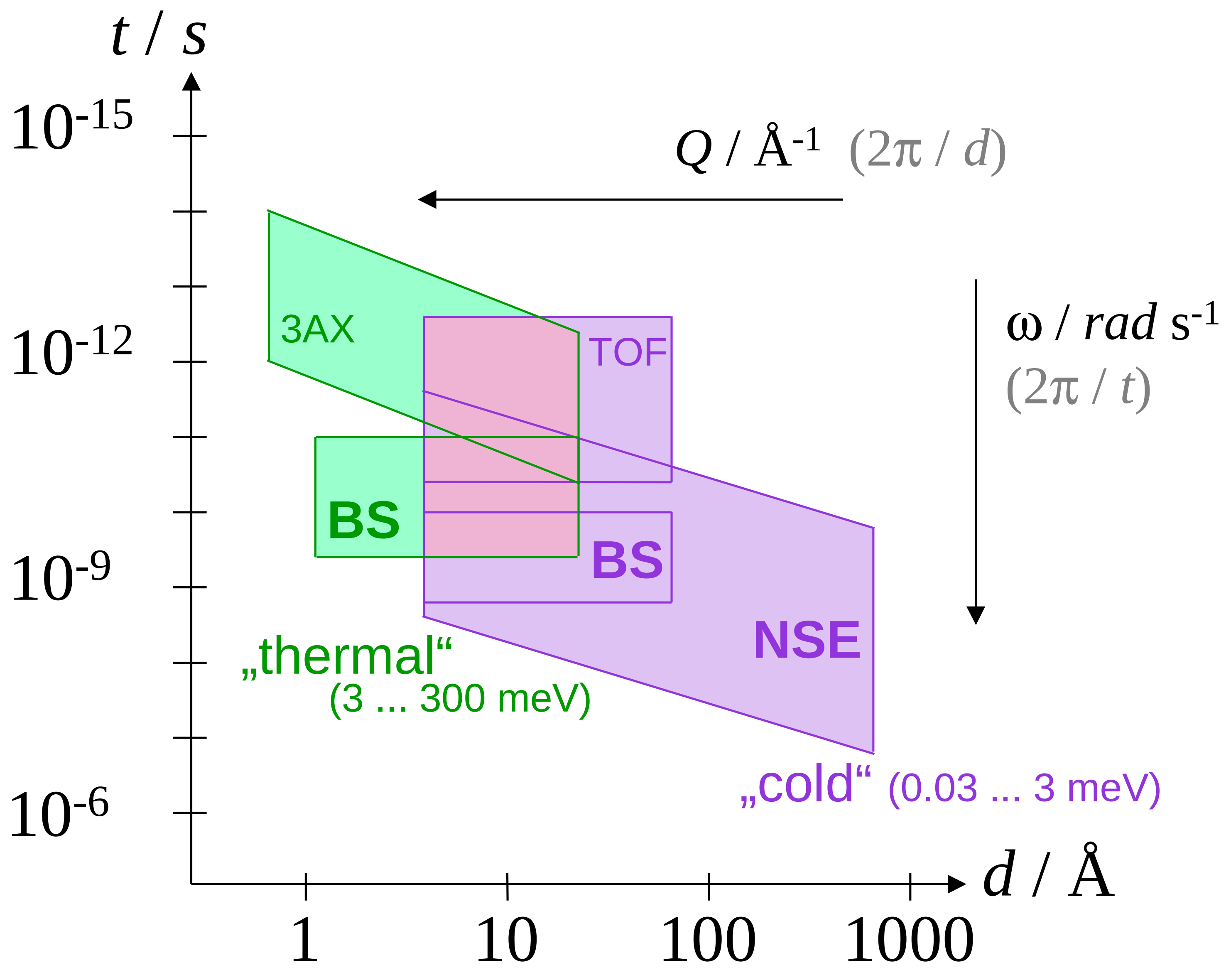
High Resolution Neutron Scattering Spectroscopy

Trieste, June 27 2002

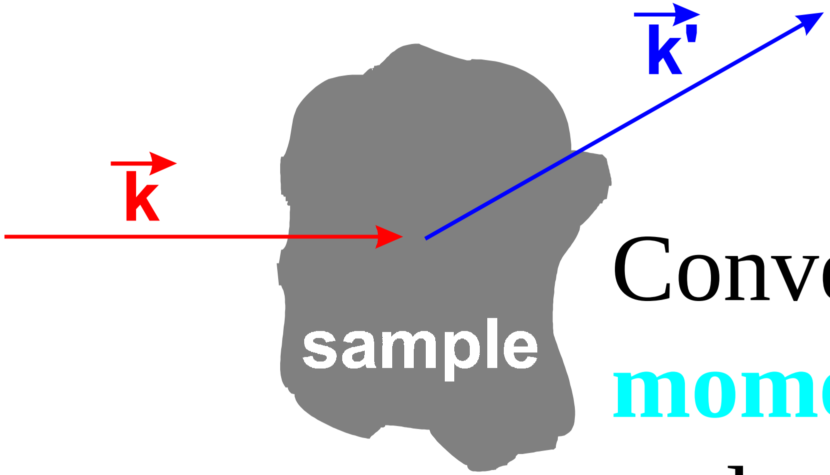
Stefan Kahle, Forschungszentrum Jülich, Germany

- Overview
- Principle of Inelastic Neutron Scattering
- Neutron Backscattering Spectroscopy
- Neutron Spin Echo Spectroscopy
- Resumé

The Inelastic Neutron Scattering Window



Principle of Inelastic Neutron Scattering



Conversion from $\vec{k}$, $\vec{k}'$ to
momentum: $\vec{Q} = \hbar\,(\vec{k} - \vec{k}')/m$
and **energy**: $\hbar\omega = \hbar^2\,(\vec{k}^2 - \vec{k}'^2)/2m$
transfer

The Experiment:

a) choose $\{\vec{k}, \vec{k}'\}$

b) record scattering probability or neutron counts ($I \sim S(\vec{Q},E)$)

Questions

- What is the relation between counts I and $S(\vec{Q},E)$?
- How does one select the average values of $\langle\vec{k}\rangle$ and $\langle\vec{k}'\rangle$, respectively ?
- How does one optimize the shape of their variances $\delta\vec{k}$ and $\delta\vec{k}'$?

Relation Between Neutron Counts I and S(Q,E)

$$I = A(\vec{k}) \cdot V(\vec{k}) \cdot t_{eff} N \cdot S(Q,E) \cdot V'(\vec{k}')$$

$$= \begin{pmatrix} flux \\ source \end{pmatrix} \cdot \begin{pmatrix} sharpness \\ monochromator \end{pmatrix} \cdot \begin{pmatrix} volume \\ sample \end{pmatrix} \cdot \begin{pmatrix} response \\ sample \end{pmatrix} \cdot \begin{pmatrix} sharpness \\ analyzer \end{pmatrix}$$

Make factors *A(k)* and $t_{eff}N$ large

Relax ‘sharpness’ without loosing information on S(Q,E)

How to "Measure" (or Select) the Energy of a Neutron

- Measure the time of flight (**velocity**)

