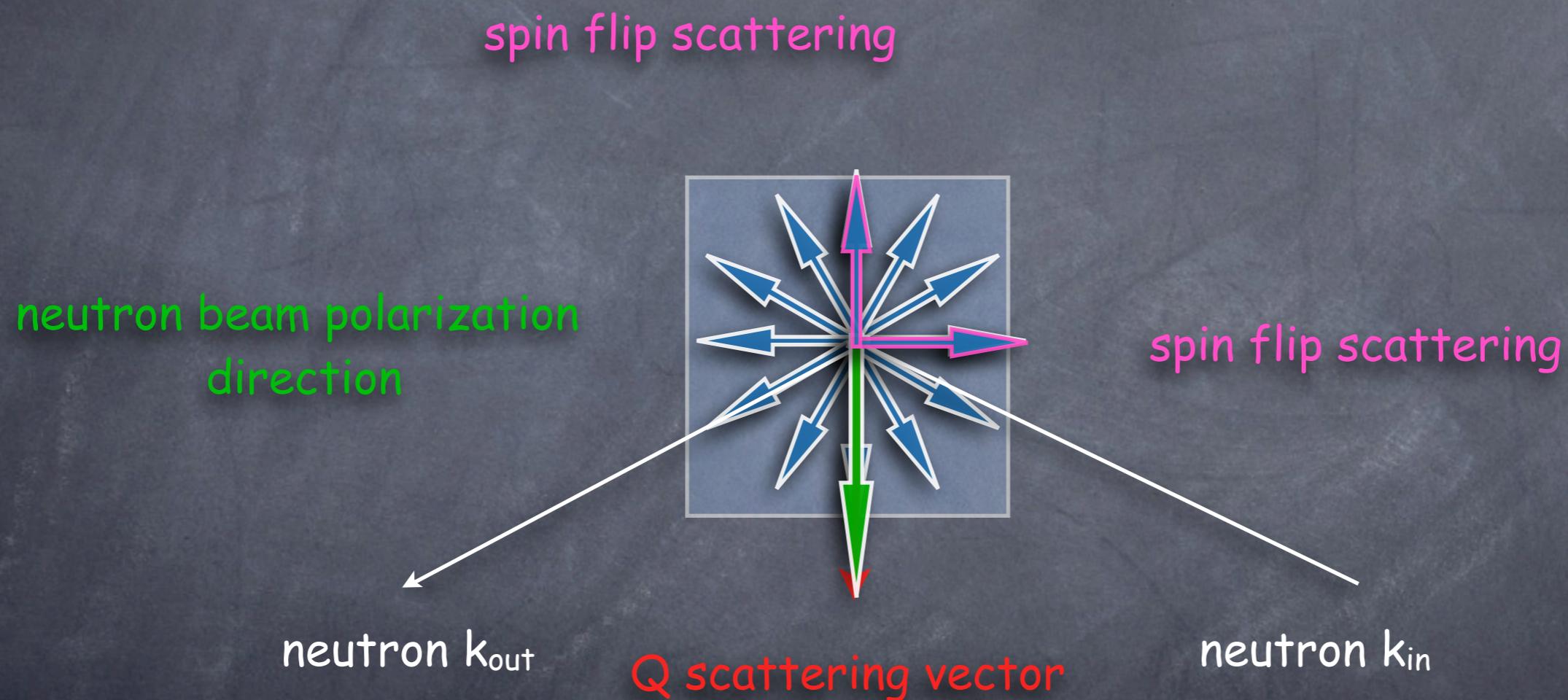
- Unpolarized neutrons
- comparable intensity to nuclear
- identified by a priori knowledge
- temperature dependence



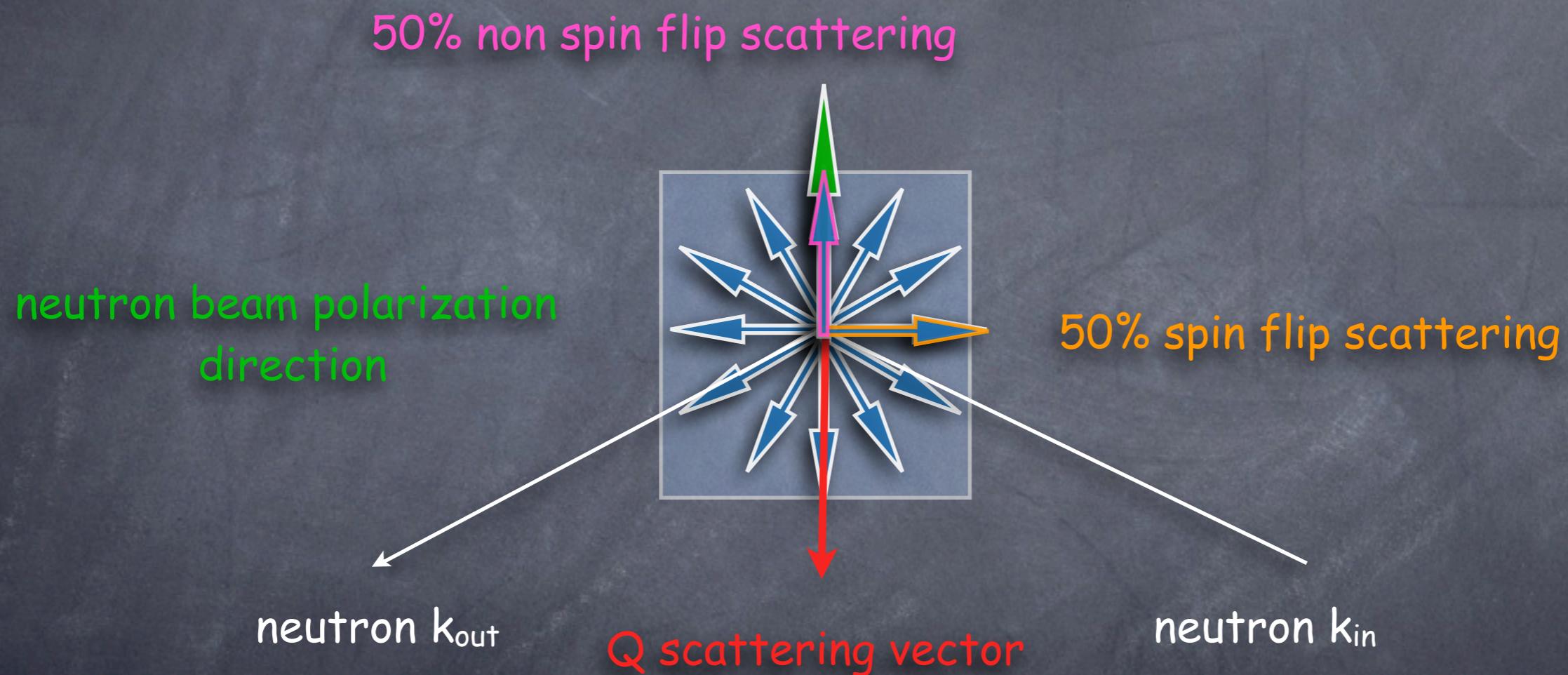
# Polarized Neutrons



# Polarized Neutrons



# Polarized Neutrons



# Polarized Neutrons



# Polarized Neutrons

$$UP_X = N + \frac{1}{2}M + \frac{1}{3}I$$

$$DOWN_X = \frac{1}{2}M + \frac{2}{3}I$$

$$UP_Z = N + \frac{1}{2}M + \frac{1}{3}I$$

$$DOWN_Z = \frac{1}{2}M + \frac{2}{3}I$$

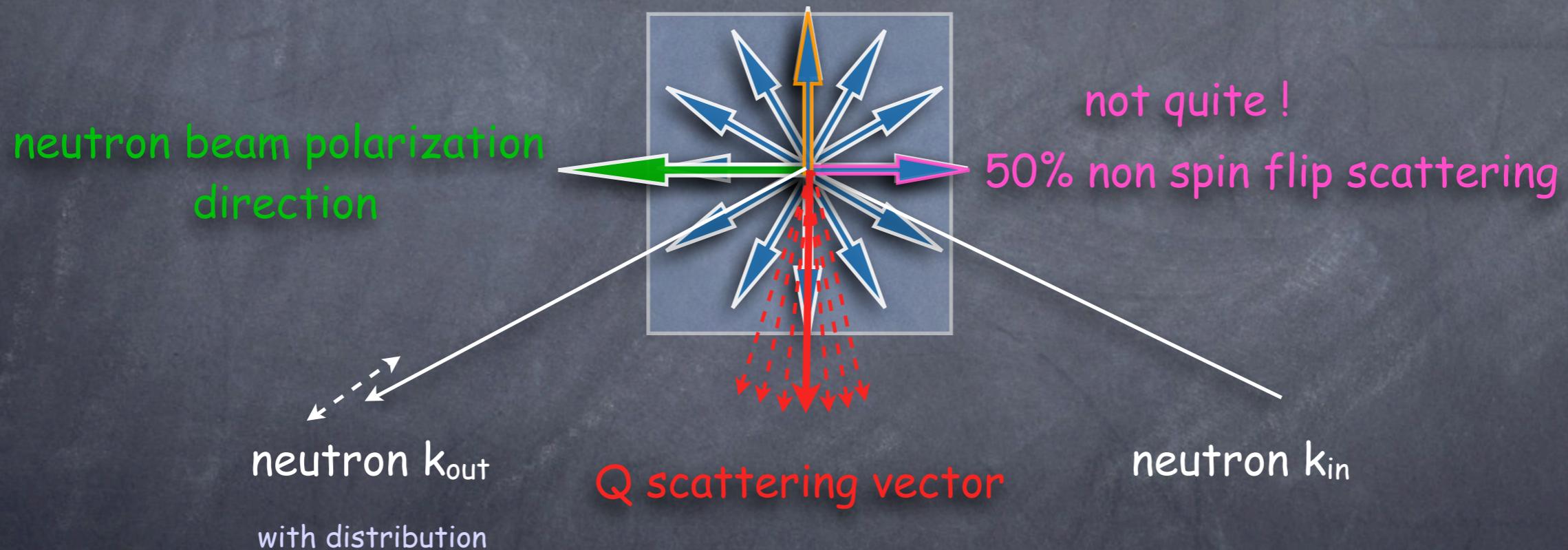
$$UP_Y = N + \frac{1}{3}I$$

N the nuclear scattering  
M the magnetic scattering  
I the incoherent scattering

$$DOWN_Y = M + \frac{2}{3}I$$

When the scattering is non negligibly quasielastic

50% spin flip scattering



# Polarized Neutrons

$$UP_X = N \frac{1+fg}{2} + \frac{1}{2}M - \frac{gf}{2}M \sin^2 \epsilon + \frac{3-gf}{6}I$$

$$DOWN_X = N \frac{1-g}{2} + \frac{1}{2}M + \frac{g}{2}M \sin^2 \epsilon + \frac{3+g}{6}I$$

$$UP_Z = N \frac{1+fg}{2} + \frac{1}{2}M + \frac{3-gf}{6}I$$

$$DOWN_Z = N \frac{1-g}{2} + \frac{1}{2}M + \frac{3+g}{6}I$$

$$UP_Y = N \frac{1+fg}{2} + \frac{1-gf}{2}M + \frac{gf}{2}M \sin^2 \epsilon + \frac{3-gf}{6}I$$

$$DOWN_Y = N \frac{1-g}{2} + \frac{1+g}{2}M - \frac{g}{2}M \sin^2 \epsilon + \frac{3+g}{6}I$$

g is the polarizing efficiency  
f the flipper efficiency  
N the nuclear scattering  
M the magnetic scattering  
I the incoherent scattering  
 $\epsilon$  is the angle of Q to  $Q_{\text{elastic}}$

