Neutron Scattering

Part 2: Techniques

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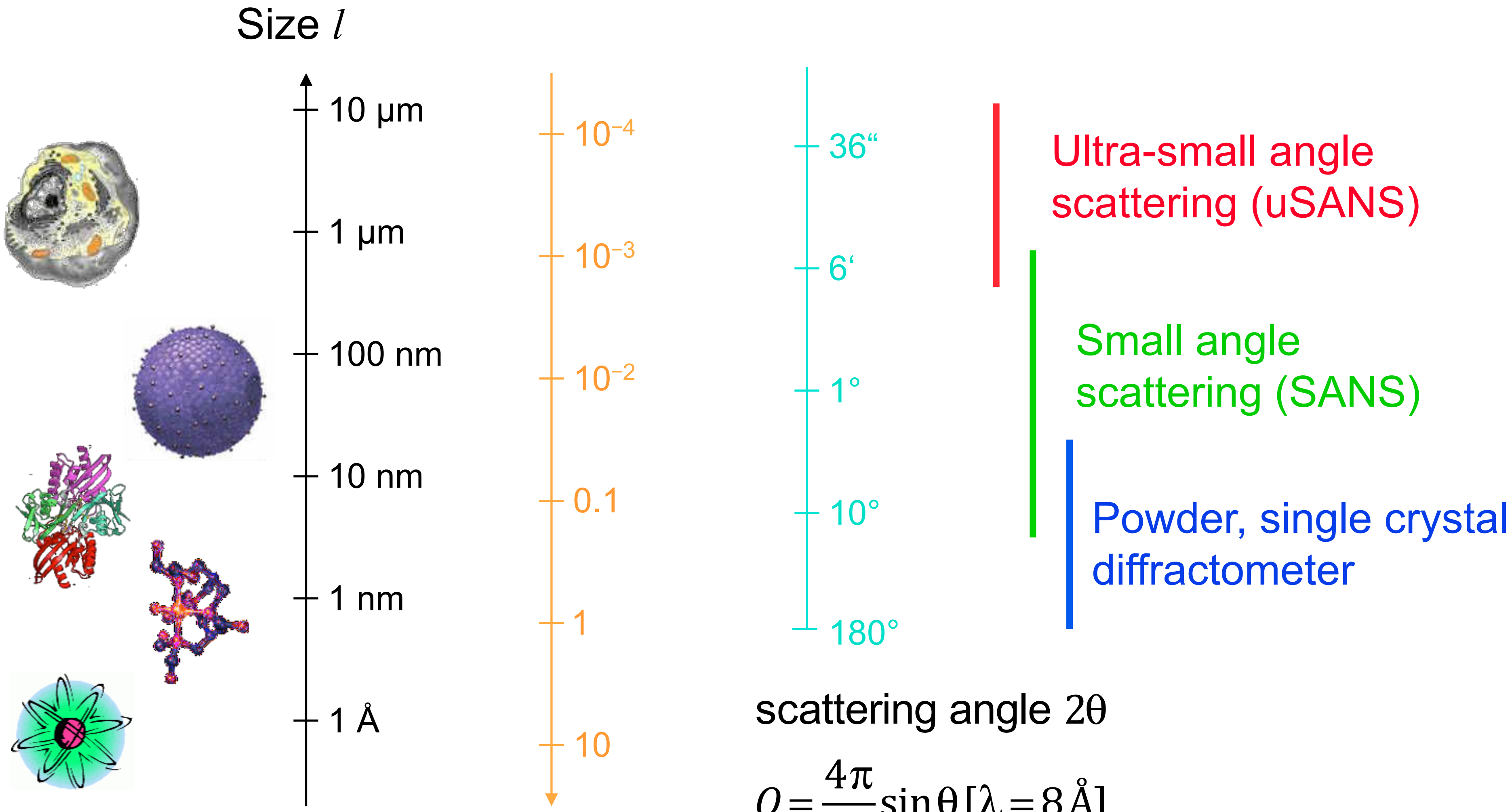
- Short remarks on elastic scattering methods
- Triple axis spectrometer
- Time-of-flight spectrometer
- Backscattering spectrometer
- Neutron spin echo spectrometer

Elastic Neutron Scattering

a.k.a.
Neutron Diffraction

Elastic scattering methods



Ultra-small angle scattering (uSANS)

Small angle scattering (SANS)

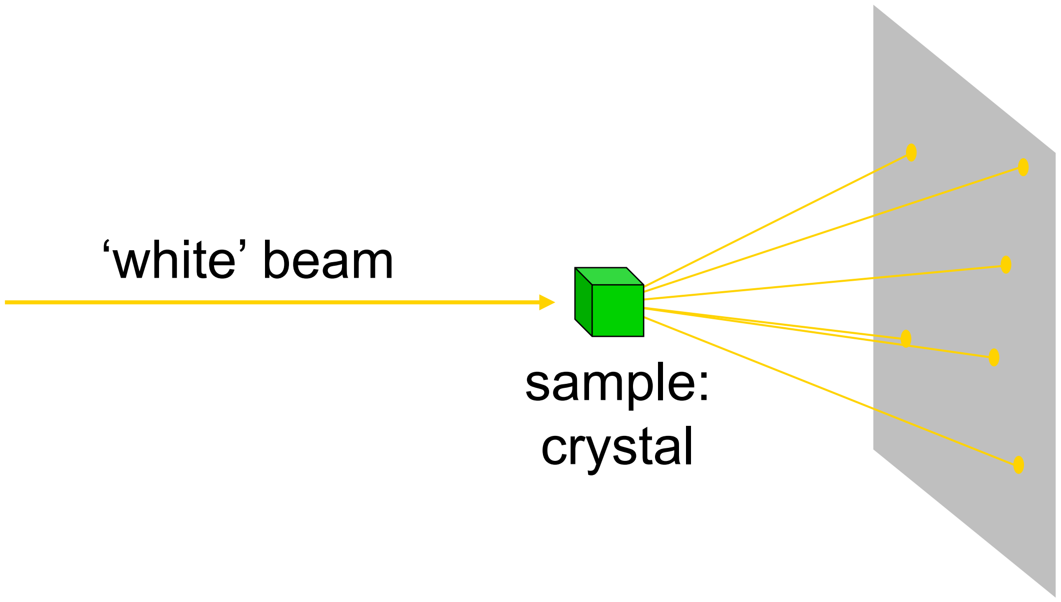
Powder, single crystal diffractometer

scattering angle 2θ

$$Q = \frac{4\pi}{\lambda}\sin\theta\,[\lambda = 8\,\text{Å}]$$

$$Q \approx \frac{2\pi}{l}\,[\text{Å}^{-1}]$$

Laue camera



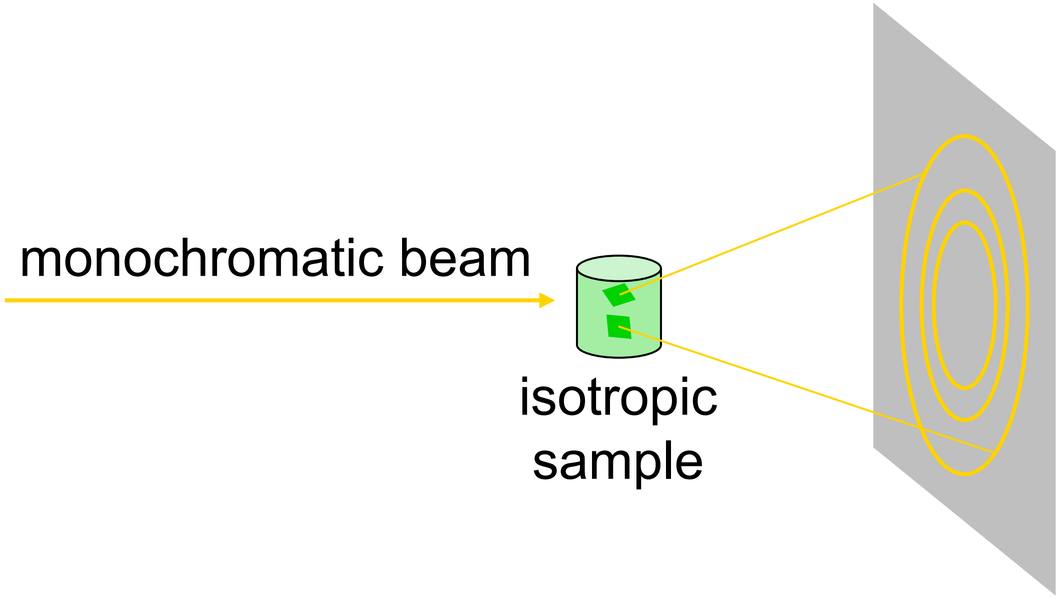
Each spot contains a single wavelength λ_{hkl} under an angle $\theta_{hkl}/2$ corresponding to a lattice plane by

$$d_{hkl} = \frac{\lambda_{hkl}}{2\sin(\theta_{hkl}/2)}$$

- Advantage:
- high information content (2D)
- Disadvantage:
- single crystal necessary

in general not for polymers, except proteins (biopolymers)

Debye-Scherrer camera



Each ring corresponds to a lattice spacing by

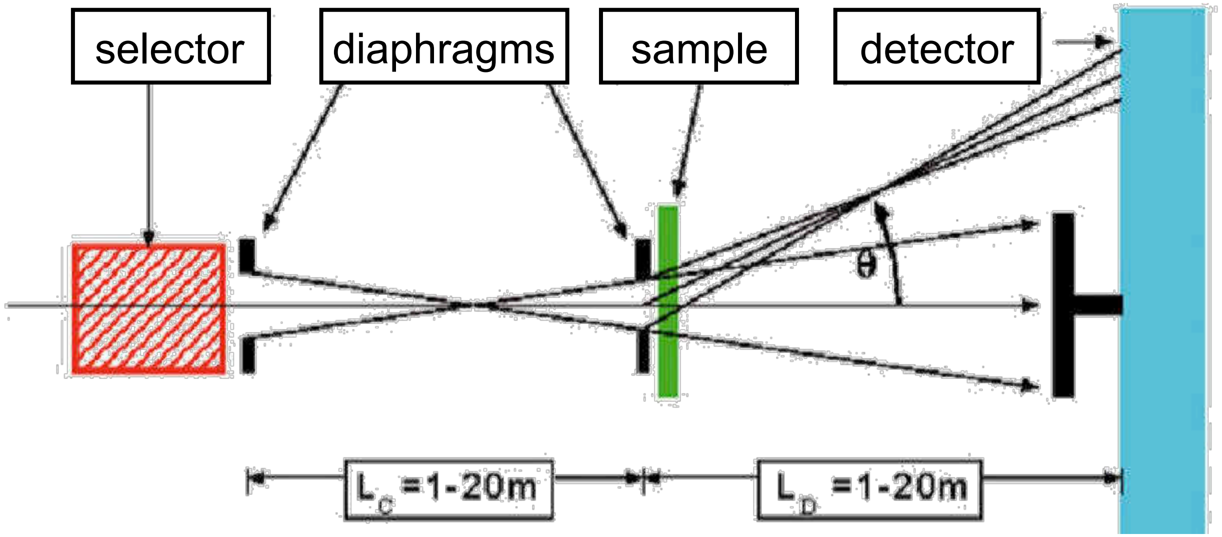
$$d_{hkl} = \frac{\lambda}{2\sin\left(\theta_{hkl}/2\right)}$$