$$E_n = \frac{m_n}{2} v_n^2$$

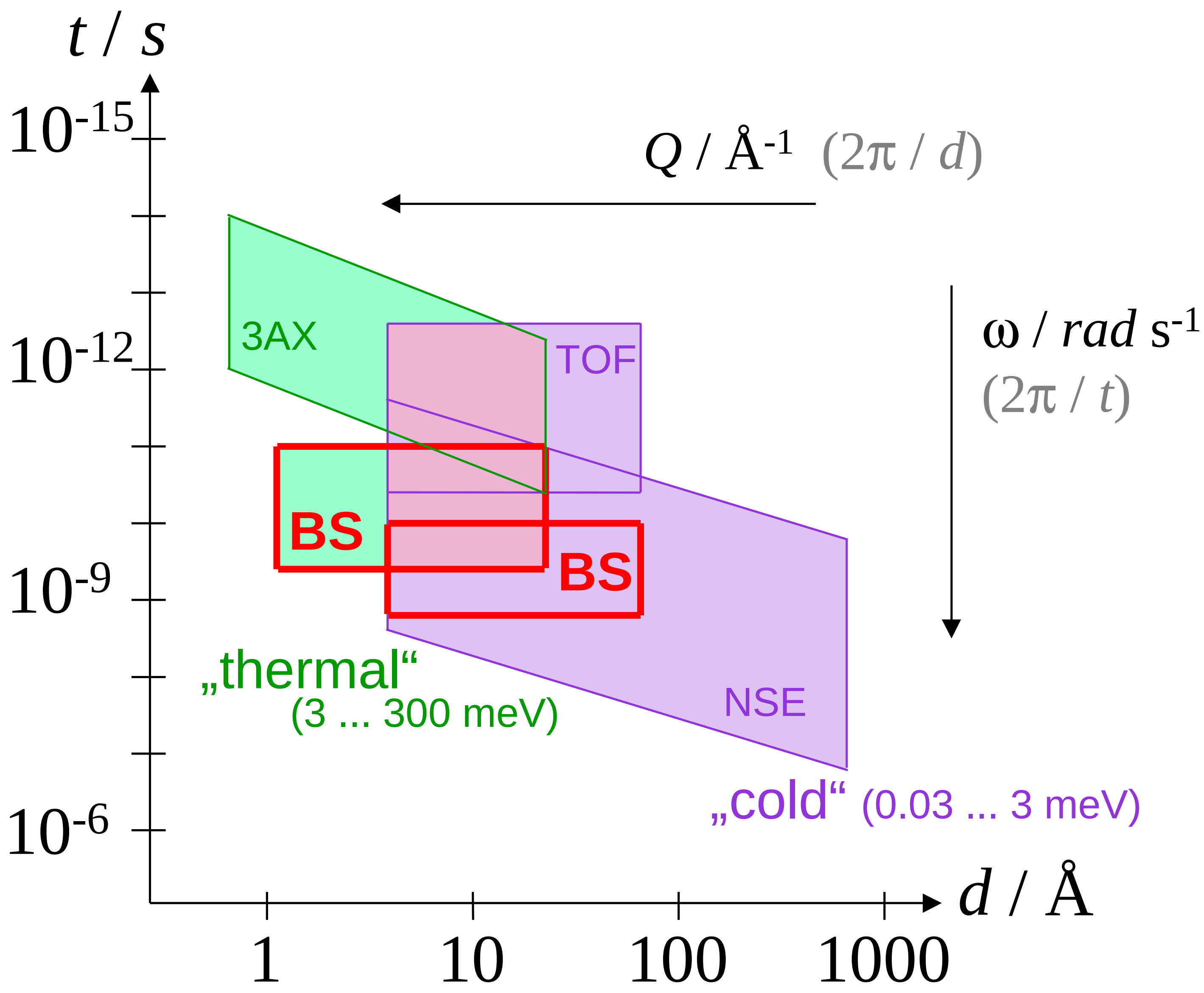
→ Time of Flight Instruments

- Using the Bragg condition (**wavelength**)