## Spin manipulation

Quantum mechanical description of the neutron spin state:

$|\chi\rangle = a|+\rangle + b|-\rangle$  where  $a$  and  $b$  can be complex and  $\sqrt{a^2 + b^2} = 1$

and conveniently  $|\chi\rangle = e^{-i\varphi/2} \cos \frac{\theta}{2} |+\rangle + e^{i\varphi/2} \sin \frac{\theta}{2} |-\rangle$

this leads to  $\langle \hat{\sigma}_x \rangle = \sin \theta \cos \varphi$ ,  $\langle \hat{\sigma}_y \rangle = \sin \theta \sin \varphi$ ,  $\langle \hat{\sigma}_z \rangle = \cos \theta$

Time evolution of the neutron spin in magnetic field

$$\frac{\partial \hat{\sigma}}{\partial t} = \frac{1}{\hbar} [\hat{\sigma}, H_s] = -\frac{\gamma}{2} [\hat{\sigma}, (\hat{\sigma} \vec{H})] = \dots = -\gamma (\vec{H} \times \hat{\sigma})$$

The Polarization of the beam  $P = \langle \sigma \rangle$  behaves as a "classical" Larmor precession

$\gamma_L = 2957 \text{ Hz/Gauss}$

$$\frac{\Delta\phi}{\Delta x} [\text{deg/cm}] = 2.65 \lambda [\text{\AA}] H [\text{Gauss}]$$

What happens if the direction of the magnetic field changes in space?

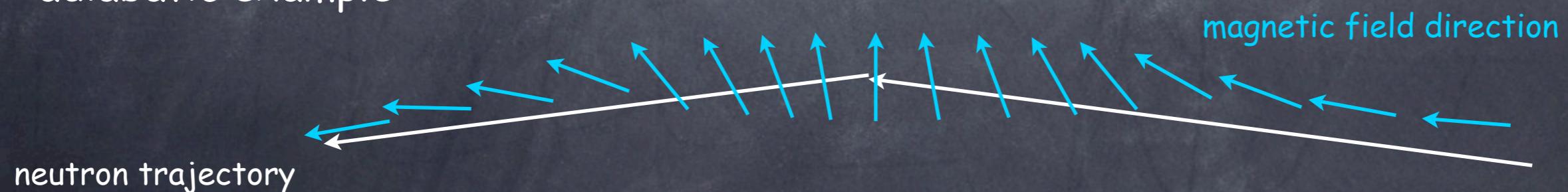
The moving neutron will see a B field which changes its direction in time

Two limiting cases

if  $\omega_B \ll \omega_L$  it will follow adiabatically

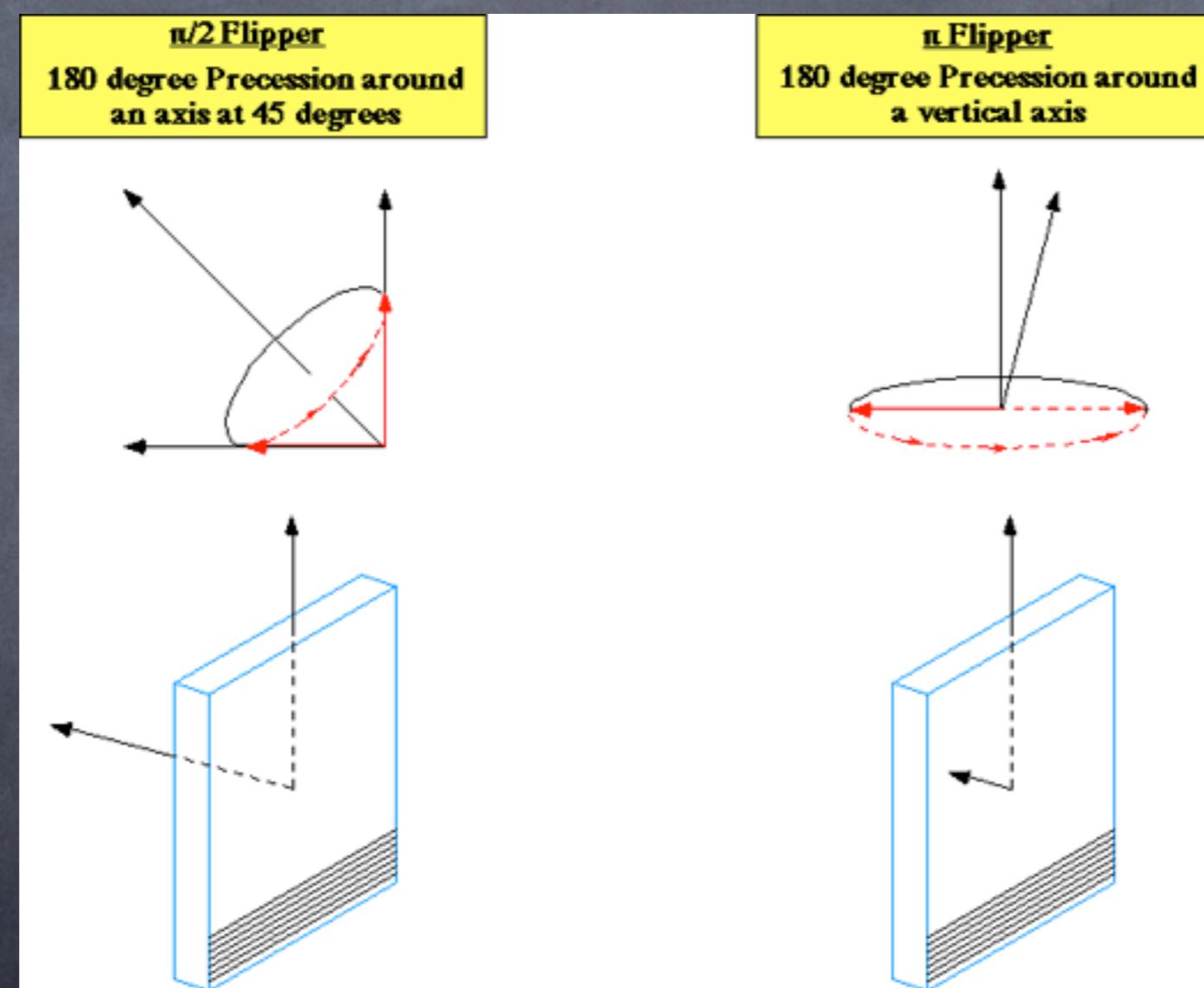
if  $\omega_B \gg \omega_L$  it will start to precess around the new field direction

adiabatic example:

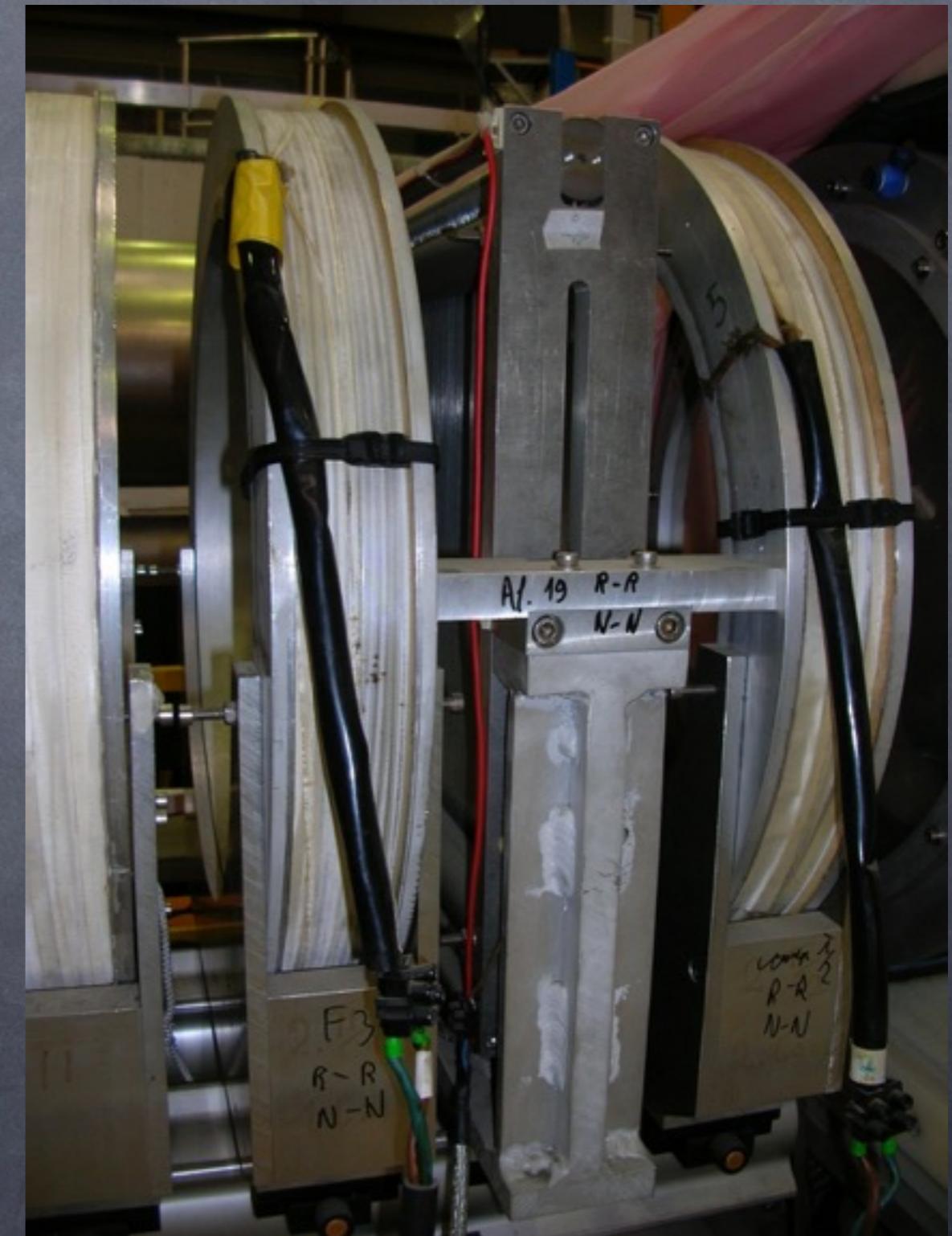
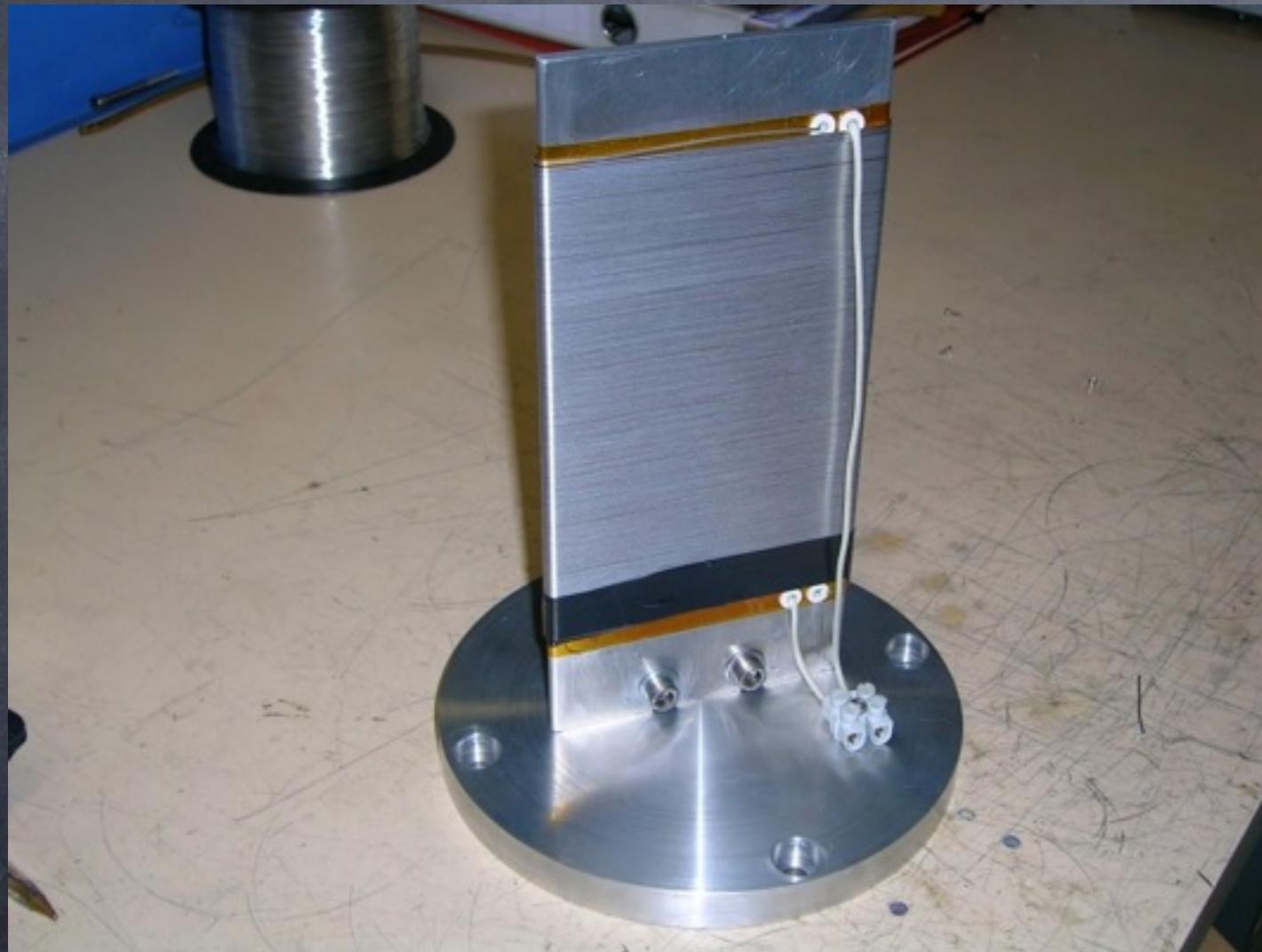


# Polarized Neutrons

Non adiabatic example : Mezei flipper

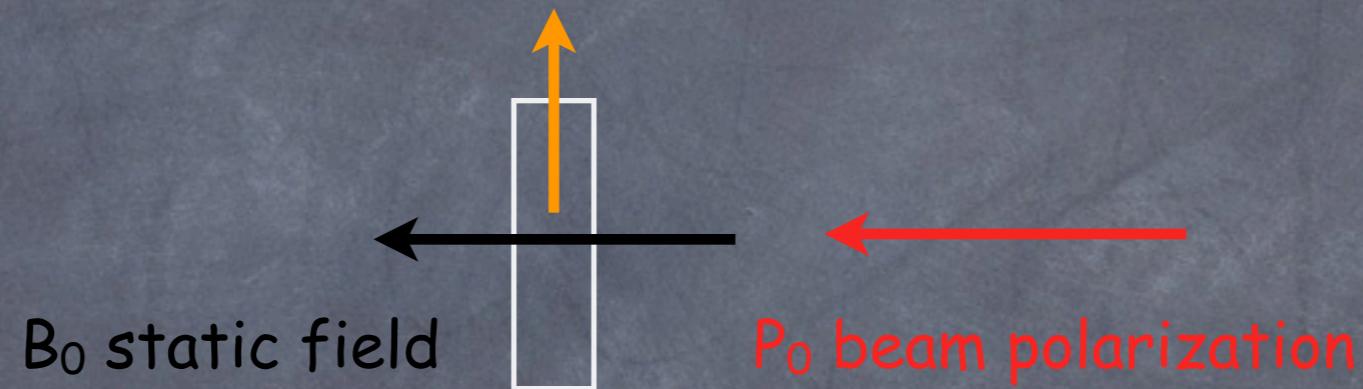


# Polarized Neutrons



RF flipper

$B_{rf}$  oscillating  $\omega_{RF}$  radiofrequency field

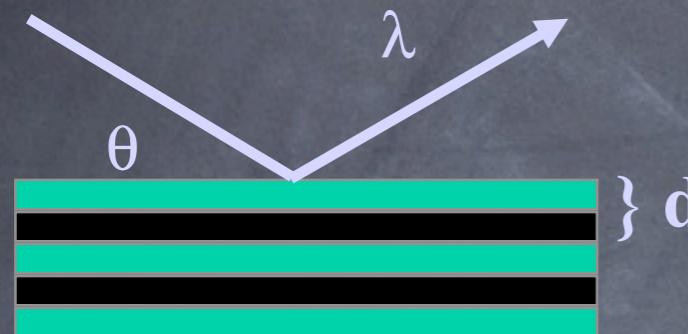


Makes up a  $\pi$  flipper

- if  $B_0 \gamma_L = \omega_{RF}$
- and  $B_{RF}$  is just enough for a  $\pi$  turn during the flight time

Haussler Xtal  $\text{Cu}_2\text{MnAl}$  (111):

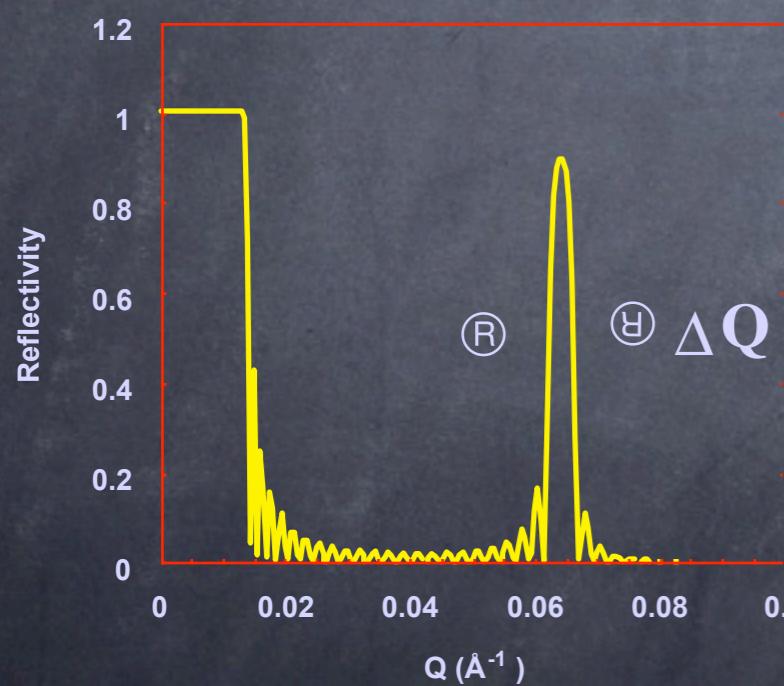
- $F_M(q) = F_N(q)$  for one of the Bragg reflections
- easy to saturate
- grow single crystal
- controlled mosaicity
- low  $\lambda/2$  contamination (or filter)