- Advantage:
- macroscopically isotropic sample sufficient (necessary)

powders, polycrystals, liquids amorphous polymers…

- Disadvantage:
- lower information content (1D)

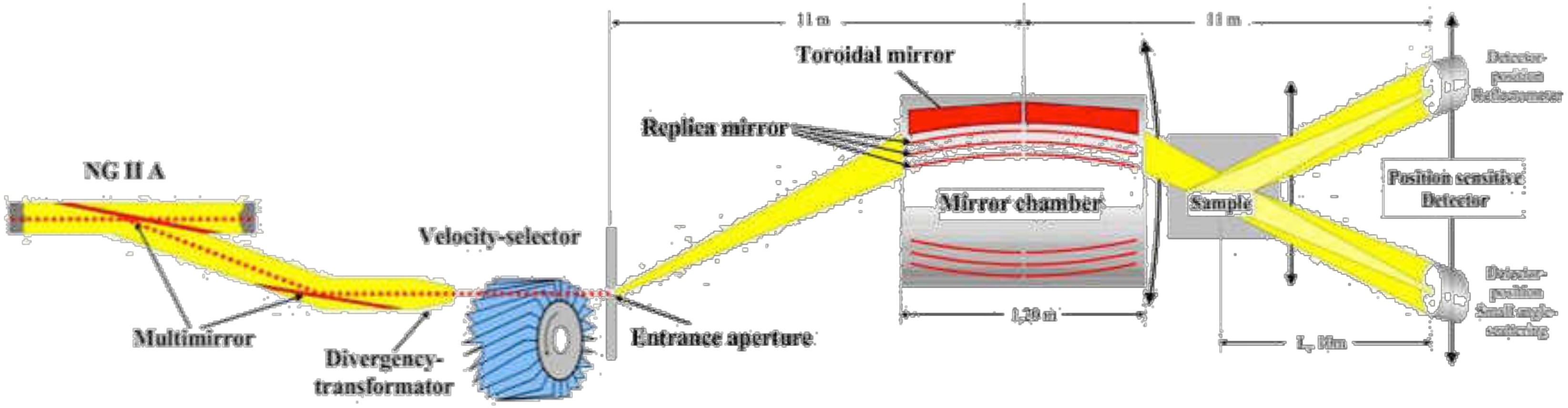
Neutron Small Angle Scattering (SANS)



SANS:

- Velocity selector:
  250 … 900 m/s ↔ 4.5 … 15 Å
- 20 m length, 2 cm diaphragms
  → min. 3 arc minutes
- $Q = 10^{-3} \ldots 0.2$ Å^{-1}
- l = 3 … 600 nm

Ultra-small-angle scattering



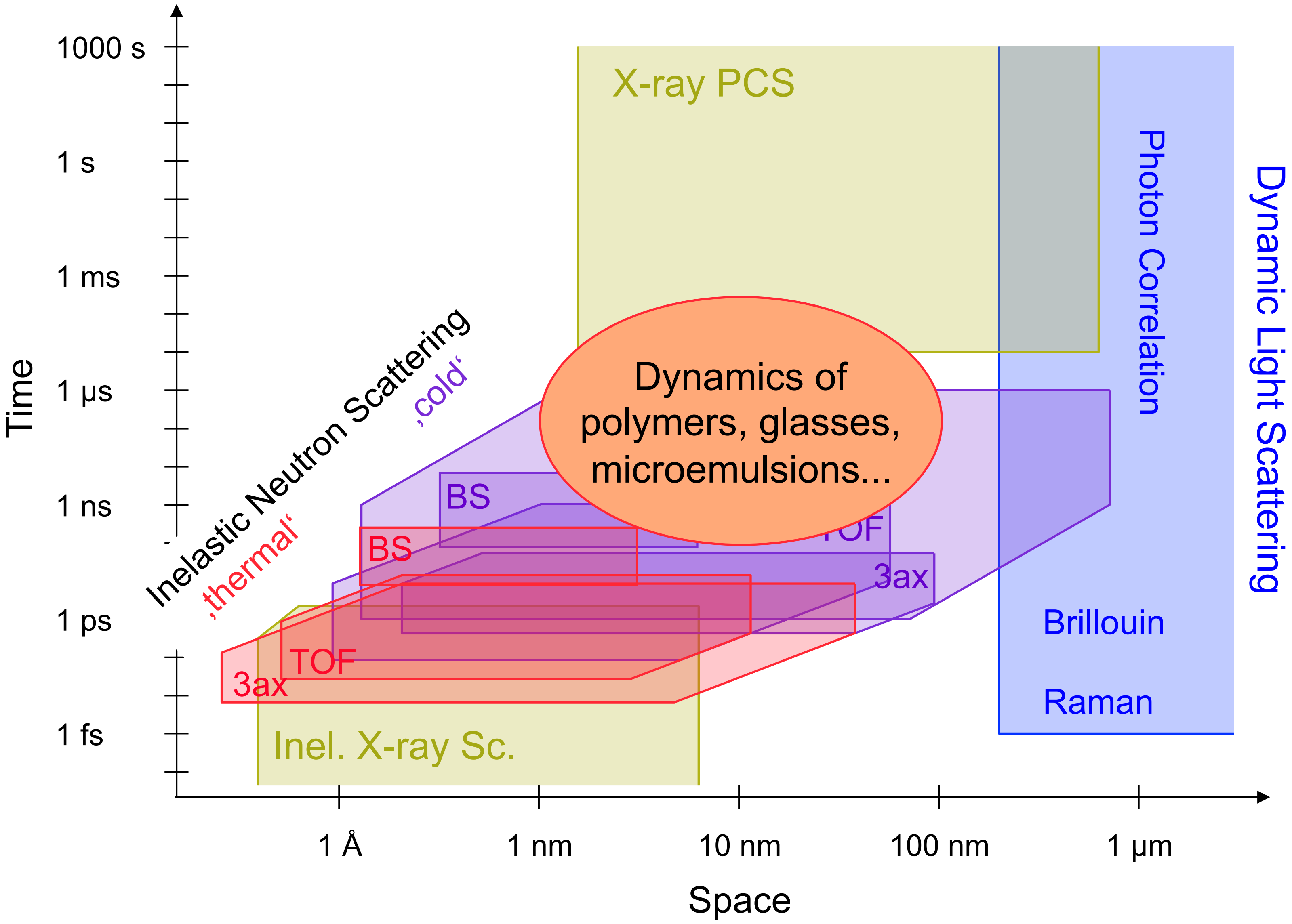
Ultra-SANS:

- 11 m length, 2 mm apertures
  → min. 36 arc seconds
- Mirror optics enables to keep intensity (alternative: lenses)
- $Q = 10^{-4} \ldots 2 \cdot 10^{-3}$ Å^{-1}
- $l = 0.3 \ldots 6$ µm

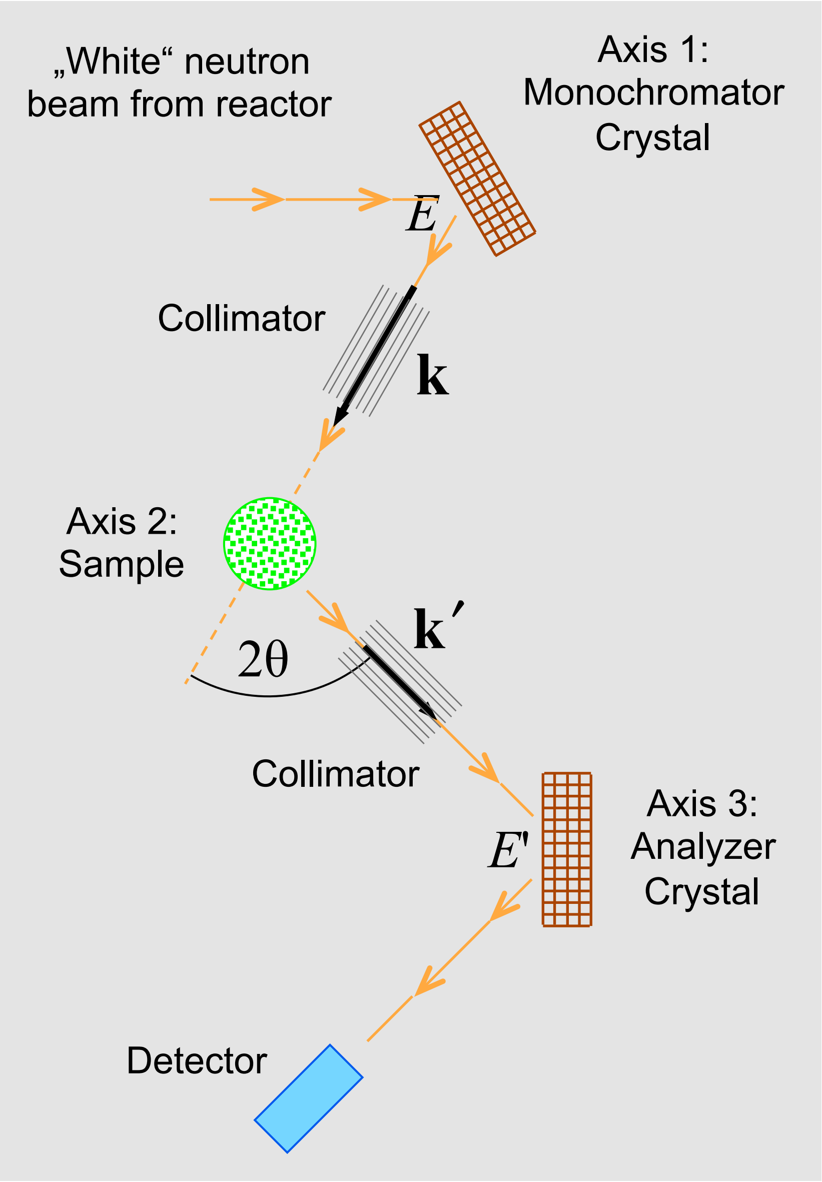
Inelastic Neutron Scattering

a.k.a.
Neutron Scattering Spectroscopy,
Dynamic Neutron Scattering, Quasielastic
Neutron Scattering …

Inelastic Scattering Methods



Triple-axis spectrometer



General construction scheme of neutron scattering spectrometers:

Primary spectrometer: selection of incident wavelength and direction

E and $\mathbf{k}$

——— sample ———

Secondary spectrometer: detection of outgoing wavelength and direction

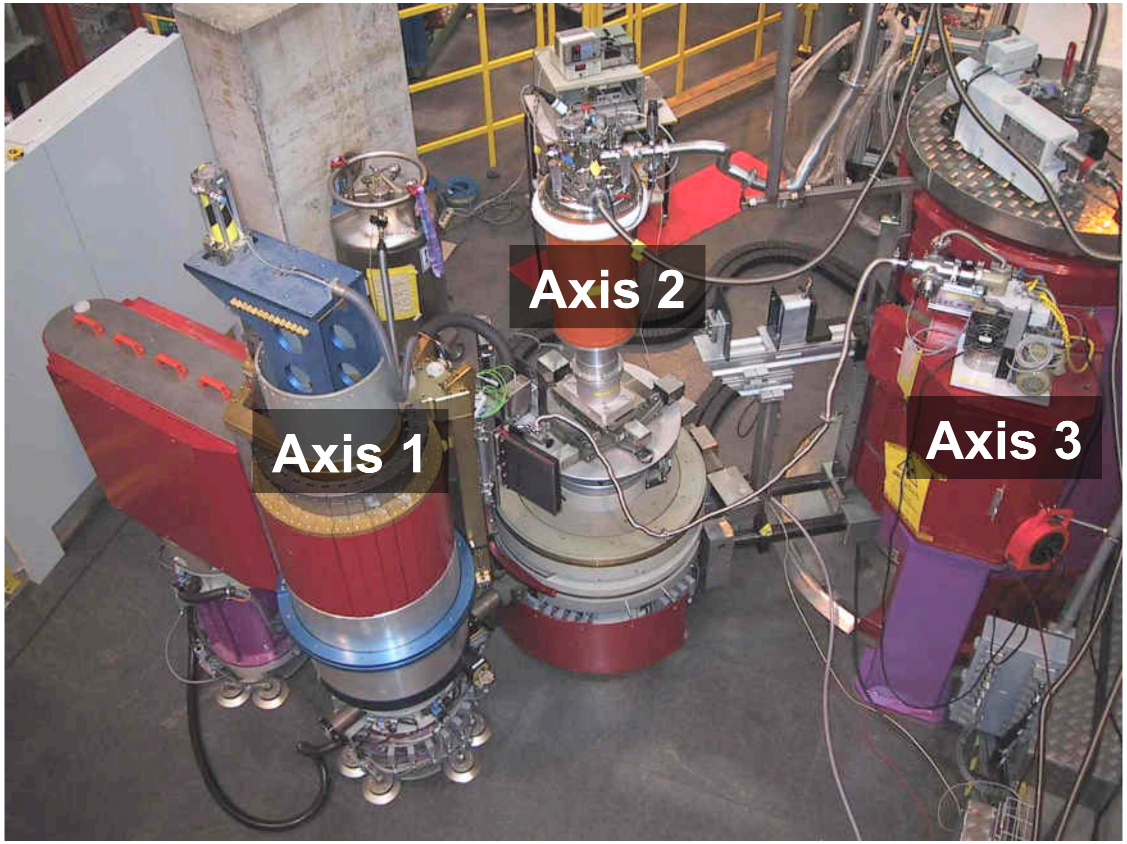
E' and $\mathbf{k}'$

$$\mathbf{Q} = \mathbf{k}' - \mathbf{k}$$

$$\hbar\omega = E' - E$$

Triple-axis spectrometer

3ax-principle requires motion of axis 3 in two dimensions: hovering airpads on ‚Tanzboden' floor.



TASP, PSI, Villigen, Switzerland

Characteristics of triple-axis spectrometers

Flexibility:

- Full control of $\mathbf{Q}$ and ω within limits of wavelengths from source (using different monochromator crystals)
- Adjustable resolution (different collimators), tradeoff resolution-intensity possible

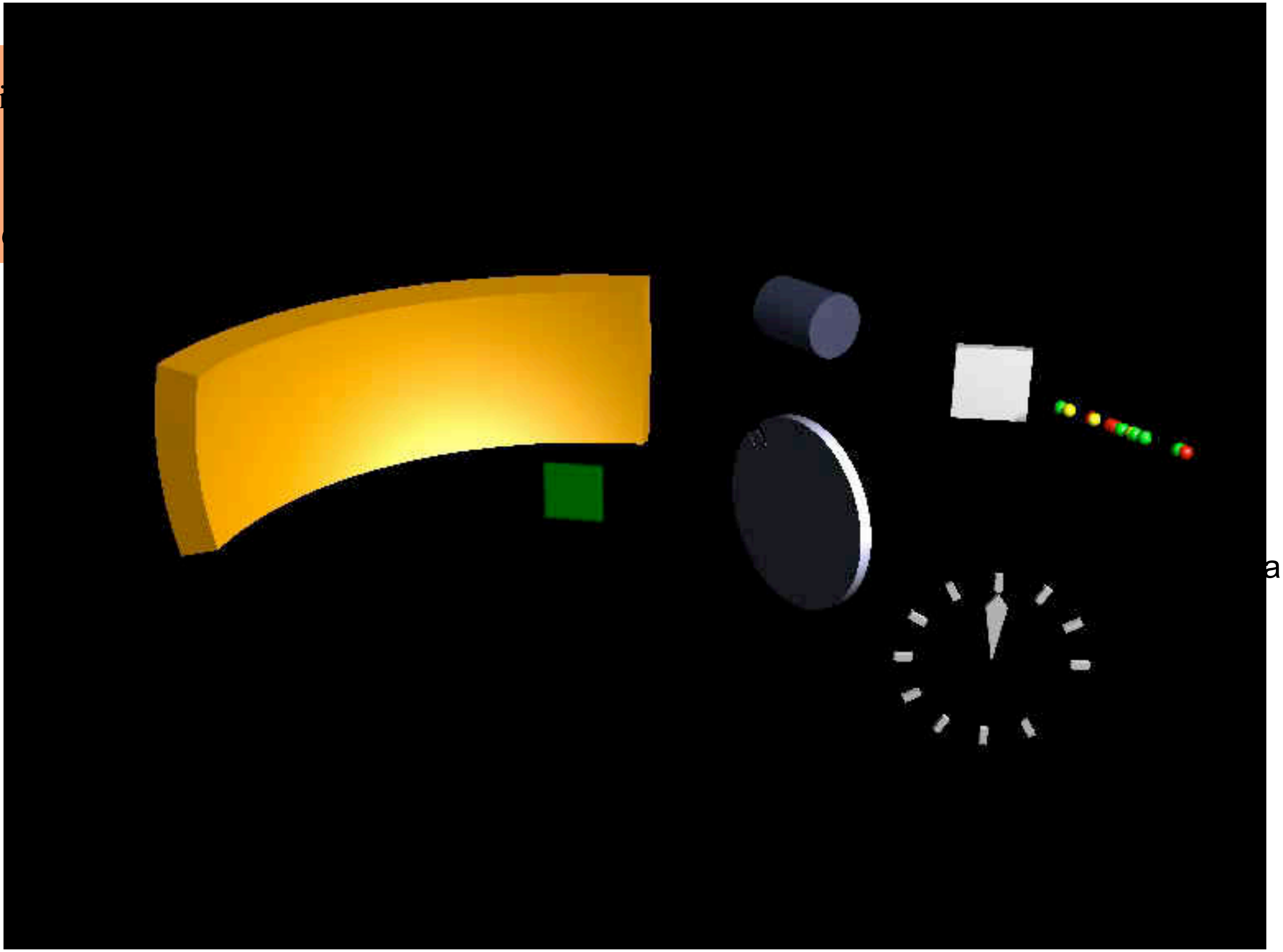
Disadvantage:

- Only one $(\mathbf{Q},\omega)$ point is measured at a time.
- Long registration time for complete spectra (hours-days)
- Better suited if only peaks have to be found (phonons, magnons)

Time-of-Flight Spectrometer

t_{fli}

$\hbar$



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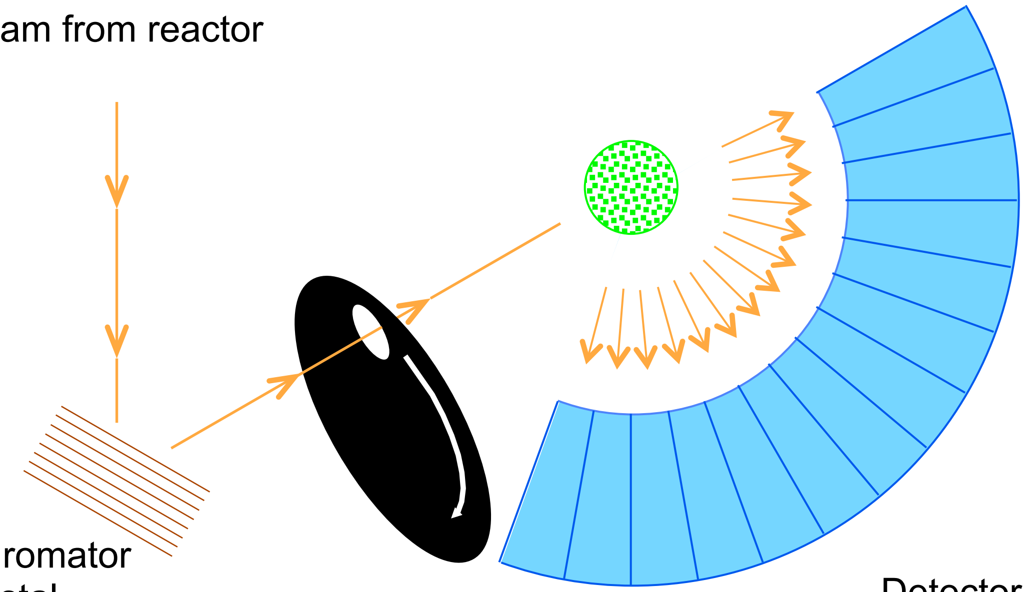
Time-of-Flight Spectrometer