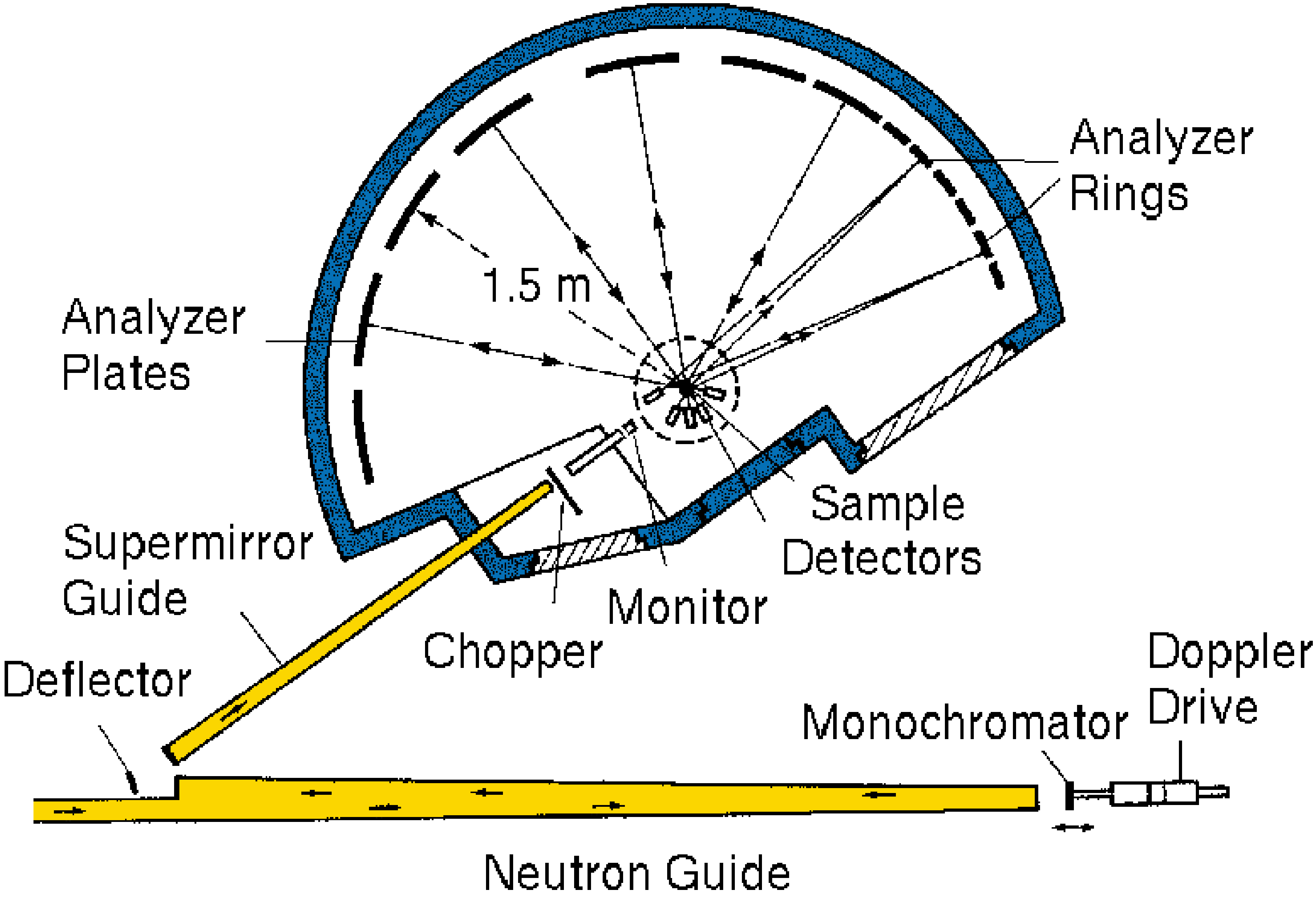
$$E_n = \frac{h^2}{2 m_n \lambda_n^2}$$

→ Crystal Spectrometers

Neutron Backscattering Spectroscopy

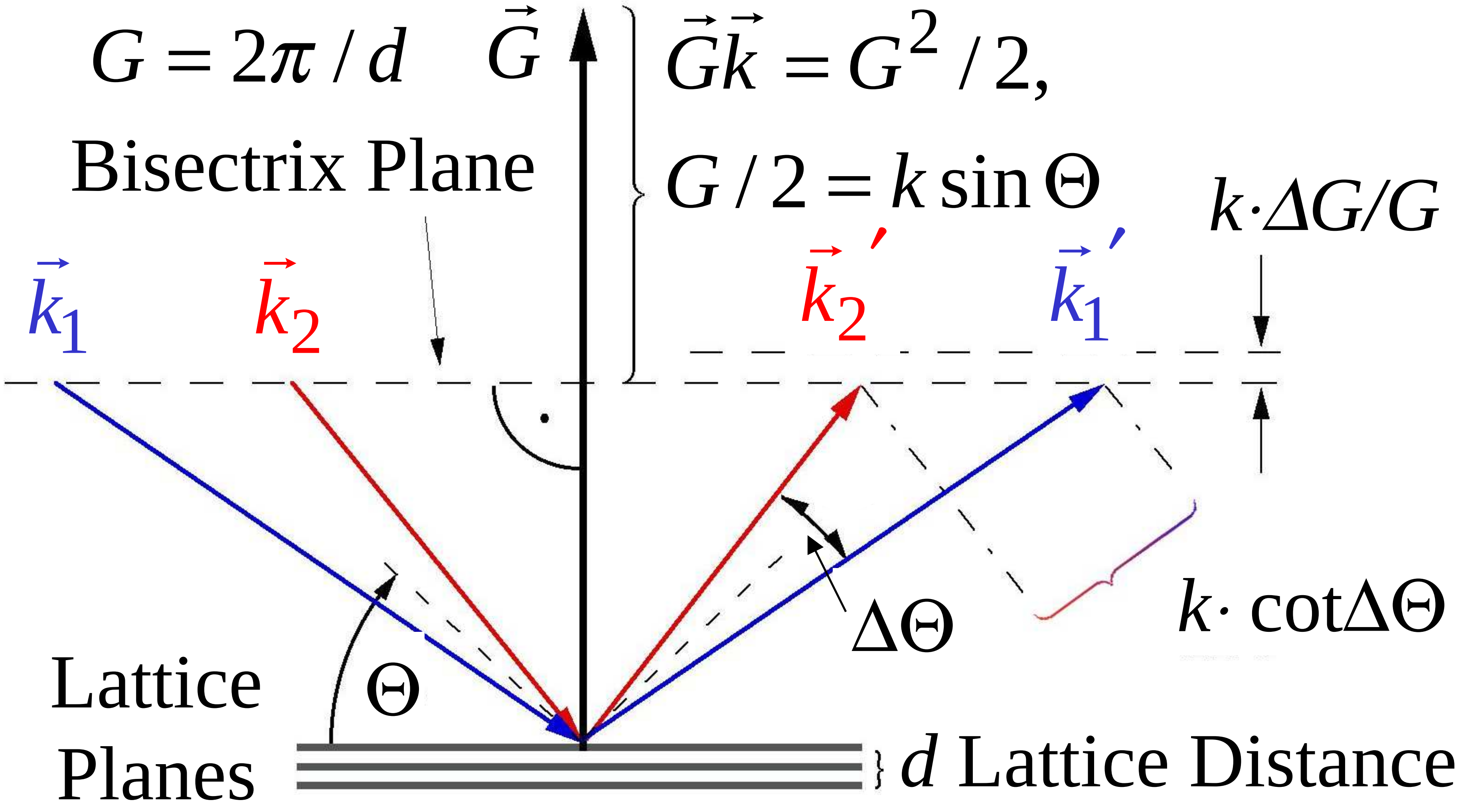


The Backscattering Instrument at FRJ2



Select Neutrons

Using a Perfect Crystal as Monochromator:

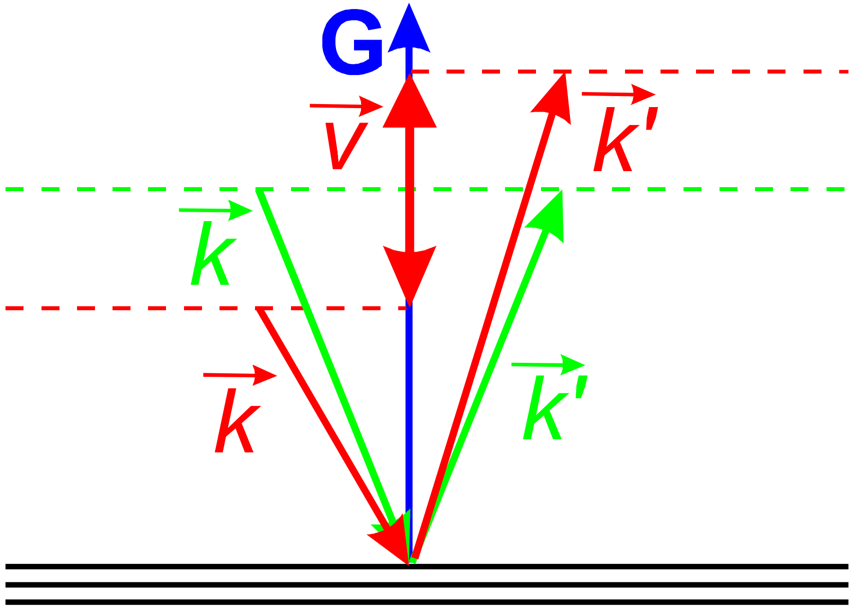


Detune of Neutron Energy; The Doppler Effect

Move Monochromator Crystal:

$$\vec{G} \to \vec{G} + \vec{G}_{\vec{v}}$$

$$\vec{k} \to \vec{k} + \vec{k}_{\vec{v}}$$



Bragg is modified:

$$G^2/2 = \vec{G}(\vec{k} + \vec{k}_{\vec{v}}) \qquad G^2/2 = (\vec{G} + \vec{G}_{\vec{v}})\vec{k}$$

Alternative: Change Lattice Vector

By Heating the Monochromator

$$\vec{G} = \vec{G}(T) \quad \text{1\% in 100K}$$

$$G^2 / 2 = \vec{G}(T)\vec{k}$$

The Analysis of the Neutron Energy

Use Perfect Crystals as Analyzer:

Only the neutrons which fulfill the Bragg condition a second time (at the analyzers) are detected!

Profit: Energy resolution is given by the monochromator and analyzer quality (in order of μeV)

Handicap: About 10^5 n/s at the sample but 0.1..1 n/s in each detector, only

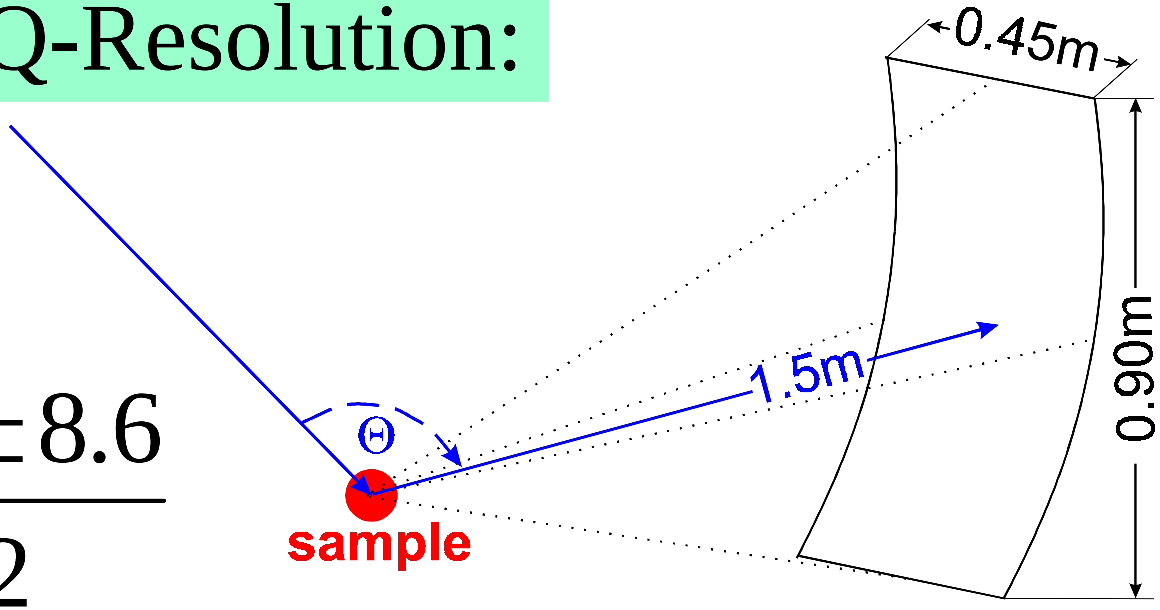
More Intensity: Increase Solid Angle

Decrease of the Q-Resolution:

$$Q = \frac{4\pi}{\lambda} \sin\frac{\Theta}{2}$$

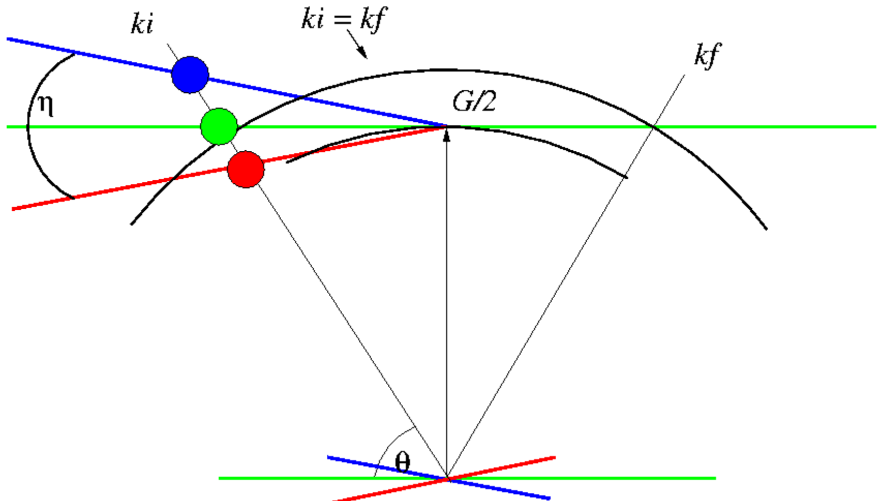
$$Q = \frac{4\pi}{6.3\text{Å}} \sin\frac{90 \pm 8.6}{2}$$