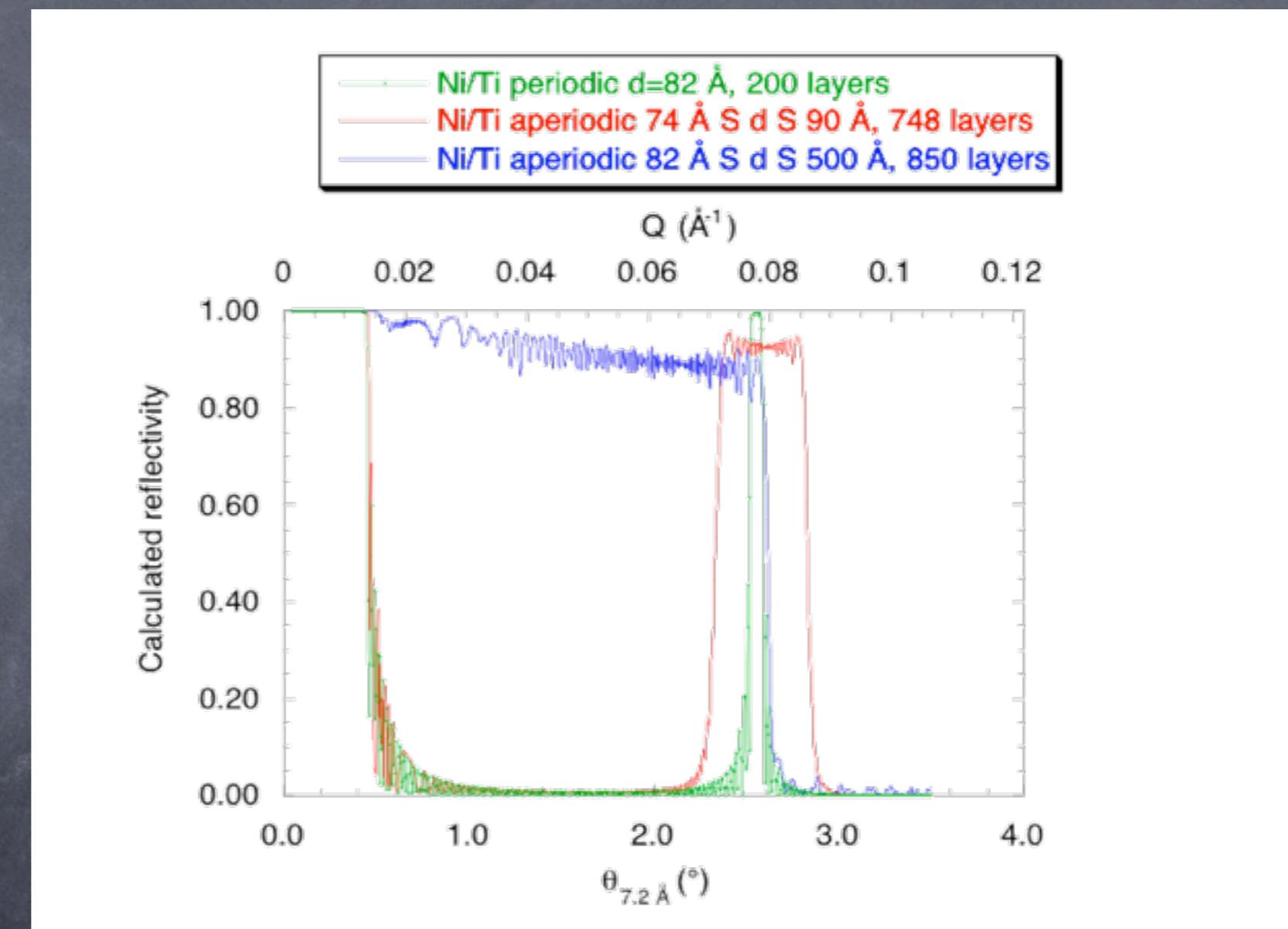
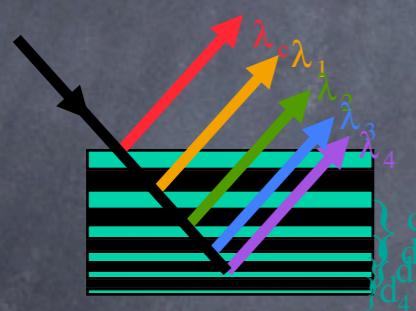
$$R = \frac{4N^2 d^4 (f_1 - f_2)^2}{\pi^2 n^4}$$