$$t_{\text{flight}}, \theta$$
$$\Downarrow$$
$$\hbar\omega, Q$$

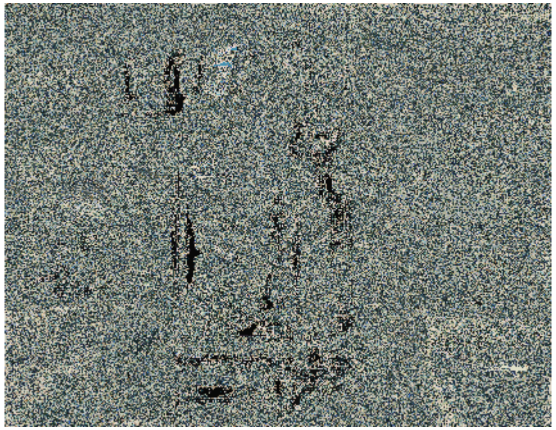


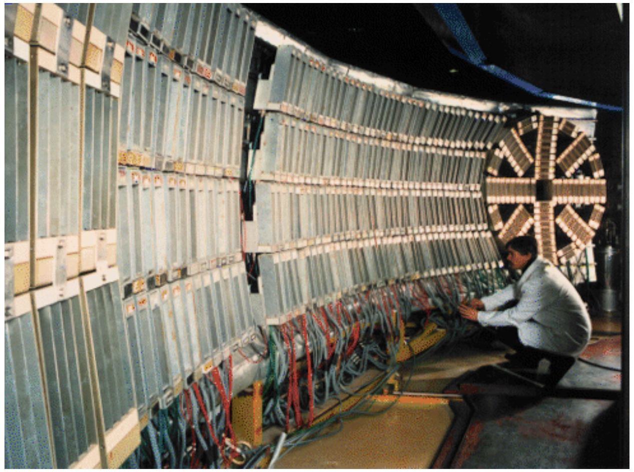
„White“ neutron
beam from reactor

Monochromator
Crystal

Chopper

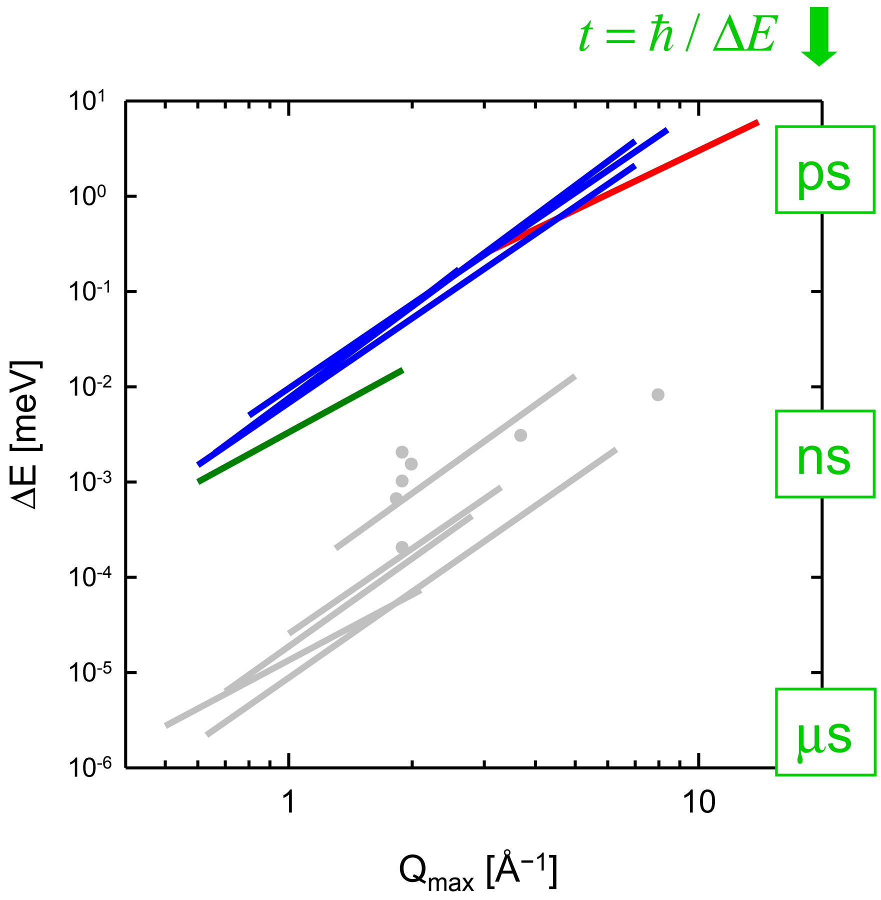
Detector Bank





IN6, IN5, ILL,
Grenoble, France

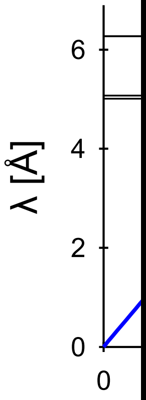
Specifications of TOF Instruments

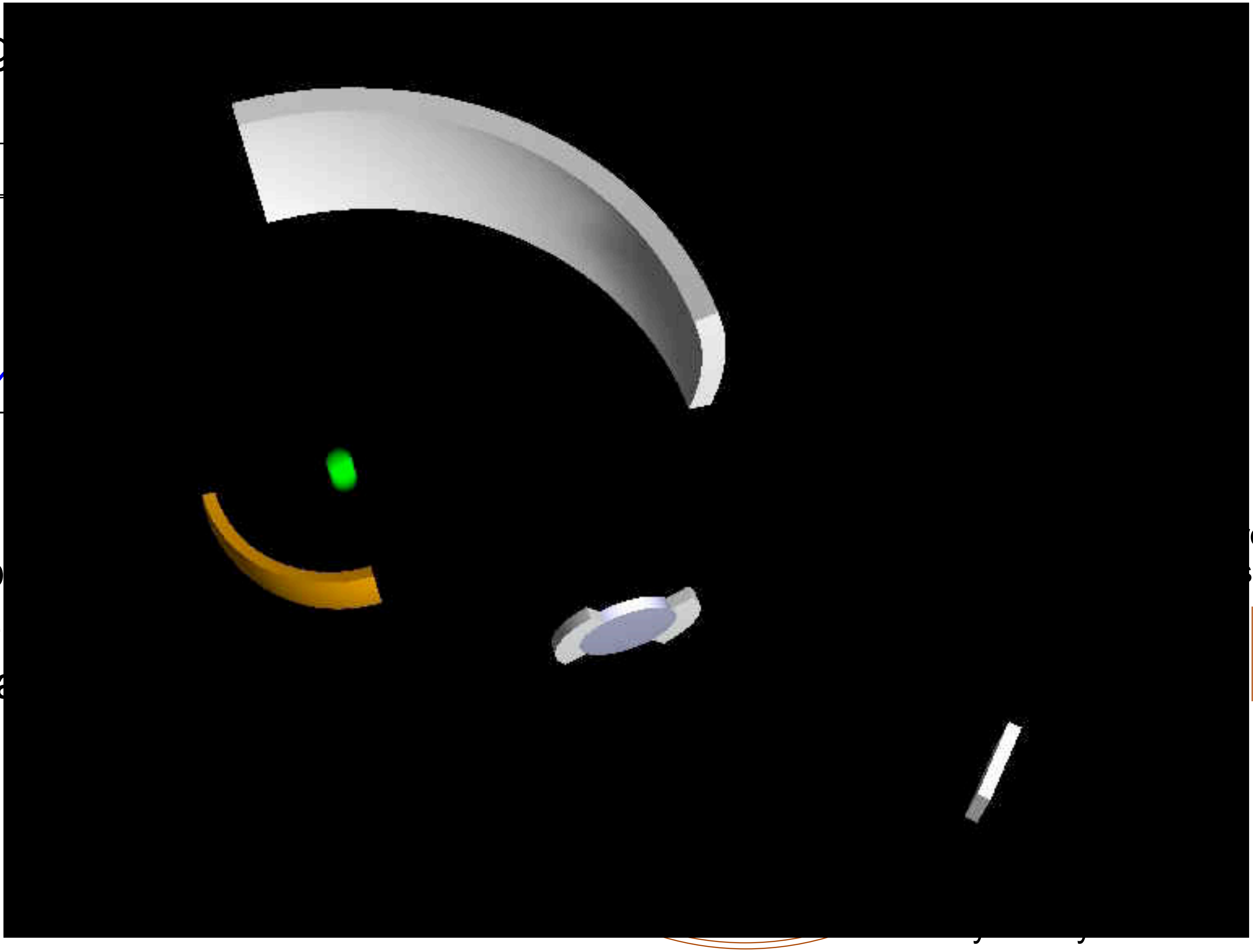


IN6:	cold neutrons, crystal monochromator
IN5, NEAT, TOFTOF:	cold neutrons, chopper monochromator
IRIS:	cold neutrons,spallation source, inverse geometry
IN4:	hot neutrons, crystal monochromator

Backscattering Spectrometer

Bragg





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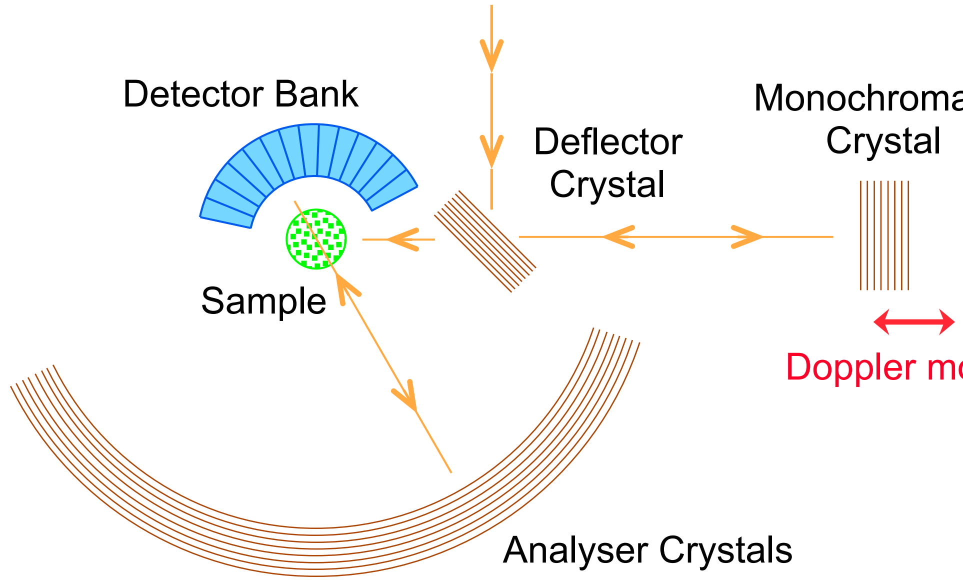
Backscattering Spectrometer