$$\approx (1.4 \pm 0.1)\ \text{Å}^{-1}$$

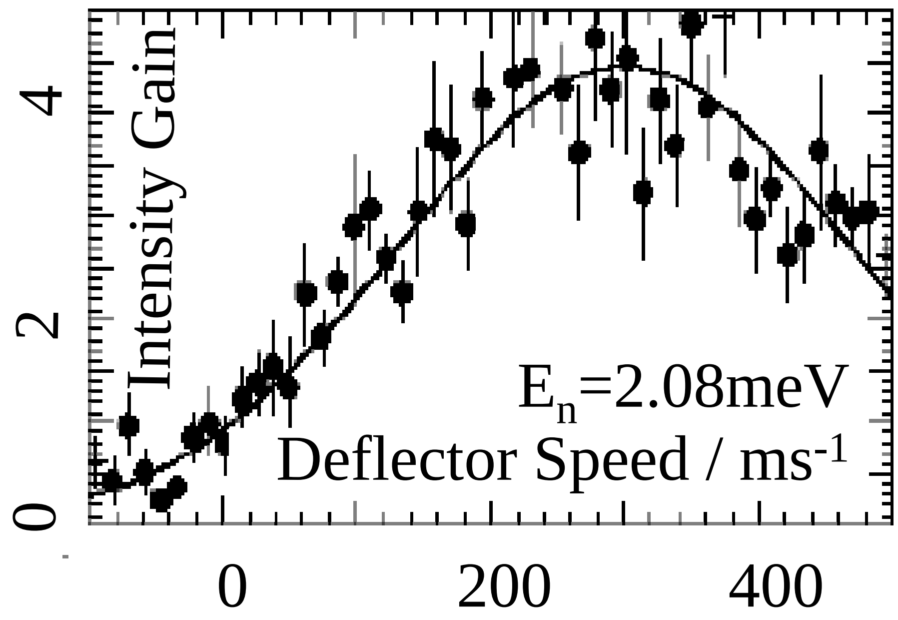


More Intensity: Phase Space Transformator

Convert Energy Spread to Beam Divergence



Move Deflector **Mosaic**-Crystal



Bragg scattering at a crystal at rest

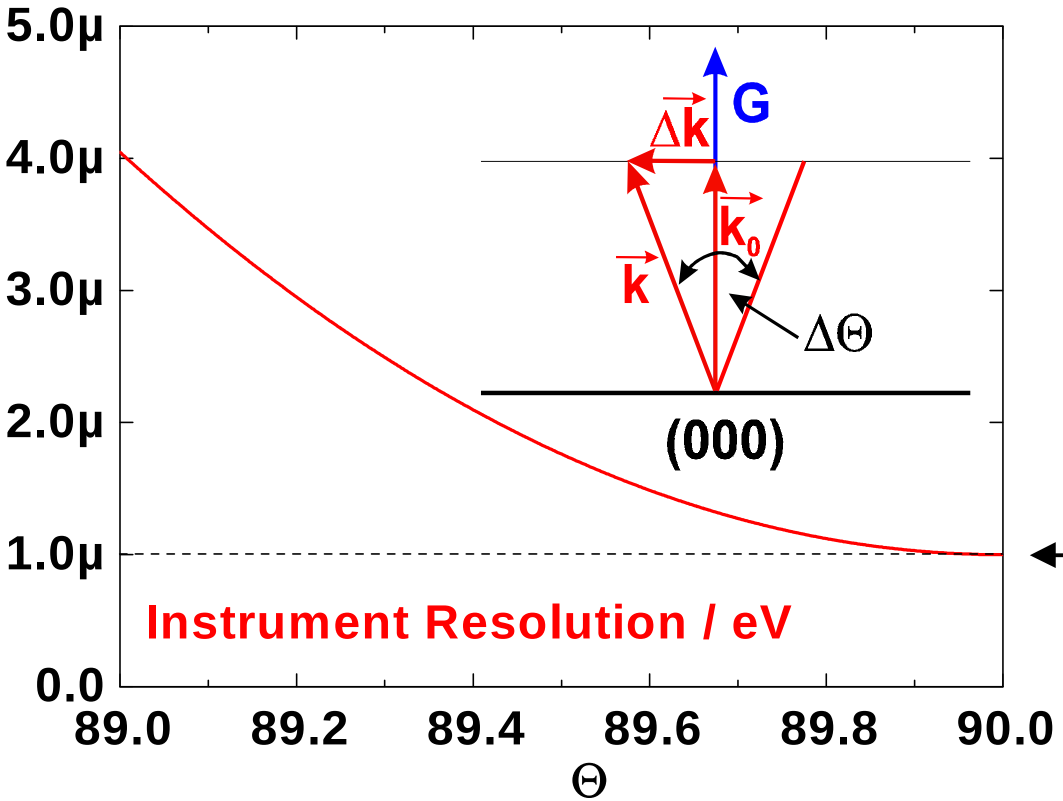
$G/2 = k \sin(\Theta)$

Bragg scattering at a moving crystal $G/2 = k' \sin(\Theta+\eta')$

k_f is adapted, i.e. the neutron is accelerated or slowed down

“from white to wide”

The Energy Resolution of the Instrument

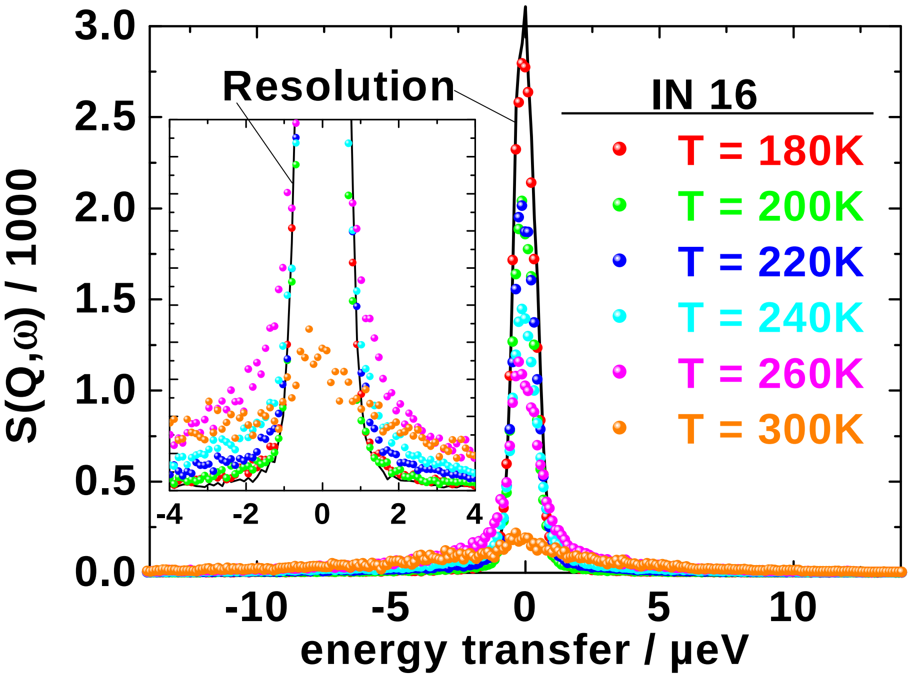


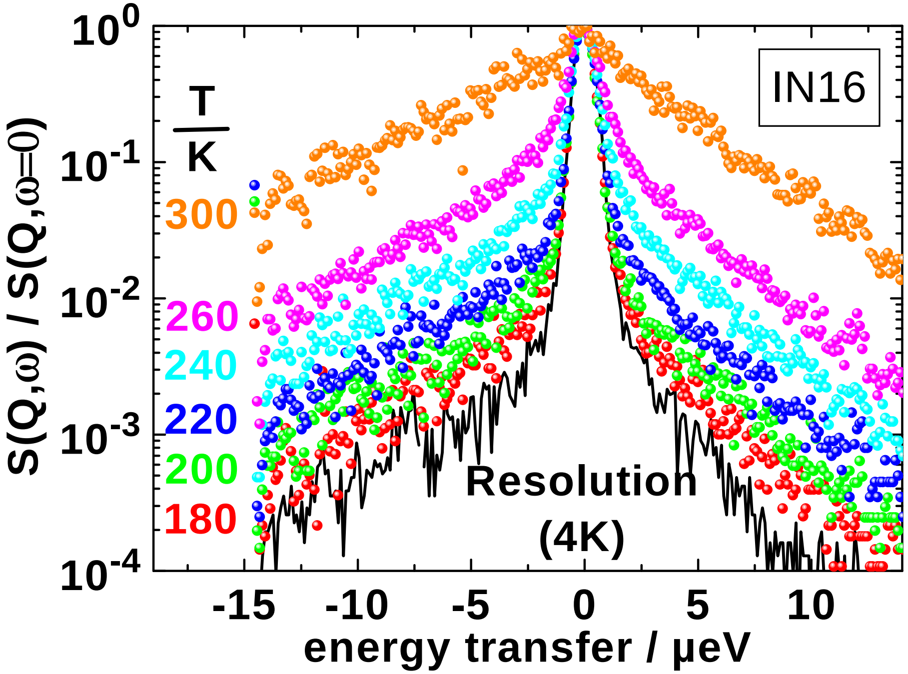
$$\frac{\Delta G}{G} = \frac{\Delta d}{d}$$

$$\frac{\Delta k}{k} = \frac{\Delta \lambda}{\lambda} = \frac{\Delta E}{2E} = \frac{\Delta G}{G} + \cot \Theta \Delta \Theta$$