$$\frac{\Delta \lambda}{\lambda} = \frac{2d^2 (f_1 - f_2)}{\pi}$$

$$\theta \sim \frac{\lambda}{2d}$$

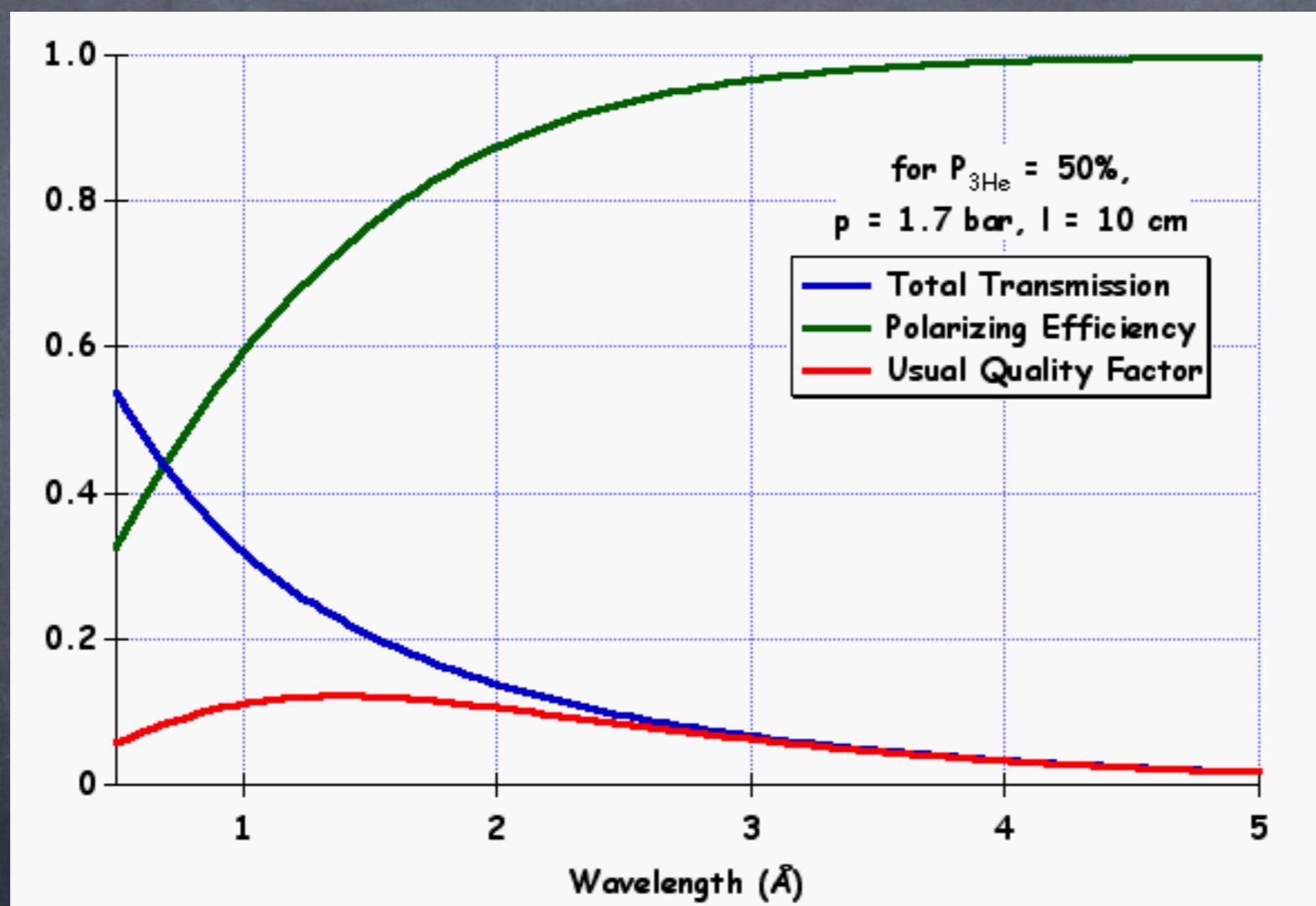


# Polarized Neutrons



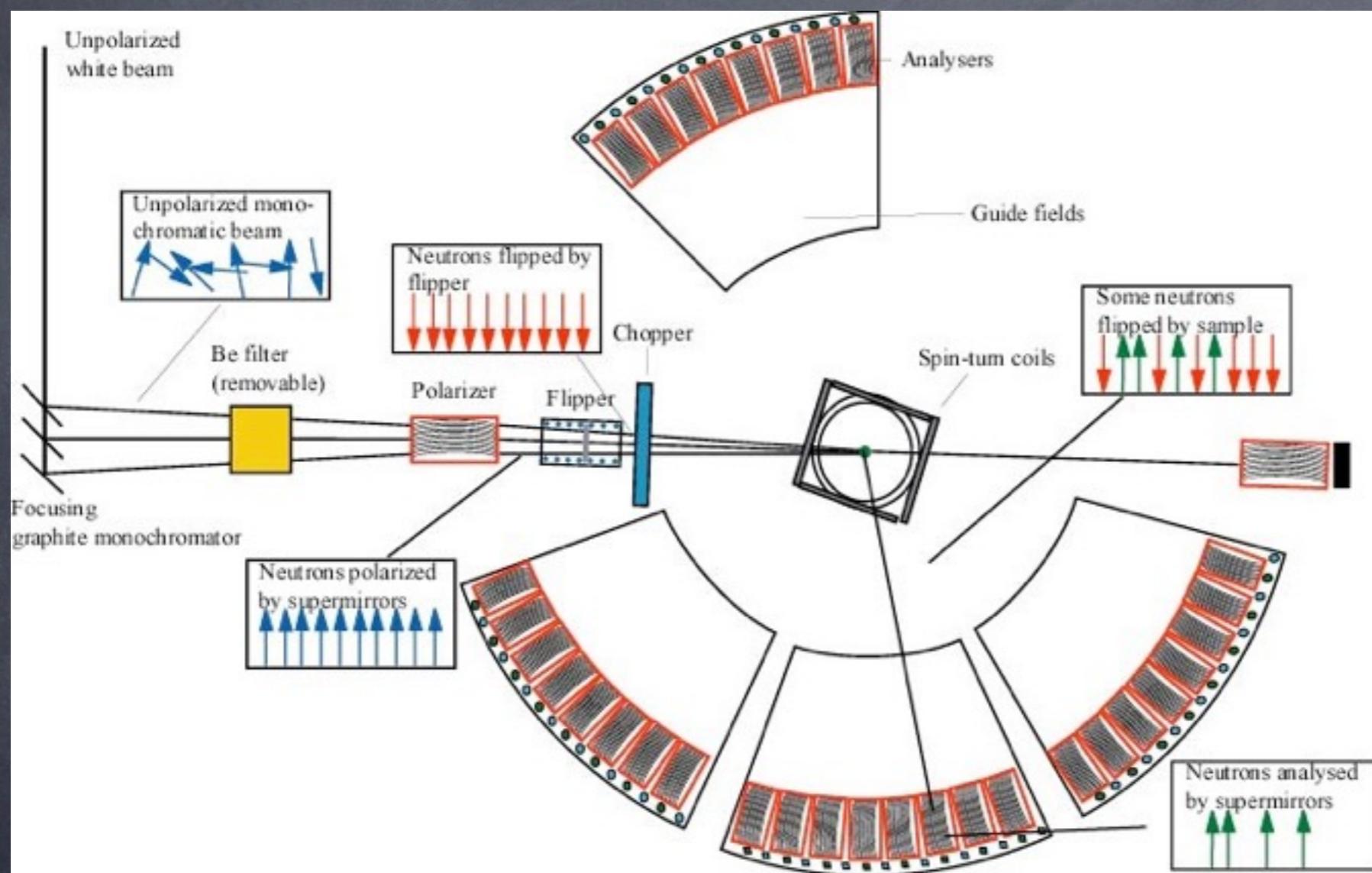
# Polarized Neutrons

$\text{He}^3$  absorbs only neutrons with spin antiparallel to the nuclear spin



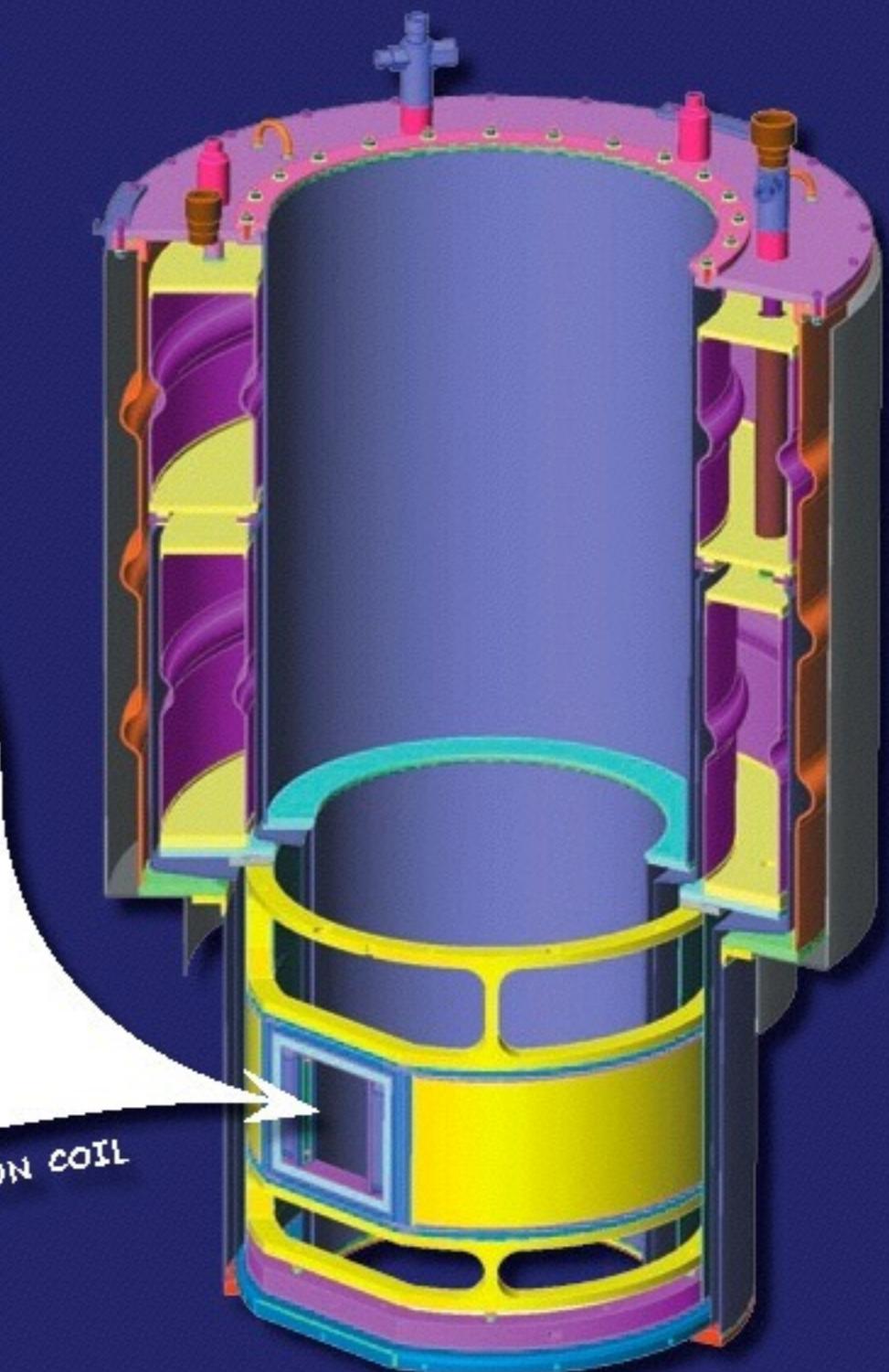
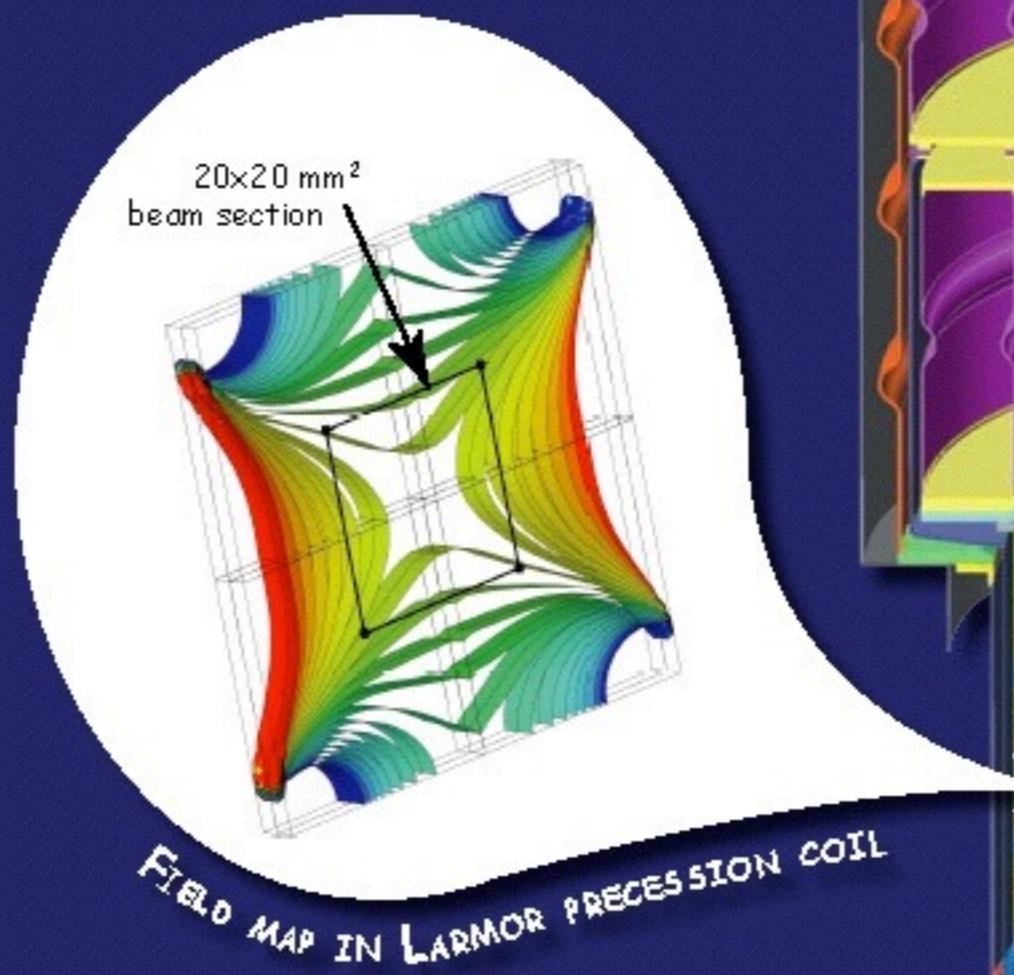
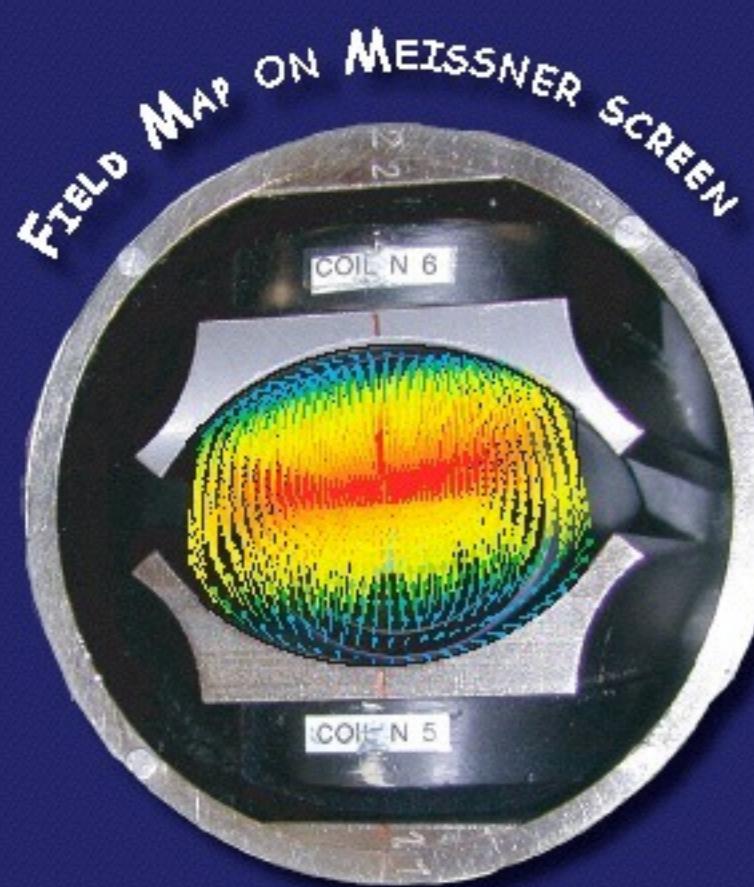
## Instruments

# Polarized Neutrons



# Polarized Neutrons

A 3<sup>rd</sup> generation Cryopad has recently been designed to carry out elastic and inelastic scattering experiments with 0.5 deg precision.