„White“ neutron
beam from reactor

Detector Bank

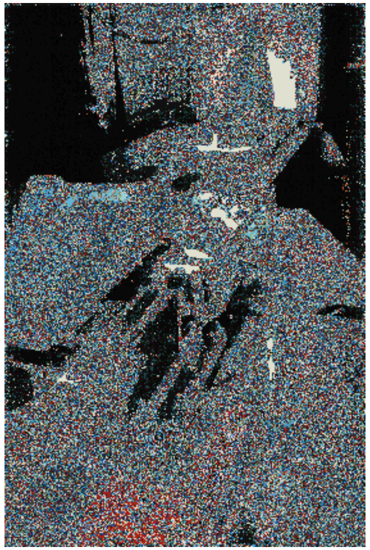
Deflector
Crystal

Monochromator
Crystal

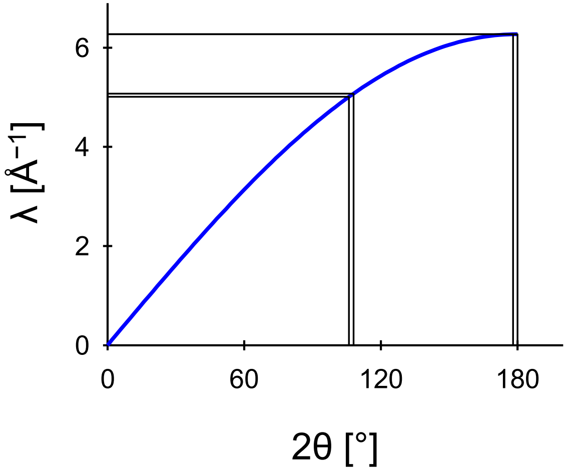
Sample

Doppler motion

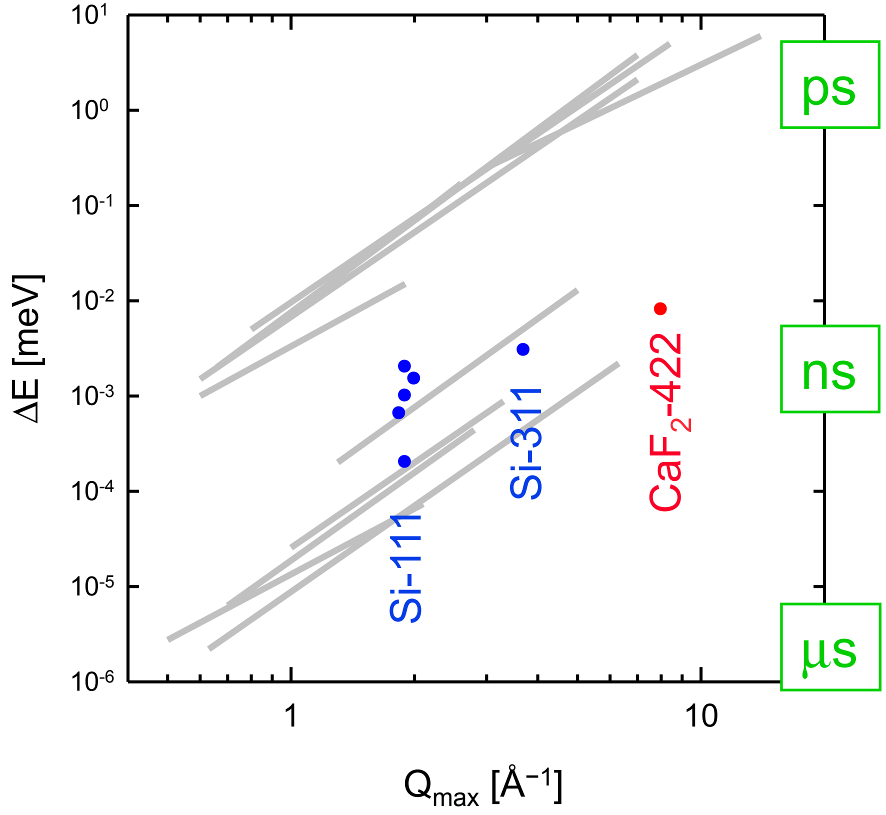
Analyser Crystals



IN10, ILL,
Grenoble, France



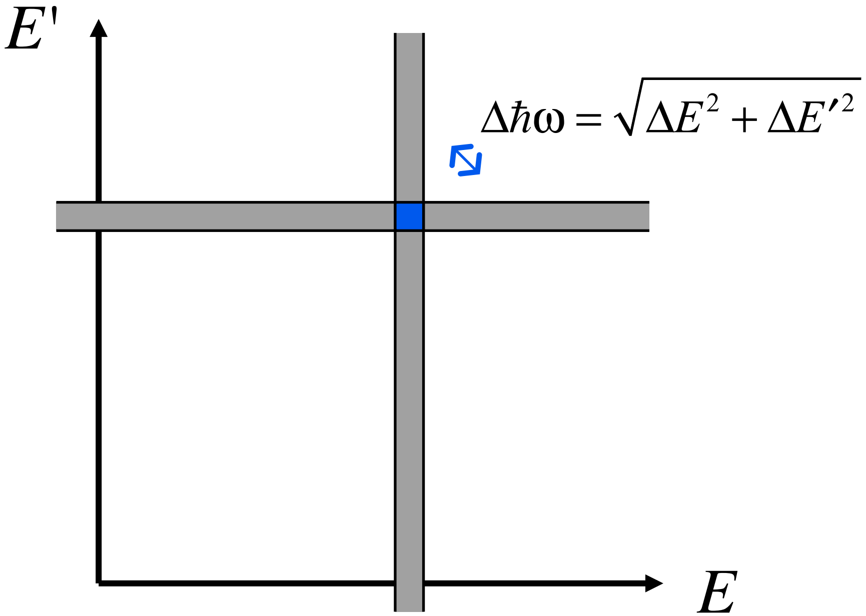
Specifications of BS Instruments



IN16, PI:	(Si-111) Doppler, range 15 meV, best resolution 0.2 meV (polished)
SPHERES:	phase space transformer
IN10B:	(Si-111) thermal, range 120 meV
IN13:	(CaF_2-422) hot neutrons, thermal

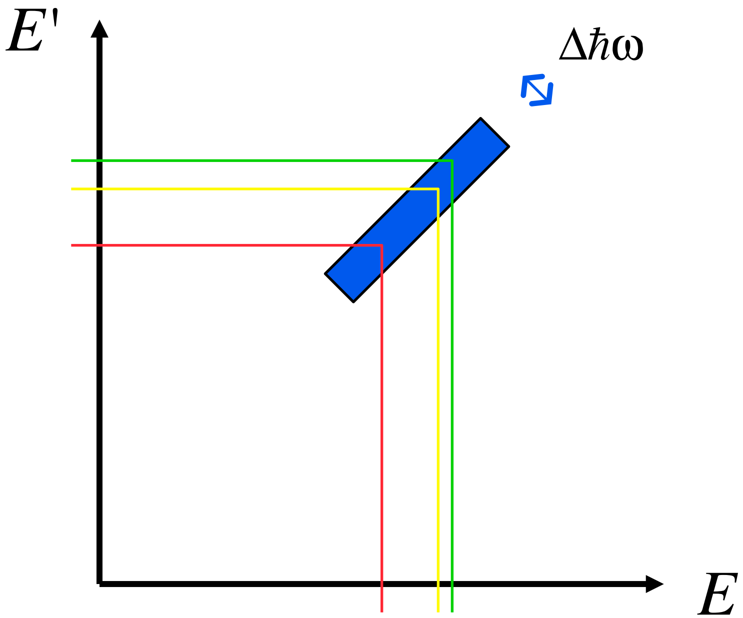
The Resolution-Intensity Dilemma

Conventional inelastic experiment:



Intensity $\propto \Delta\hbar\omega^2$!

Energy difference selection:



... needs **identification** of neutrons!

Neutron Spin

Lecture 7: Larmor precession in constant field:

Is there any information the neutron carries with itself?
— Yes:

Spin Direction

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

Neutron Spin

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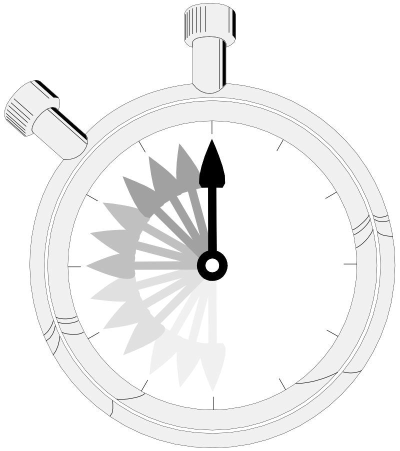
— Yes:

Spin Direction

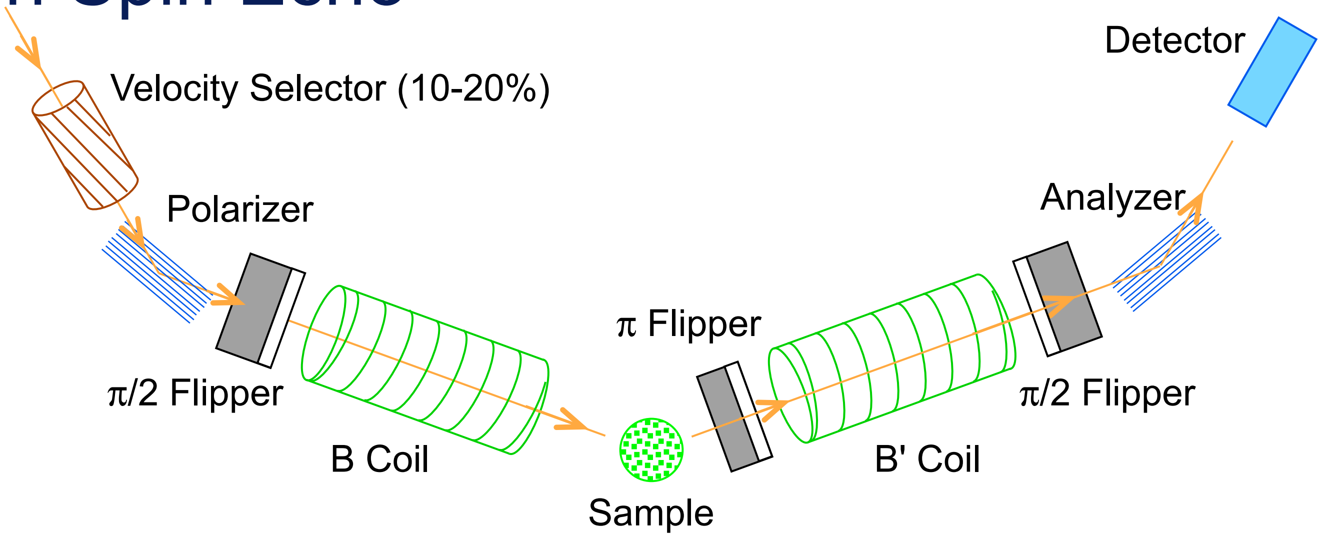
Lecture 7: Larmor precession in constant field:



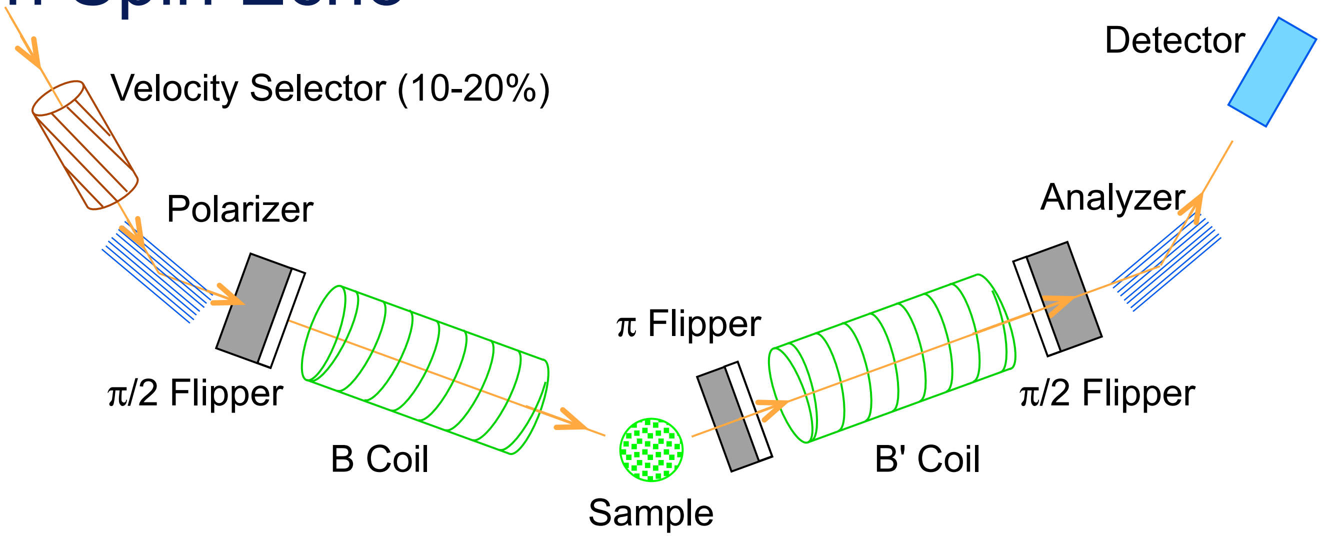
$$\omega_{\mathrm{L}} = \frac{g_{\mathrm{n}}\mu_{\mathrm{N}}}{\hbar} B \leftrightarrow 2900 \, \frac{\mathrm{rot/s}}{\mathrm{Gauss}}$$

... used as individual stop-watch

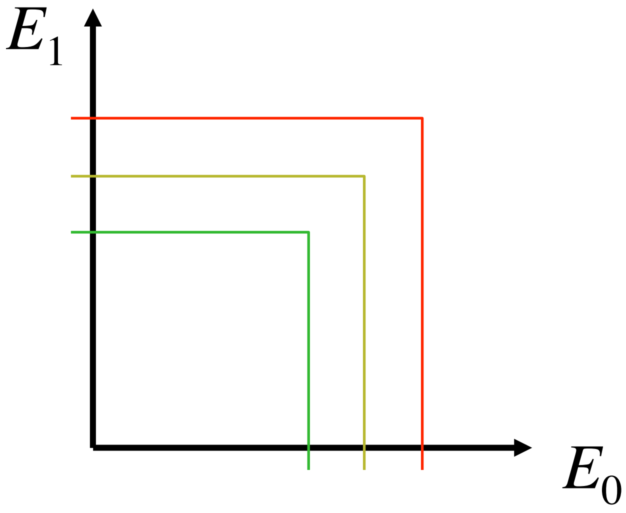
Neutron Spin Echo

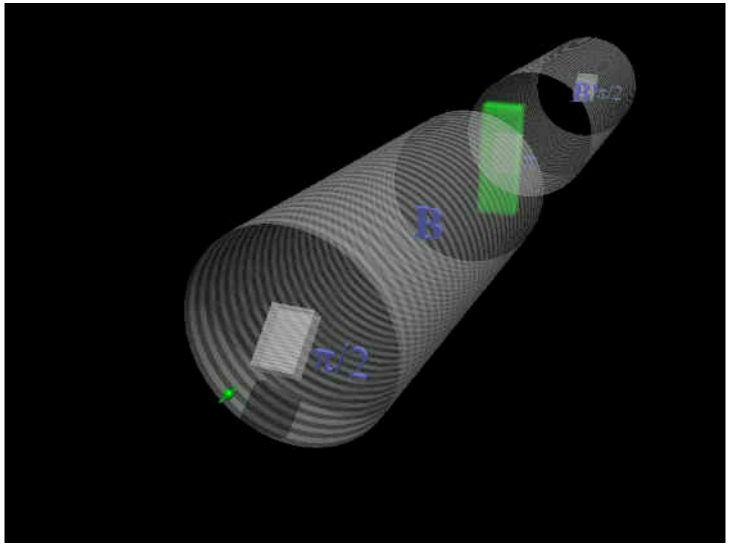


Neutron Spin Echo



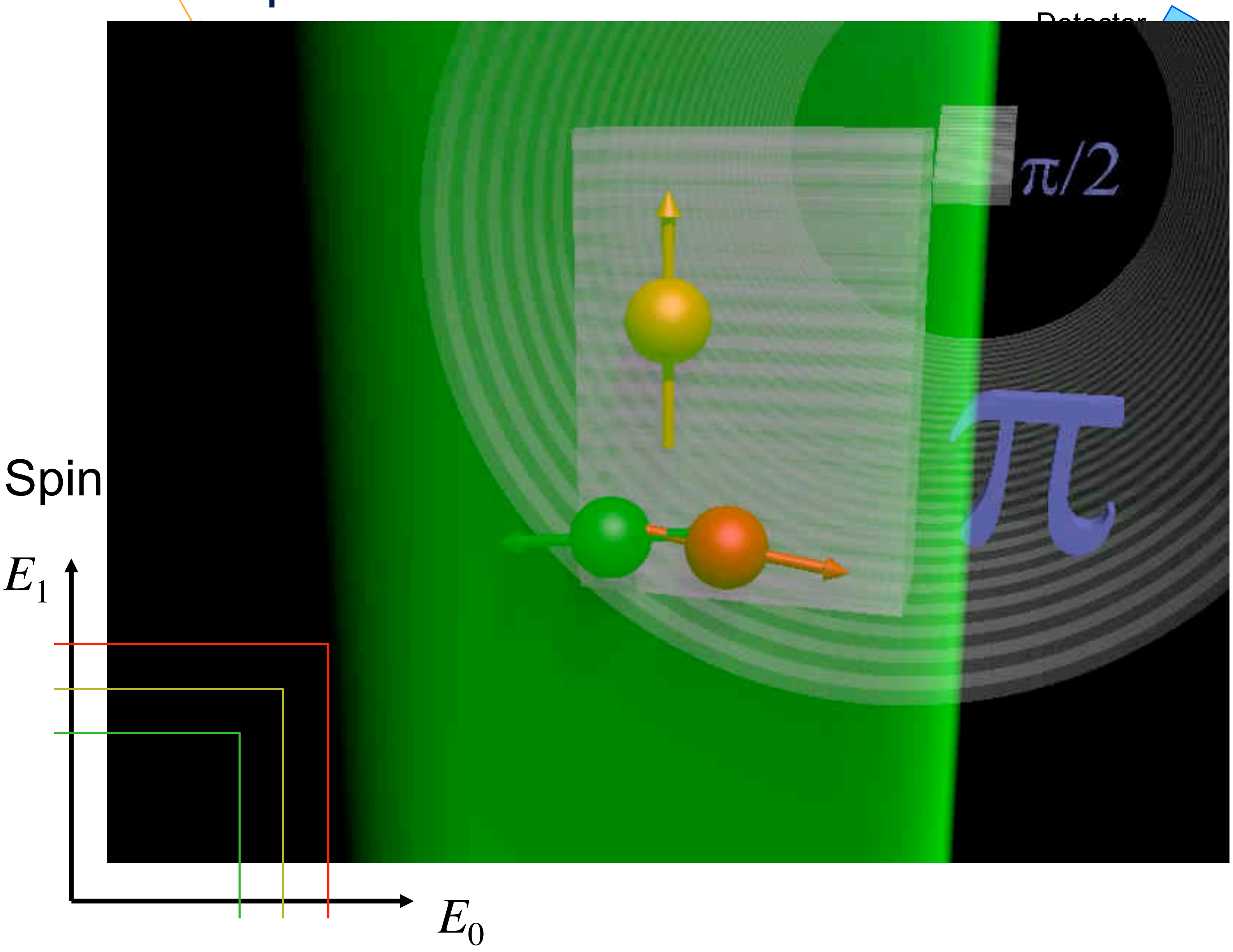
Spin development, elastic:





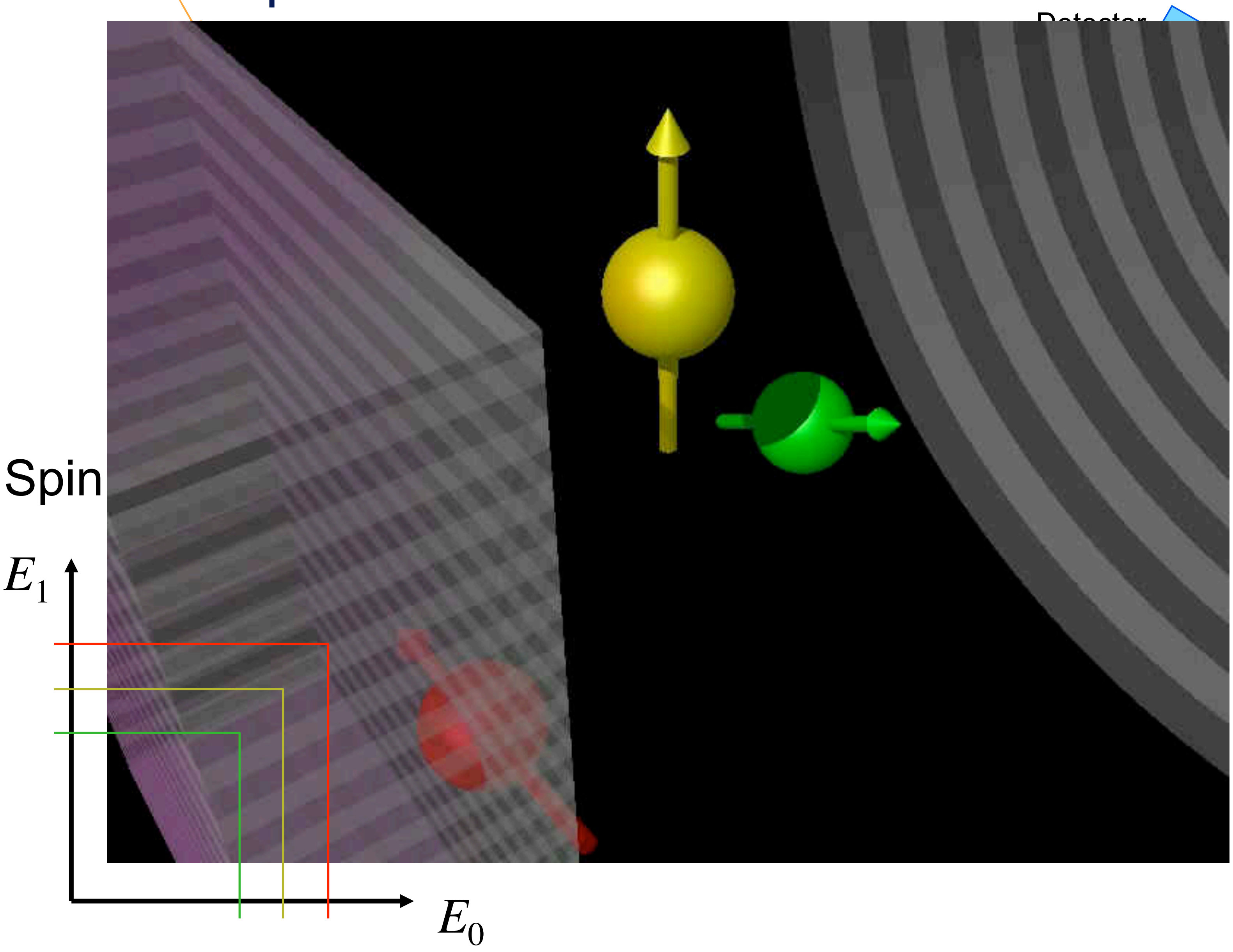
Neutron Spin Echo

Spin

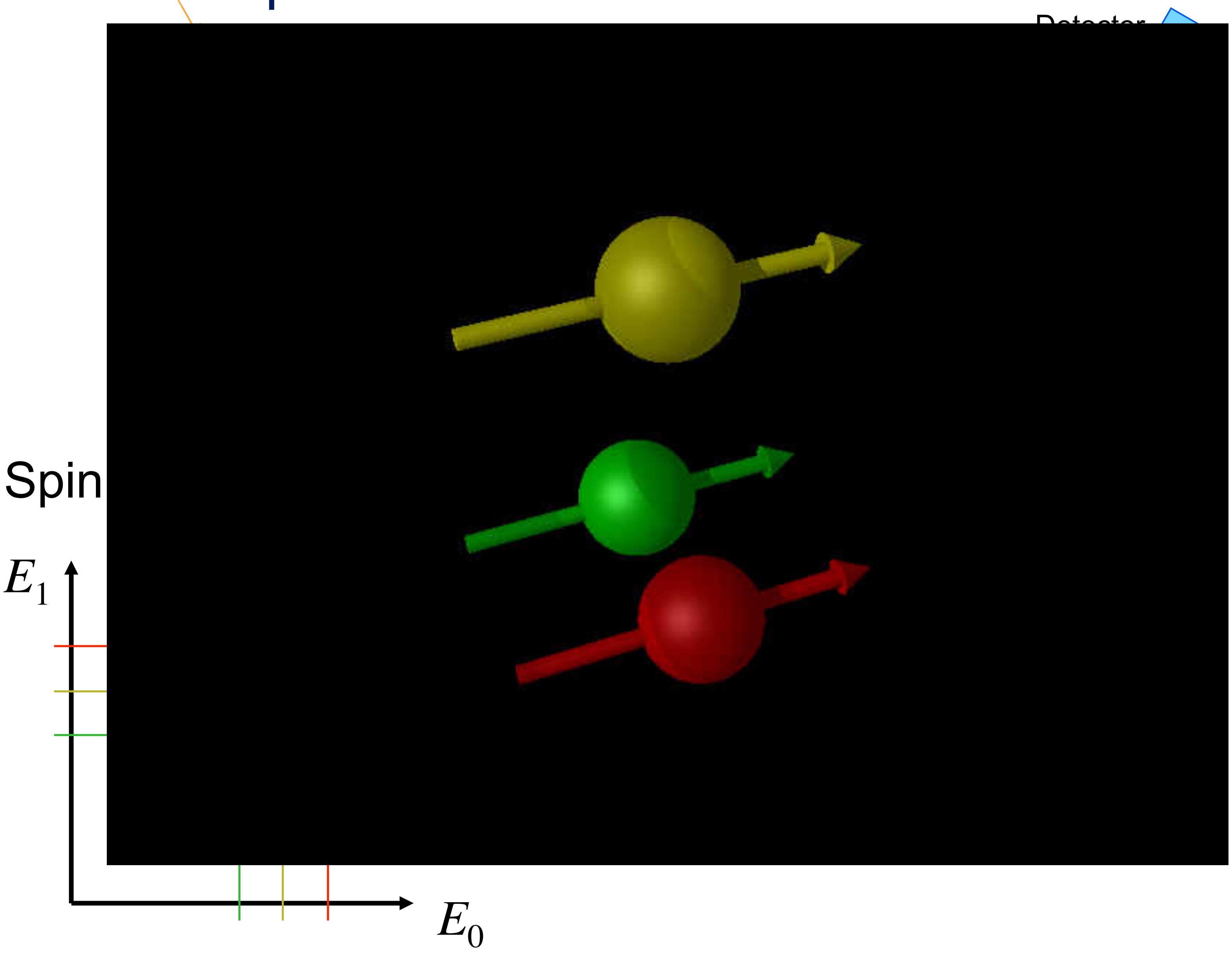


Neutron Spin Echo

Spin

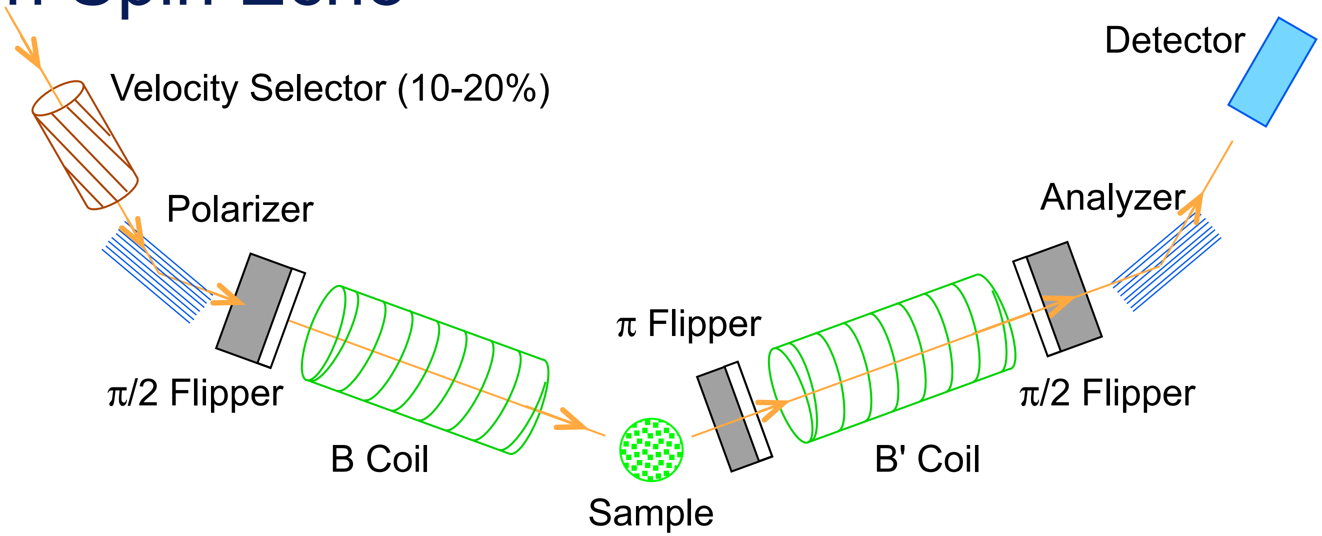


Neutron Spin Echo

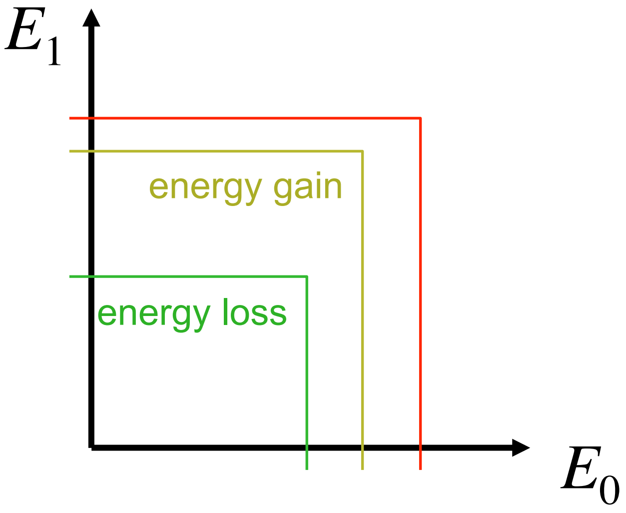


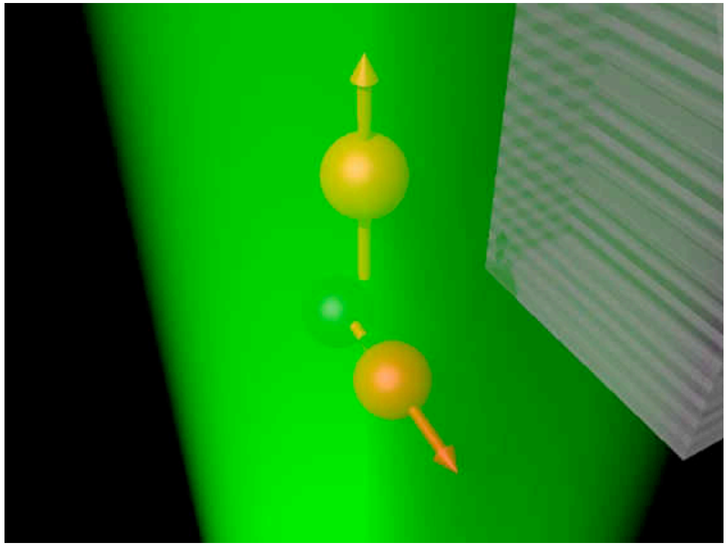
Spin

Neutron Spin Echo



Spin development, inelastic:





Neutron Spin Echo Theory

sensitivity proportional to λ^3

Precession angle mismatch:

$$\Delta\phi = \left(\frac{2\pi|g_\mathrm{n}|\mu_\mathrm{N} m_\mathrm{n}}{h^2}\right) Bl\,(\lambda_\mathrm{f} - \lambda_\mathrm{i}) \approx \underbrace{\frac{|g_\mathrm{n}|\mu_\mathrm{N} m_\mathrm{n} \lambda^3 Bl}{h^3}}_{t_\mathrm{NSE}(B)}\,\omega$$

time parameter proportional to B and current

⇒ Loss of polarization:

$$P = \cos\Delta\phi$$

... averaged over all scattered neutrons:

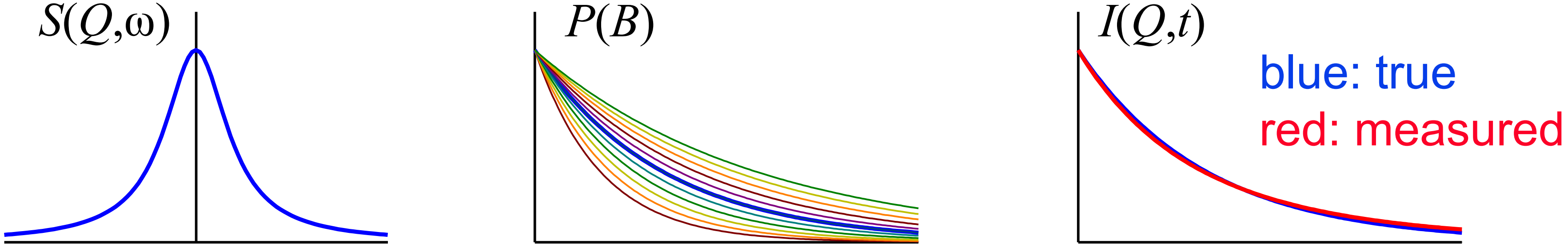
$$P(Q,t_\mathrm{NSE}) = \frac{\int_{-\infty}^{\infty} S(Q,\omega)\cos(\omega t_\mathrm{NSE})\,\mathrm{d}\omega}{\int_{-\infty}^{\infty} S(Q,\omega)\,\mathrm{d}\omega} = \frac{I(Q,t_\mathrm{NSE})}{I(Q,0)}$$

Neutron Spin Echo measures directly the normalized intermediate scattering function!