Example

Relaxation Processes in Polybutadiene

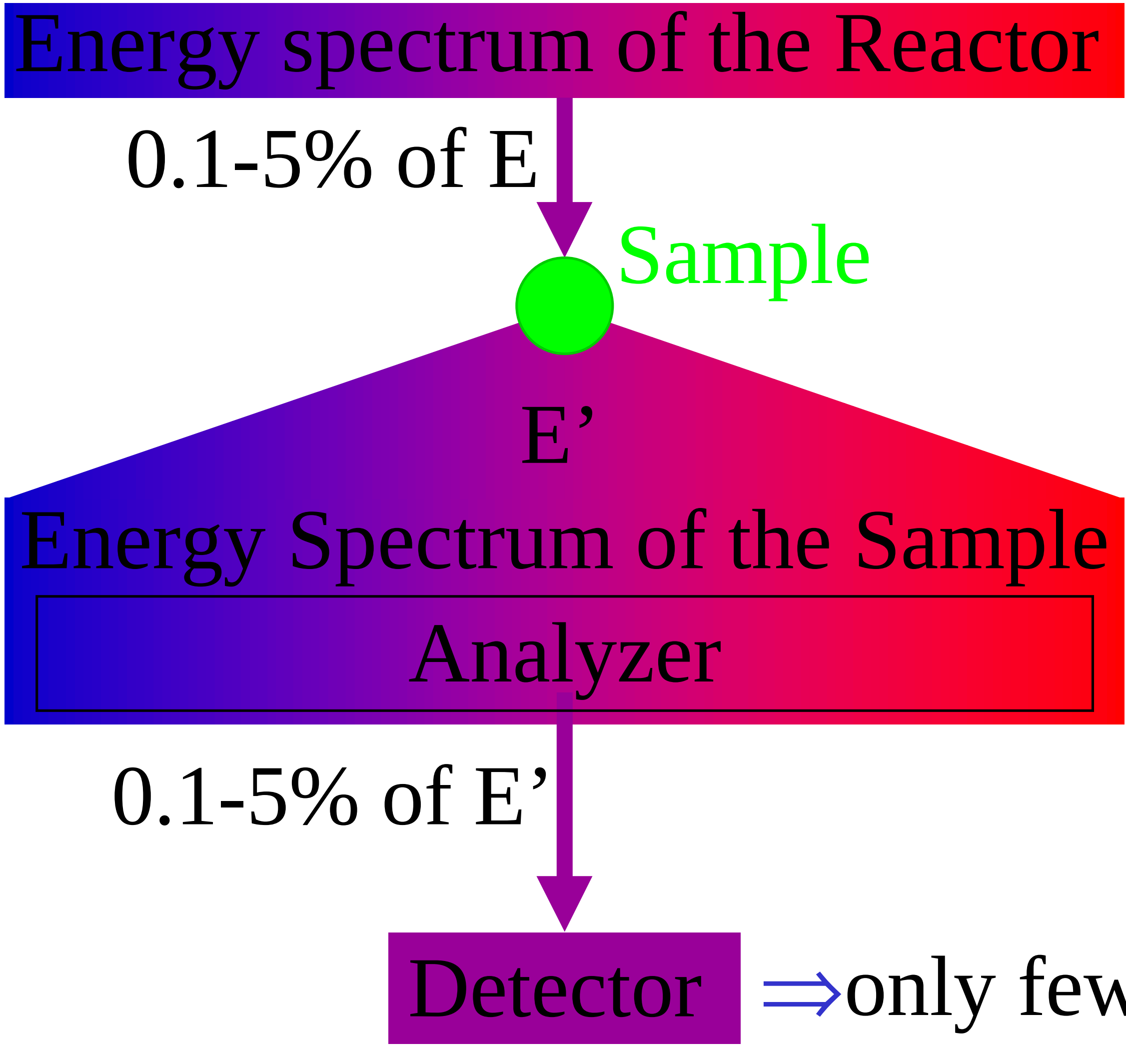




$$S_m(Q,\omega) = \int S(Q,\omega') \cdot R(Q,\omega-\omega')d\omega'$$

$$\equiv S(Q,\omega) * R(Q,\omega)$$

Limitation of the Energy Resolution



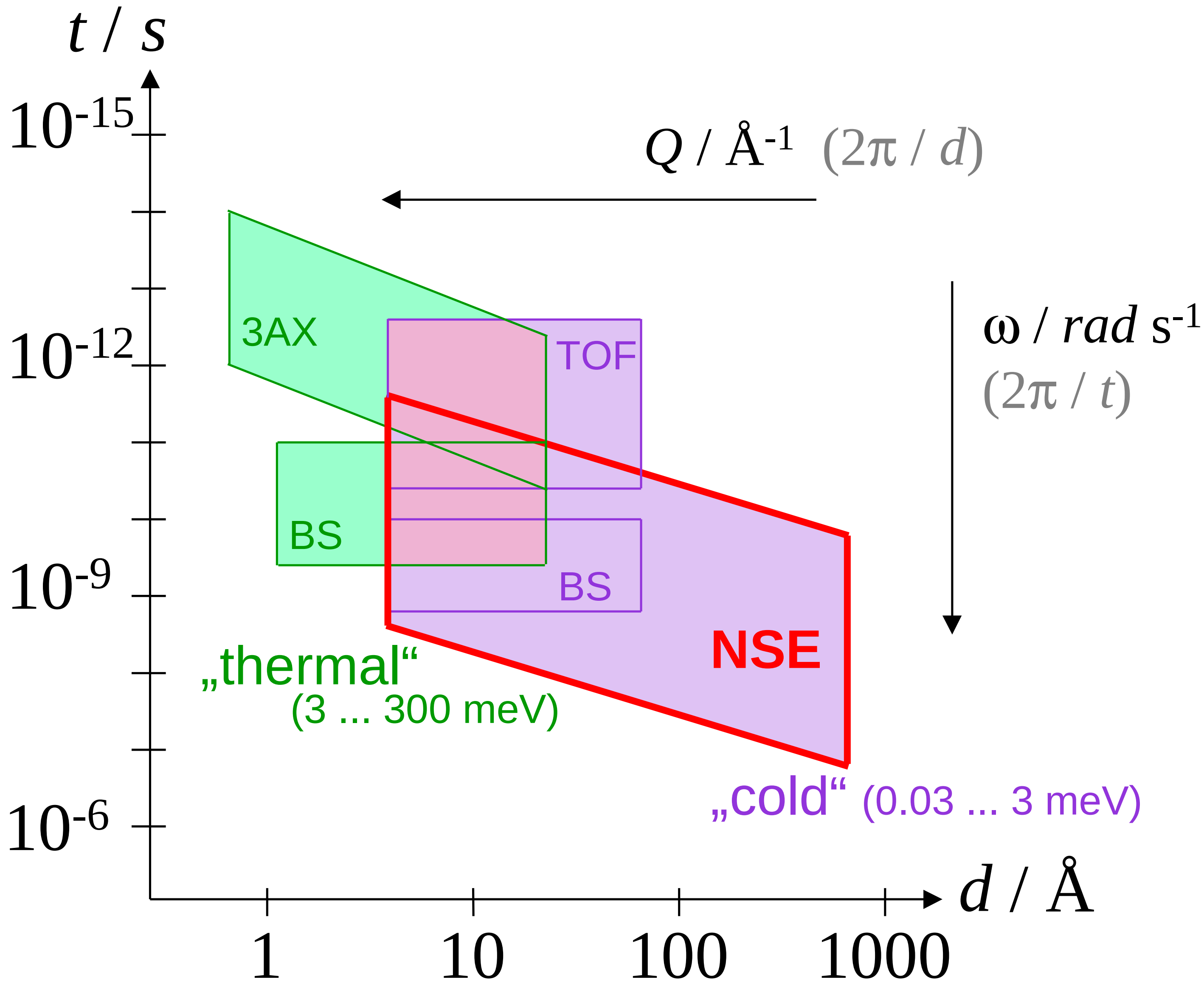
E **and** *E′* have **both** to be selected with required accuracy!