Echo condition:

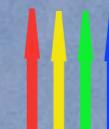
$$\int_{\pi/2}^{\pi} B_1 d\ell = \int_{\pi}^{2\pi} B_2 d\ell$$

The measured quantity is:  $S(q,t)/S(q,0)$   
where

$$t \propto \lambda^3 \int B d\ell$$

For elastic scattering:

$$\Phi_{tot} = \frac{\gamma B_1 l_1}{v_1} - \frac{\gamma B_2 l_2}{v_2} = 0$$



For omega energy exchange:

$$\Phi_{tot} = \frac{\hbar \gamma B l}{mv^3} \omega + o\left(\left(\frac{\omega}{1/2mv^2}\right)^2\right)$$



The probability of omega energy exchange:

$$S(q, \omega)$$

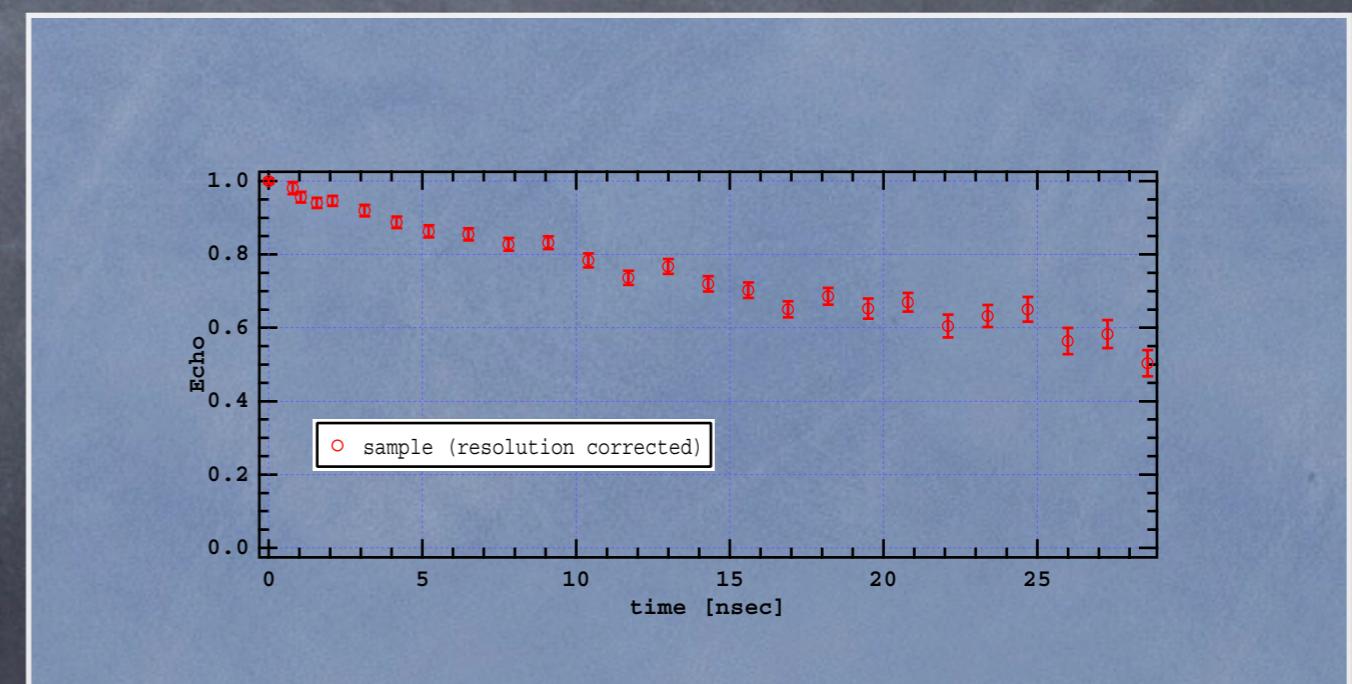
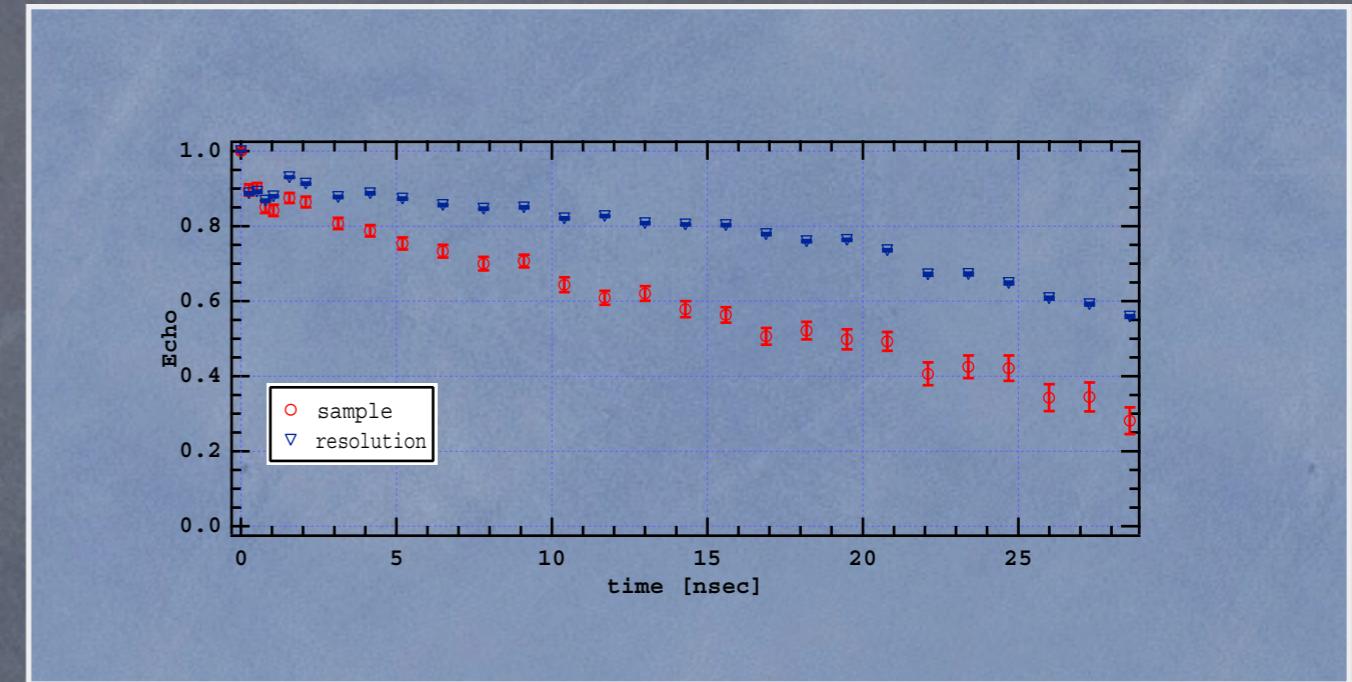
The final polarization:  $\langle \cos \varphi \rangle = \frac{\int \cos\left(\frac{\hbar \gamma B l}{mv^3} \omega\right) S(q, \omega) d\omega}{\int S(q, \omega) d\omega} = S(q, t)$