NSE is not good for non-quasielastic scattering!

Distribution of wavelengths → $P = \left\langle I\left(Q, \left(\frac{\lambda}{\lambda_0}\right)^3 t\right)\right\rangle_\lambda \Big/ I(Q,0)$

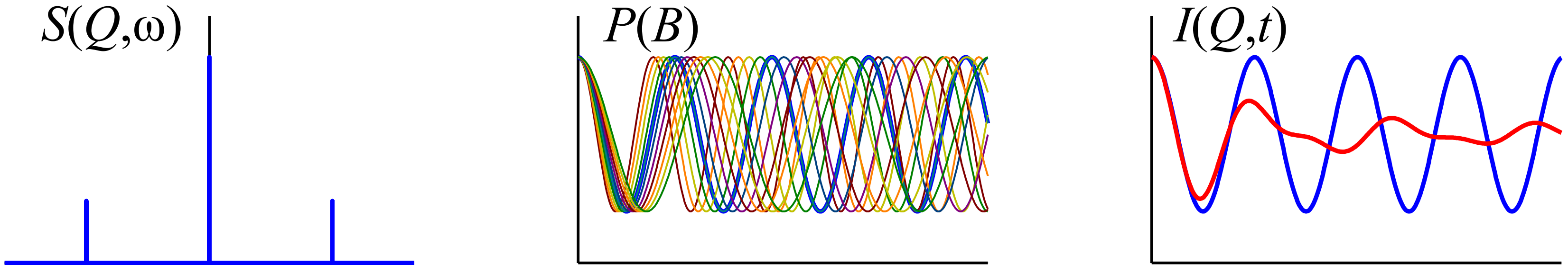
$\Delta\lambda = 20\%$ means $\Delta t = 54\%$! For quasielastic scattering:



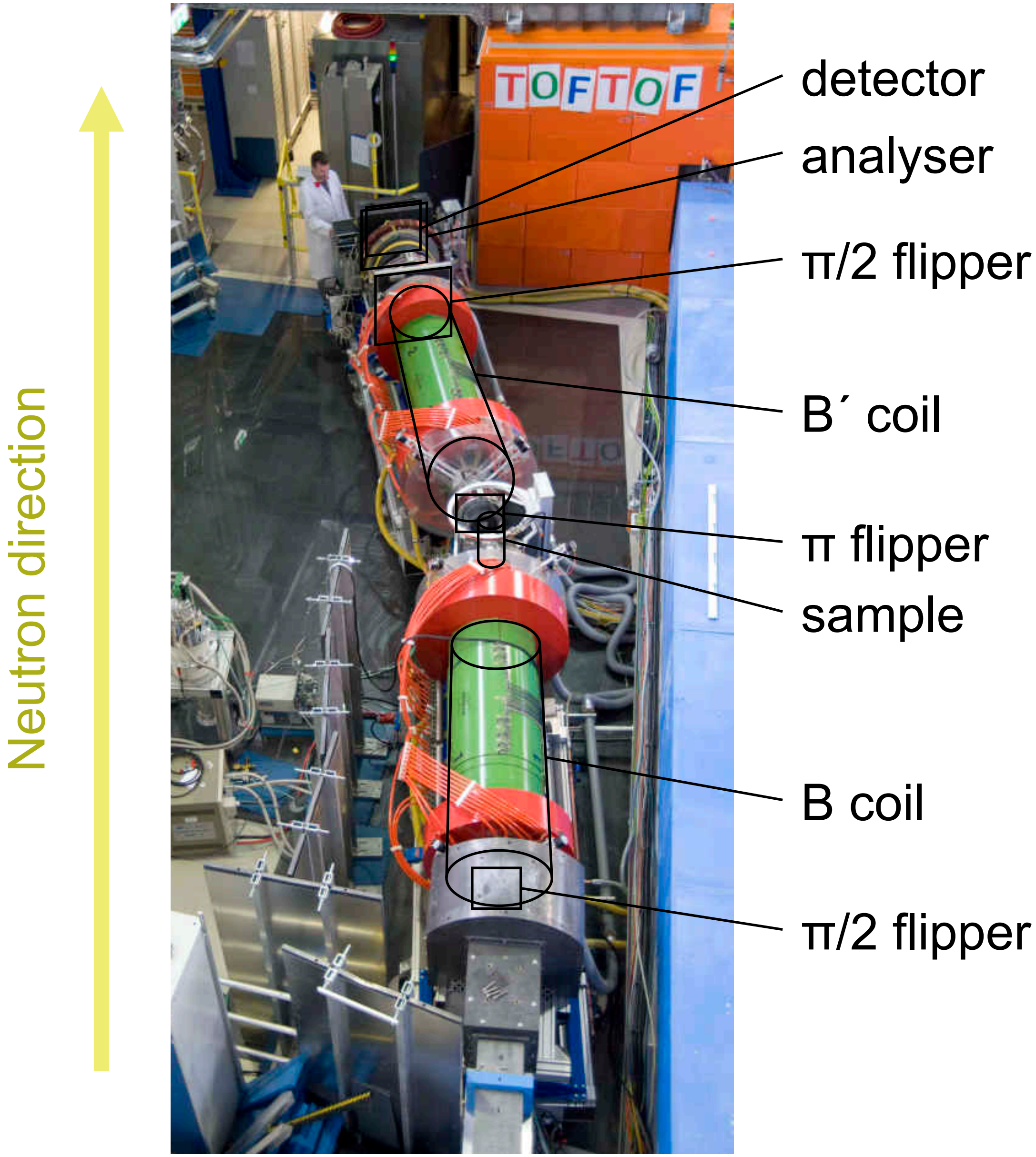
... but still the result looks ok! In addition ‘compensation’:

$\left\langle I\left(\frac{\lambda_0}{\lambda}Q, \left(\frac{\lambda}{\lambda_0}\right)^3 t\right)\right\rangle_\lambda$ for diffusion $= \exp\left(-D\left(\frac{\lambda_0}{\lambda}Q\right)^2 \left(\frac{\lambda}{\lambda_0}\right)^3 t\right) = \exp\left(-\frac{\lambda}{\lambda_0} D Q^2 t\right)$

But for non-quasielastic scattering: (even for $\Delta\lambda = 10\%$ only!)

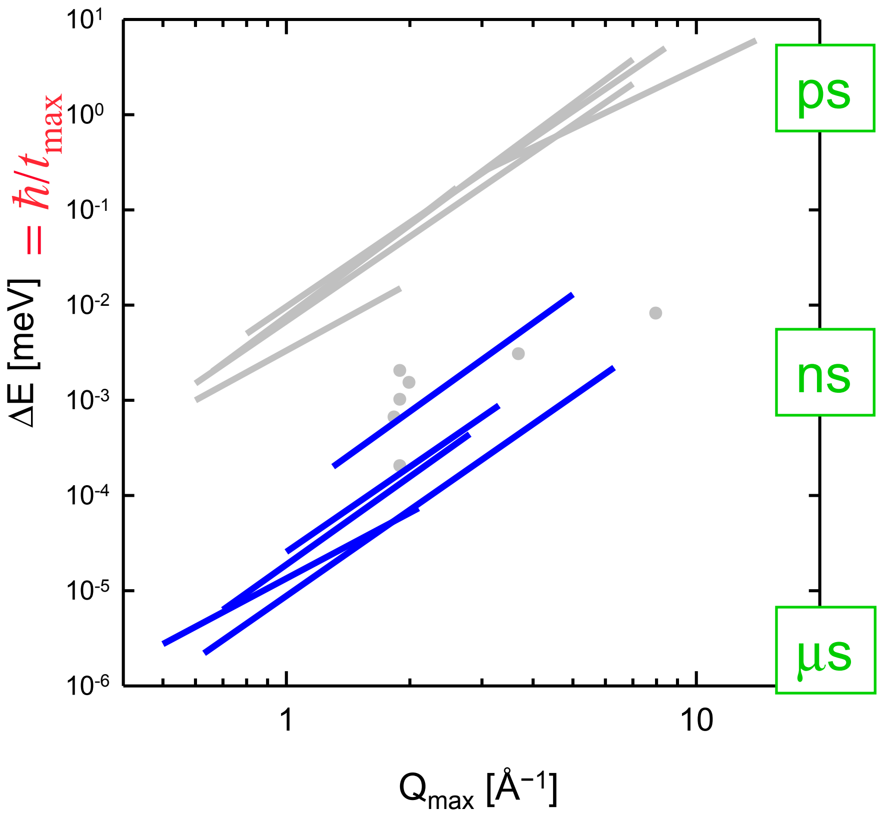


J-NSE in Munich



- ‘Standard’ set-up enhanced by multidetector: simultaneous observation of (narrow) Q range
- Highly efficient correction coils
- Time limit: 350 ns

Specifications of NSE Instruments



Special features:

J-NSE:	optimized correction coils
IN15:	focusing mirror
SPAN:	multidetector
NSE@SNS:	pulsed beam at spallation source

INS: summary of methods

3AX

ΔE > 100 µeV
t < 20 ps

- \+ flexibility of Q, ω setting and resolution
- – low efficiency hours / single-Q spectrum
- – resolution often not sufficient

TOF

ΔE > 10 µeV
t < 0.2 ns

- \+ high efficiency ≈ 2h / Q-set of spectra
- \+ simultaneously accessible Q range
- – resolution often not sufficient

BS

ΔE > 1 µeV
t < 2 ns

- \+ simultaneously accessible Q range
- \+ better than NSE for excitations
- – low efficiency ≈ 12h / Q-set of spectra
- – Doppler: short $\hbar\omega$ range (±30 µeV)

NSE

ΔE > 2 neV
t < 1 µs

- \+ measures $I(Q,t)$ directly
- – low efficiency ≈ 6h / single-Q spectrum
- – (except few) only single Q vector
- – less efficient for incoherent scattering