⇒number of detected neutrons decreases with **square** of the instrument resolution

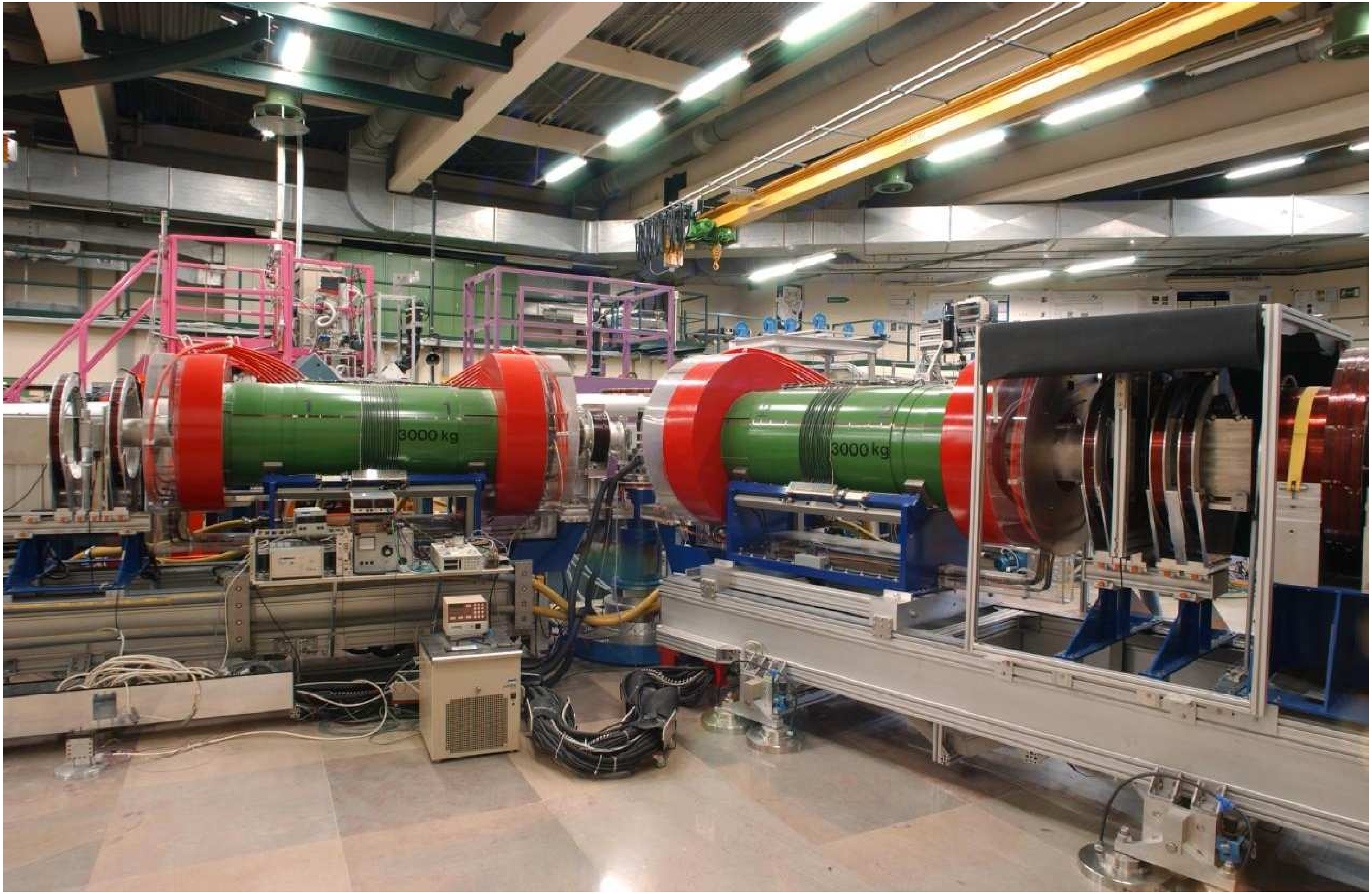
⇒only few neutrons are „used“

Can this dilemma be avoided?

Neutron Spin Echo Spectroscopy



The Neutron Spin Echo Instrument at FRJ2



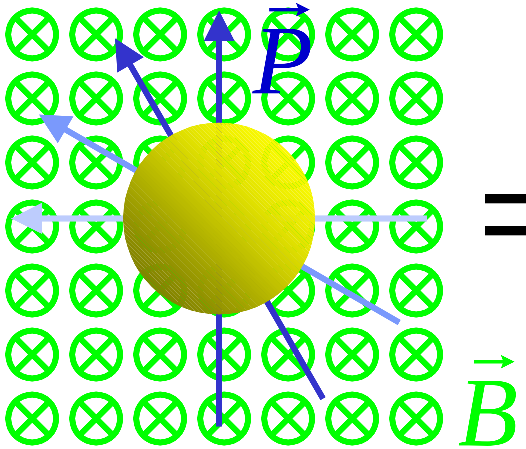
Neutron Spin Echo – The Main Idea

Is there any information the neutron carries with itself? — Yes! $\longrightarrow$ **Spin Direction**

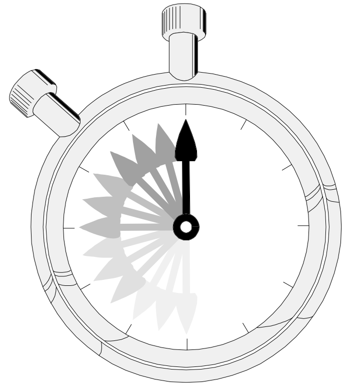
Spin (Lamor) precession in a magnetic field:

Bloch equation:

$$\frac{d\vec{P}}{dt} = \frac{g_n \mu_N}{\hbar}(\vec{P} \times \vec{B})$$



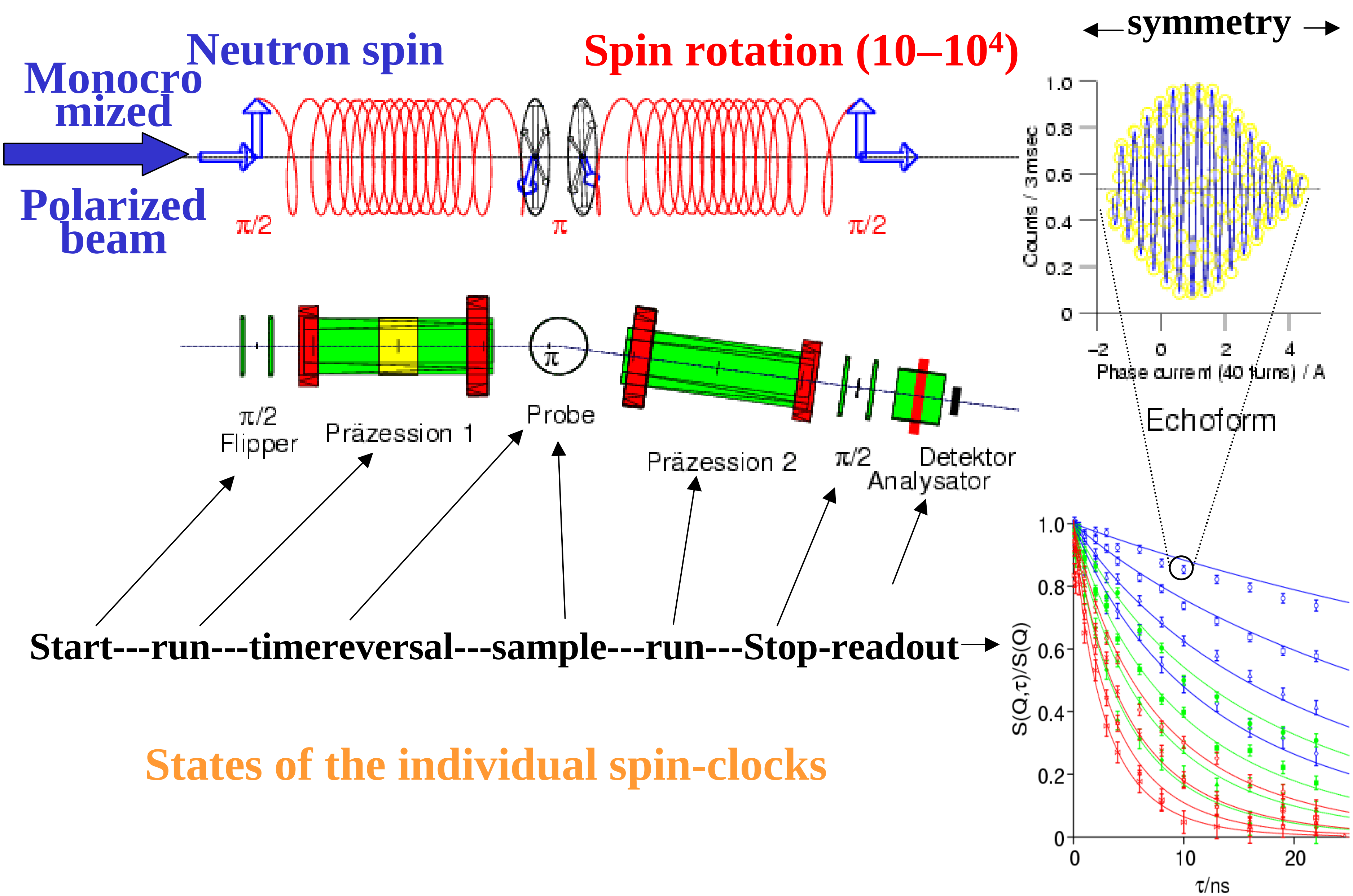
=



$$\omega_L = \frac{g_n \mu_N}{\hbar}\vec{B} \leftrightarrow 2900 \frac{rot}{s \cdot Gauss}$$