# Polarized Neutrons

As measures the fourier transforme

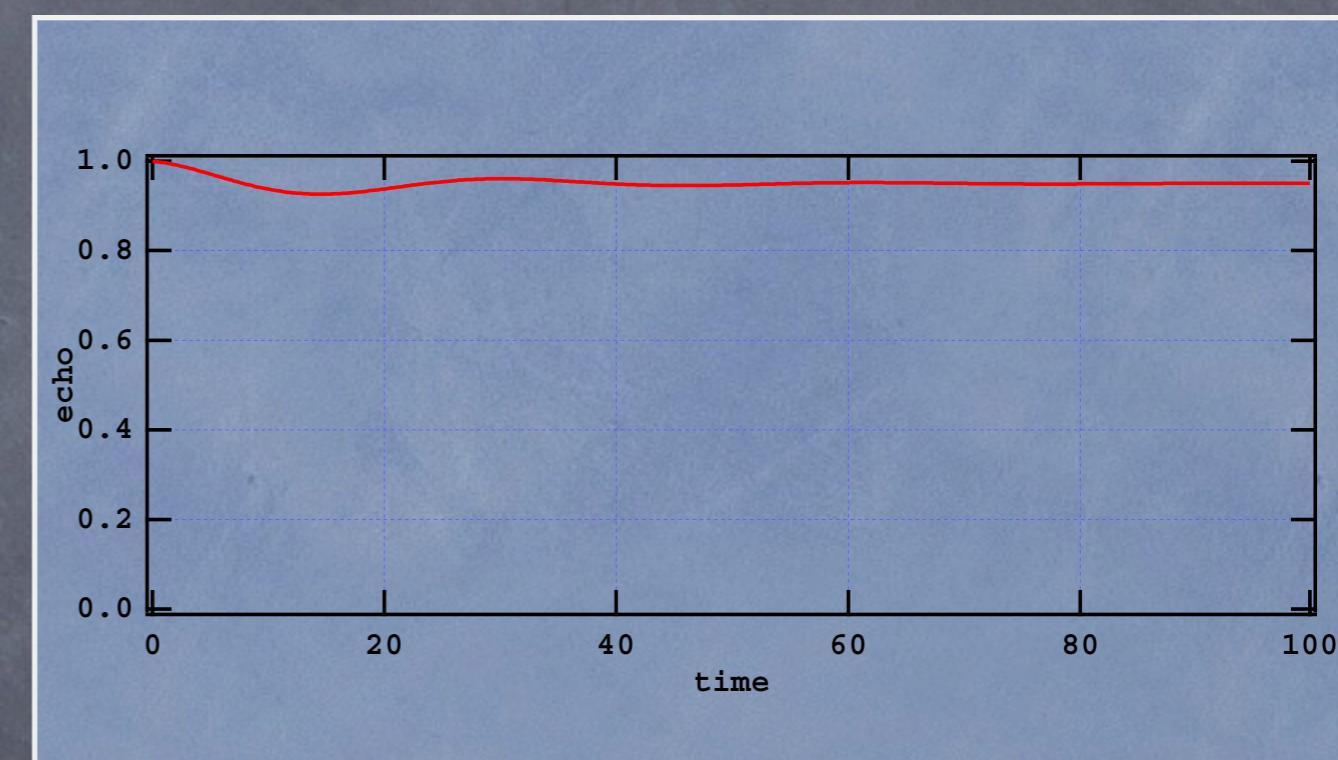
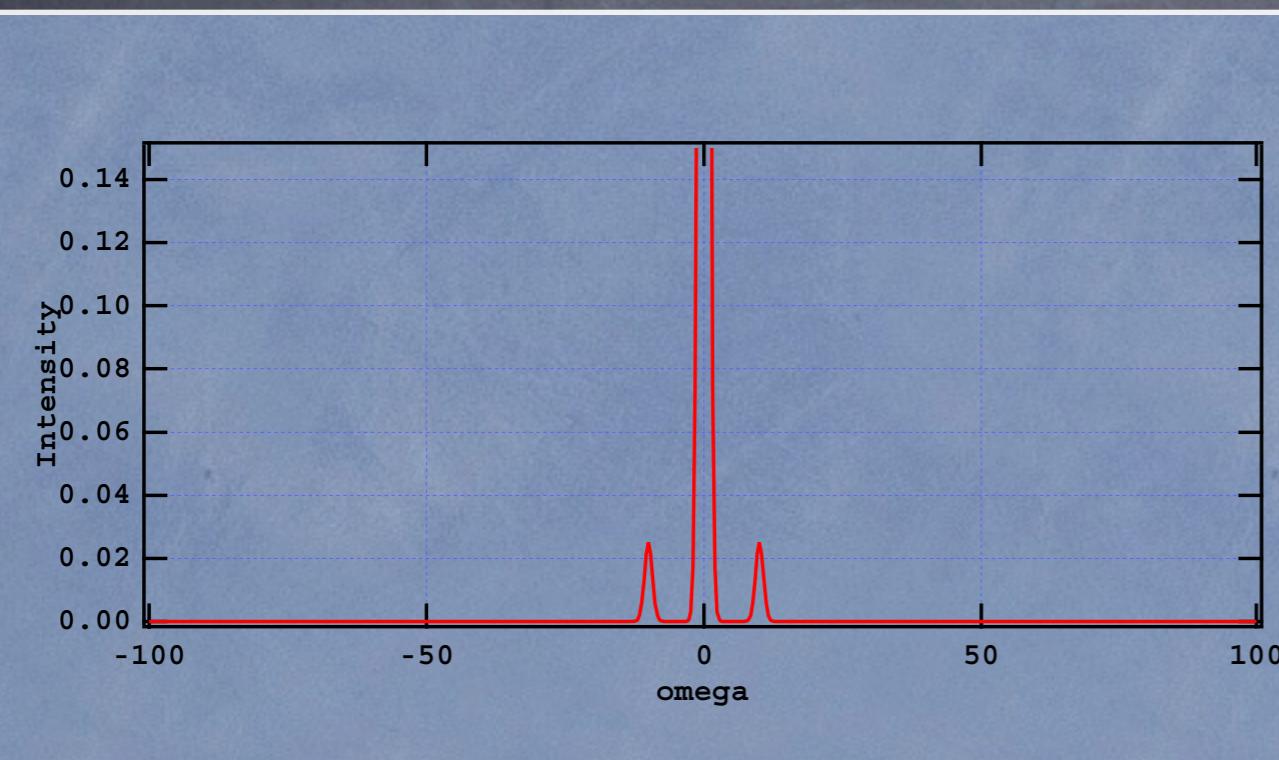
$$S(q,t)$$

the instrumental resolution is a simple division instead of deconvolution



# Polarized Neutrons

Say you have a weak but well defined excitation



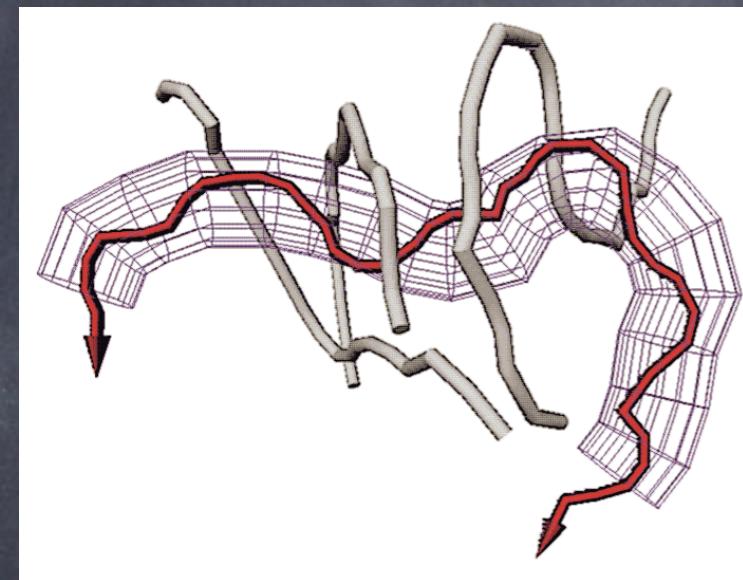
$$S(q, \omega) = 0.95 \cdot \delta(\omega) + 0.025 \cdot (\delta(\omega - \omega_0) + \delta(\omega + \omega_0))$$

$$S(q, t) = 0.95 + 0.05 \cdot \cos(\omega_0 t)$$

Bad signal to noise,  $\Delta\lambda/\lambda \Rightarrow$  no good for Spin Echo

# Polarized Neutrons

Reptation

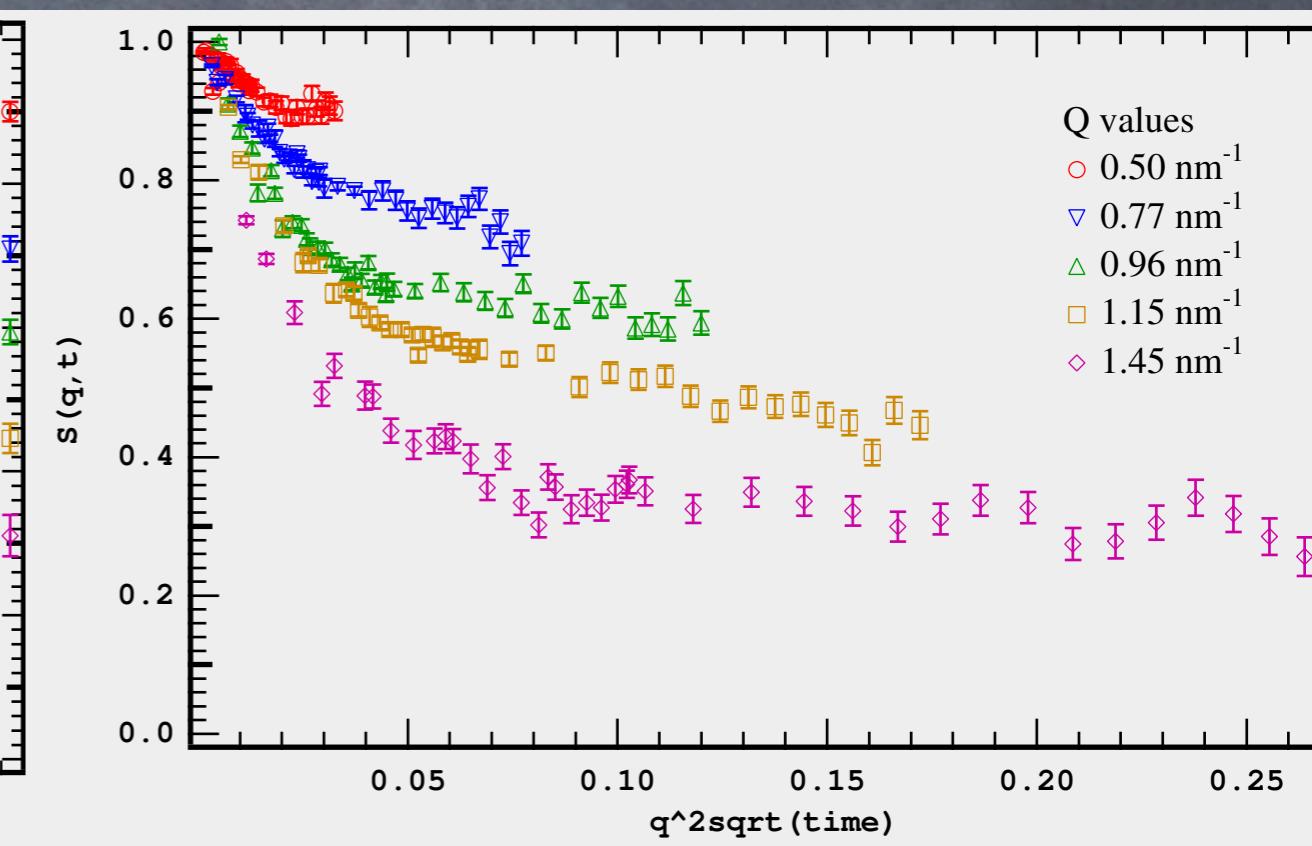
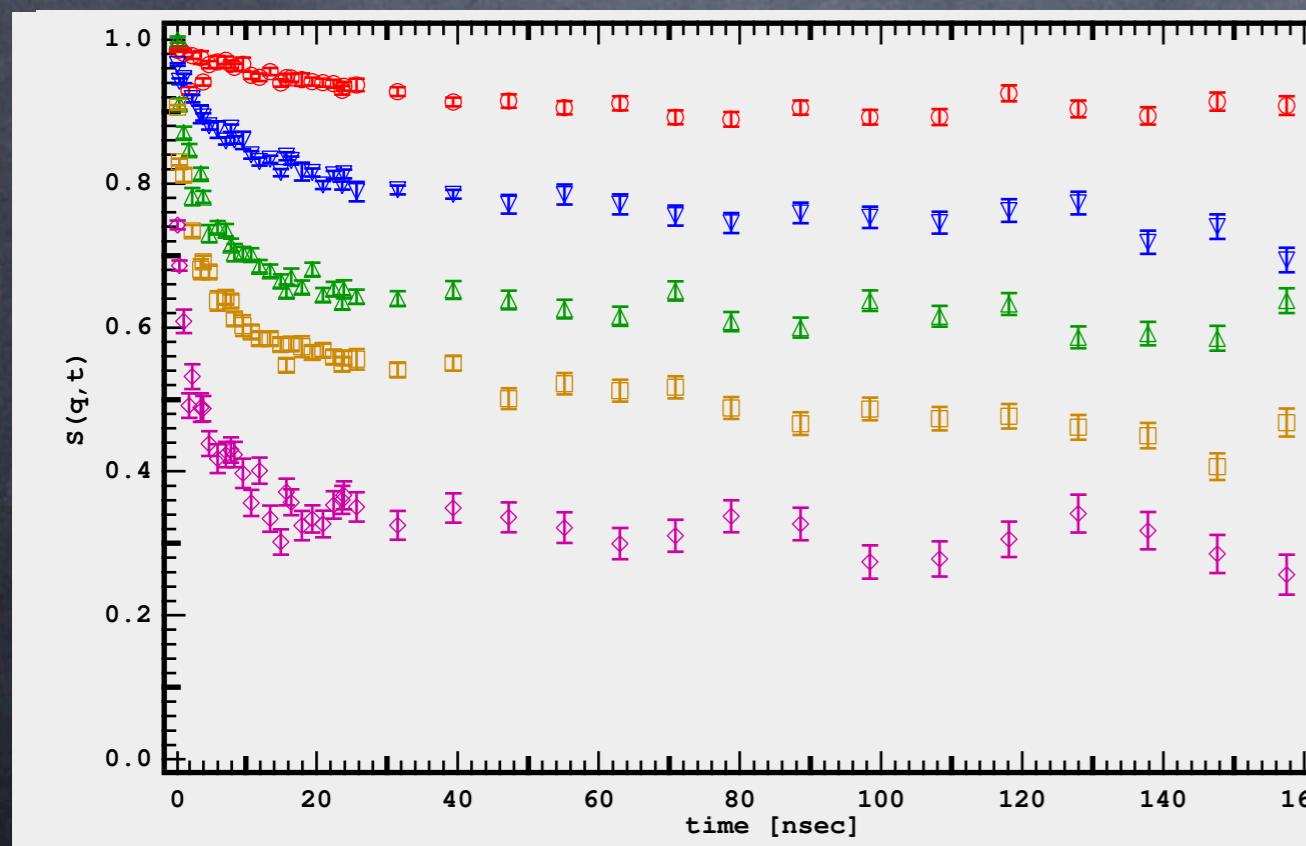