... used as individual stop-watch

Principle of the Neutron Spin Echo Spectrometer

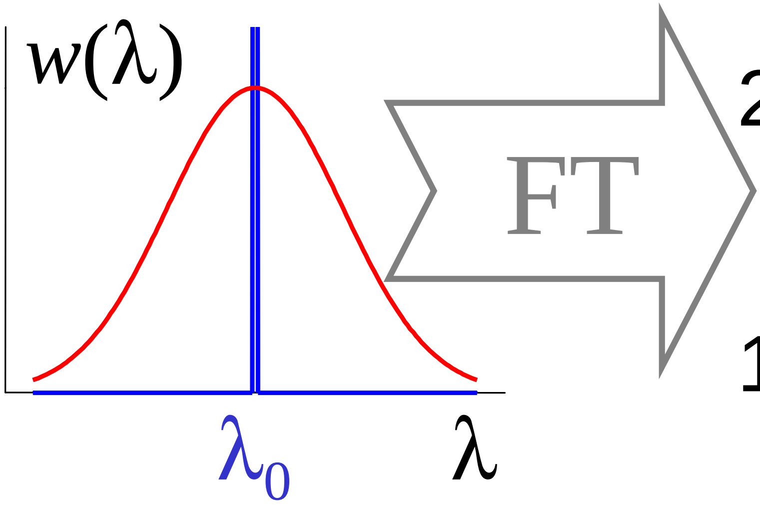


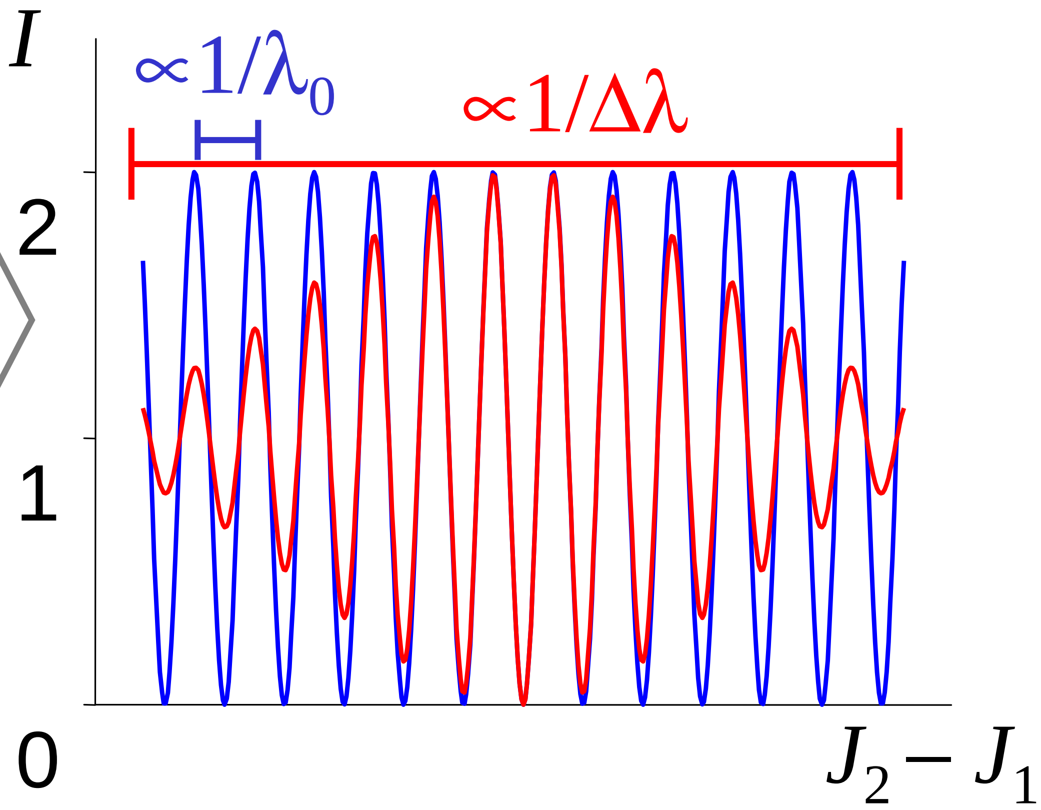
States of the individual spin-clocks

What is the Origin of the Echo?

The Elastic Case

$$I \sim \int (1 \pm \cos(\lambda \gamma (m_n / h)(J_2 - J_1)) w(\lambda) d\lambda)$$

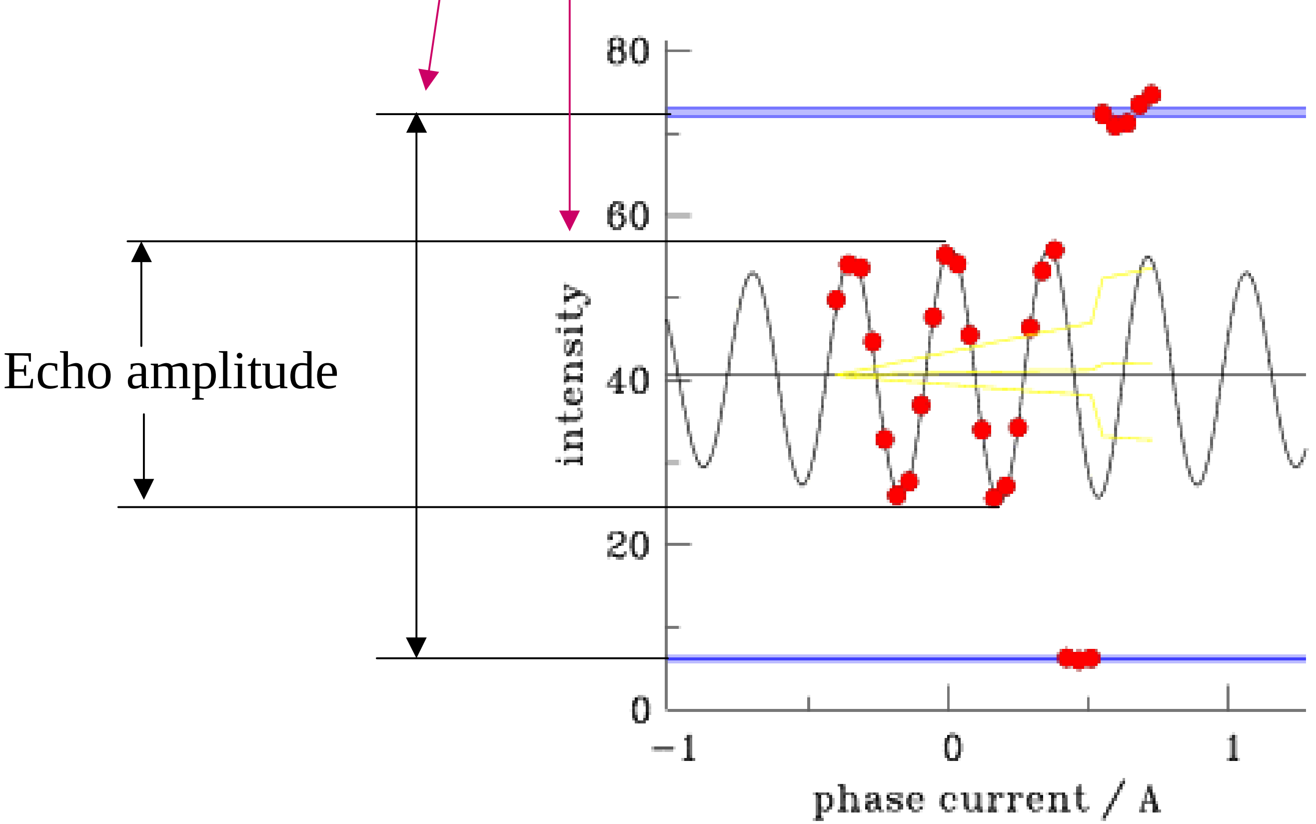




$$J = \int \vec{B} d\vec{l}$$

The NSE Signal (where is the information?)