10% marked polymer chain(H) in deuterated matrix of the same polymer melt

at short time => Rouse dynamics  $1/\tau \sim q^4$

at longer times starts to feel the "tube" formed by the other chains (deGennes)

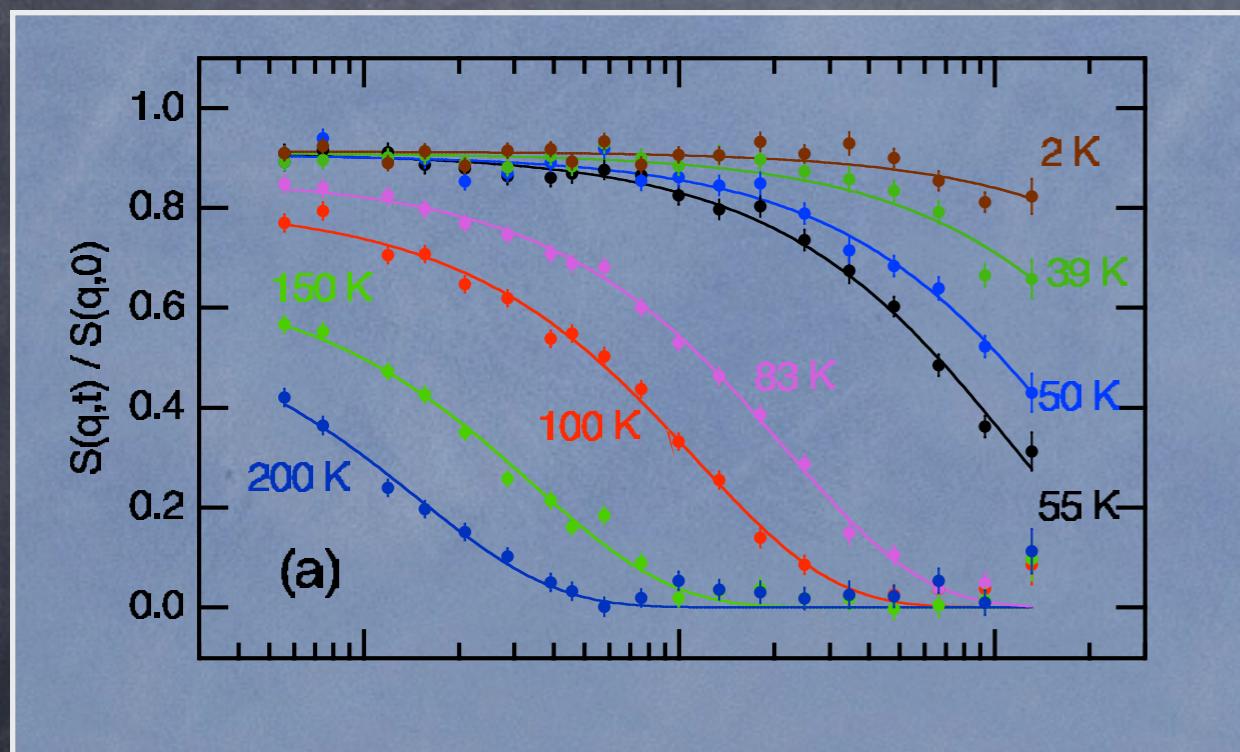
D. Richter, B. Ewen, B. Farago, et al., Physical Review Letters **62**, 2140 (1989).



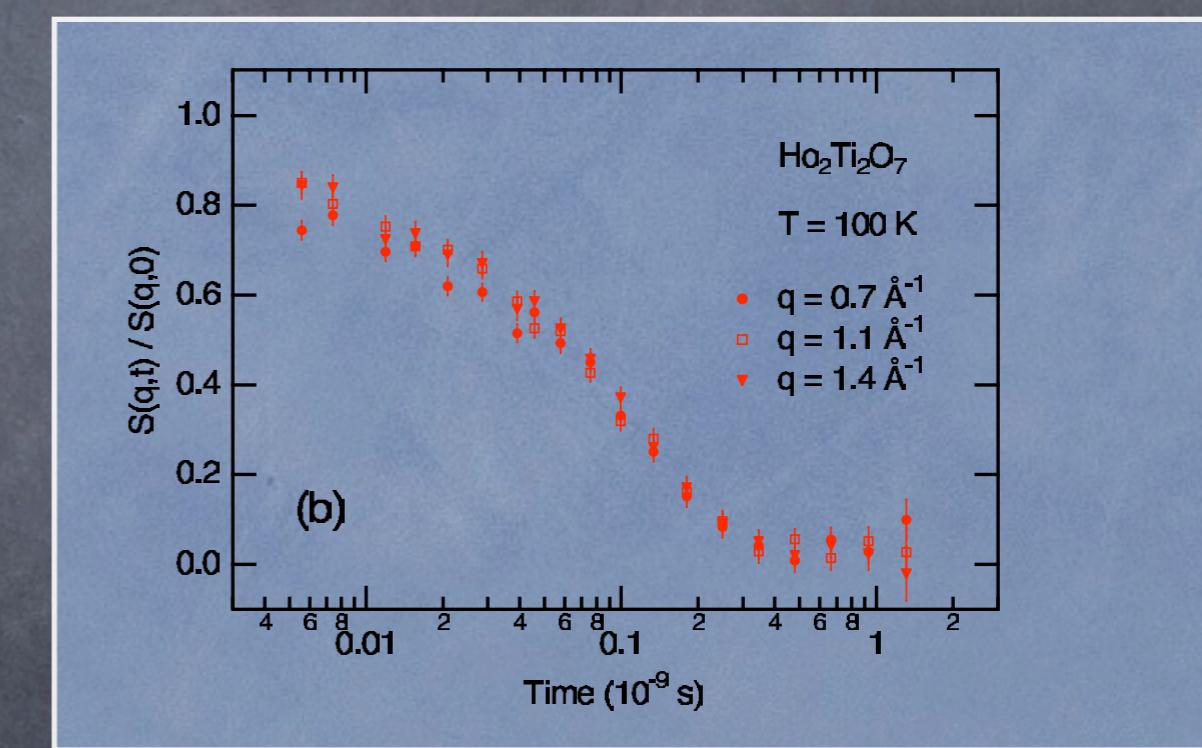
'spin ice' materials  $\text{Ho}_2\text{Ti}_2\text{O}_7$ ,  $\text{Dy}_2\text{Ti}_2\text{O}_7$  and  $\text{Ho}_2\text{Sn}_2\text{O}_7$   
 the spin is equivalent to the H displacement vector in water ice

Paramagnetic echo => Only magnetic scattering gives echo !

Single exponential thermally activated



$Q$  independent relaxation



G. Ehlers , Cornelius , A L, Orendac , M, Kajnakova , M, Fennell , T, Bramwell , S  
 T, Gardner , Journal of Physics Condensed Matter 15, L9 (2003).

# Polarized Neutrons

It's over folks !  
thanks...