$$I = \eta\frac{1}{2}\left[S(Q) + \underbrace{\int \cos\Big(\underbrace{\gamma J \frac{m_n^2}{h^2 2\pi}\lambda^3}_{t}\;\omega\Big) S(Q,\omega)\,d\omega}_{S(Q,t)}\right]$$



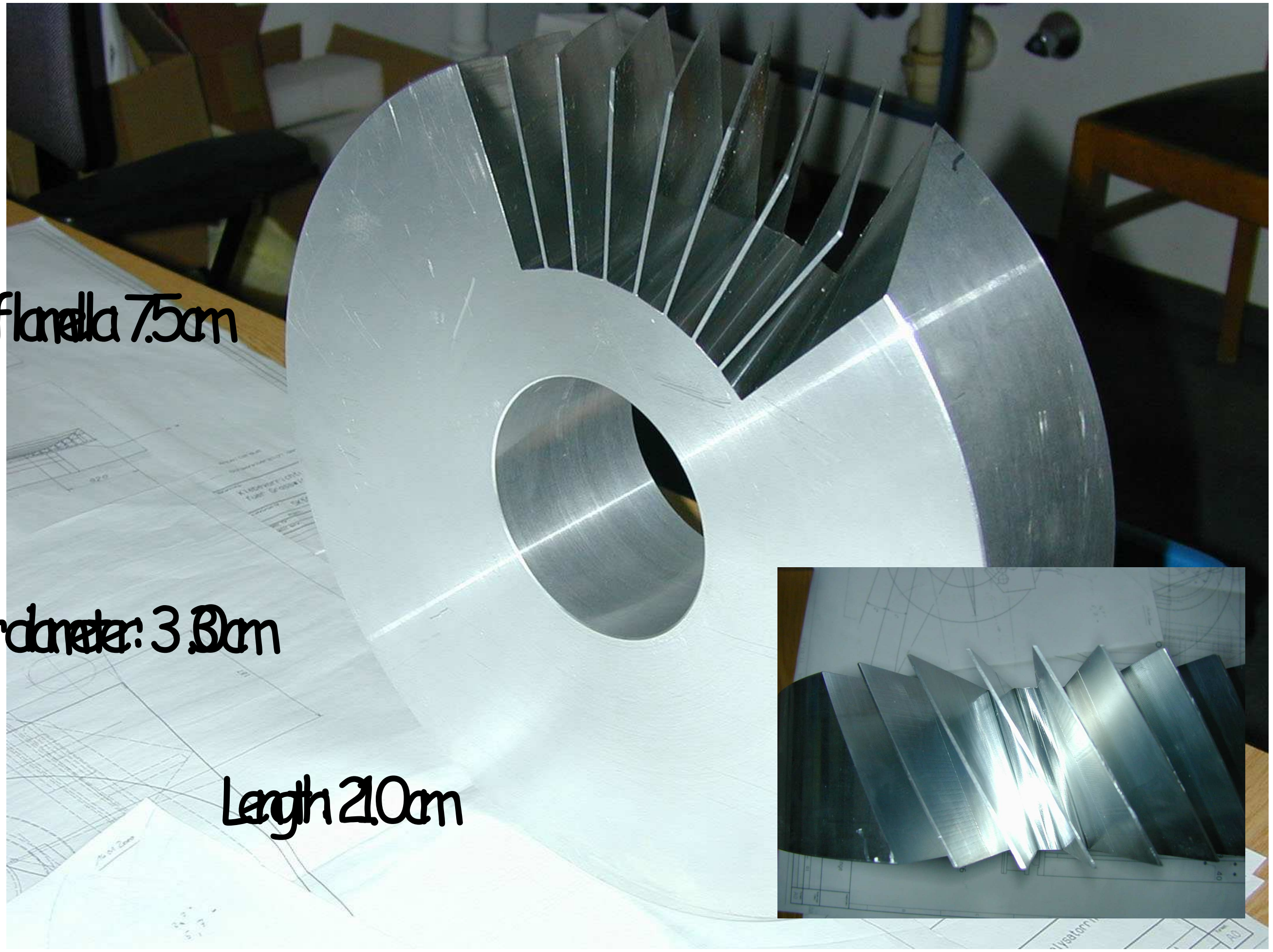
$$\frac{\mathbf{S(Q,t)}}{\mathbf{S(Q)}}$$

finally

Select Neutrons

Use a Rotating Turbine

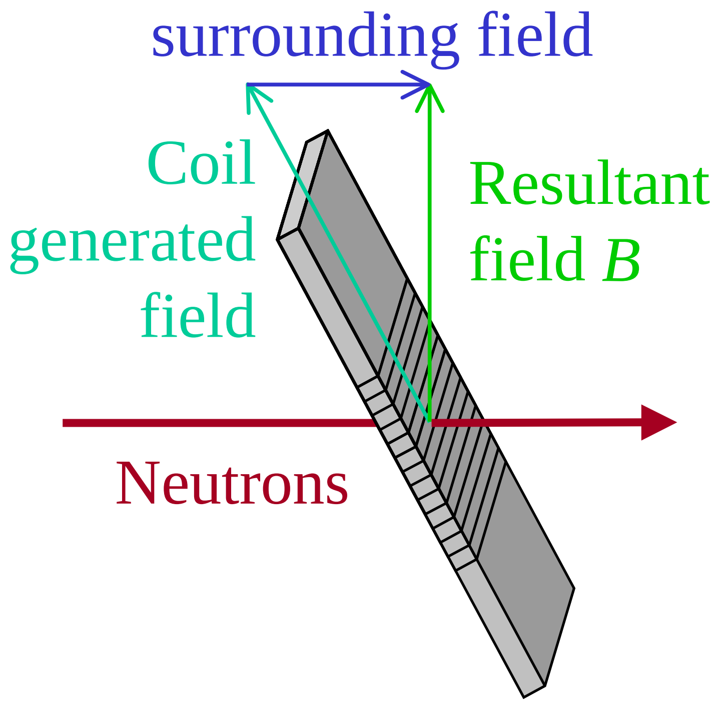
$$\Delta E / E = 10..20\%$$

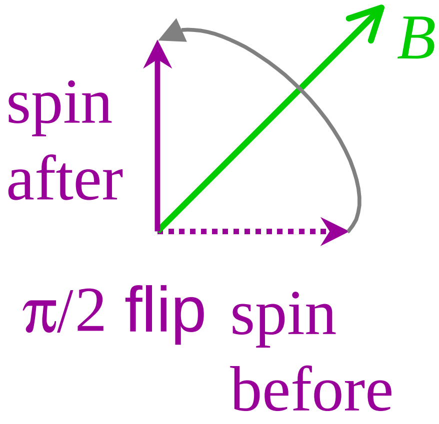


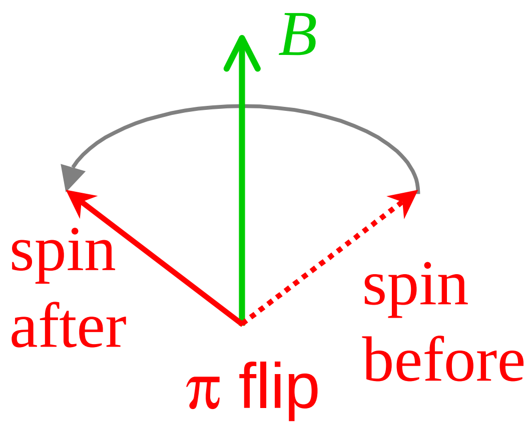
The Spin Flippers

Mezei coil

From Bloch equation: $\psi / t = \frac{g_n \mu_N}{\hbar} B$







Backscattering Spectrometer Resume

- ⇒ Dynamic Range **$10ps \le t \le 3ns$**
- ⇒ ω Space Spectrometer **$S(Q,\omega)$**
- ⇒ Resolution Correction **$I(Q,\omega)=S(Q,\omega)*R(Q,\omega)$**
- ⇒ High Resolution but low Intensity
- ⇒ Highly Sensitive for Background Neutrons

Neutron Spin Echo Spectrometer Resume

- ⇒ Highest Resolution and Intensity
- ⇒ Direct measurement of velocity differences
- ⇒ Fourier Spectrometer **$S(Q,t)$**
- ⇒ Resolution Correction **$I(Q,t) = S(Q,t) \cdot R(Q,t)$**
- ⇒ Dynamic Range **$2ps \le t \le 200ns$**

Thanks for the Support

- ⇒ H. Grimm
- ⇒ O. Kirstein
- ⇒ M. Monkenbusch
- ⇒ D. Richter
- ⇒ R. Zorn

Jülich Neutrons for Europe

More information: http://www.neutronscattering.de