Forschungszentrum Jülich

Neutron Spin-echo Spectroscopy

Part 1: generic technique and application (continuous & pulsed)

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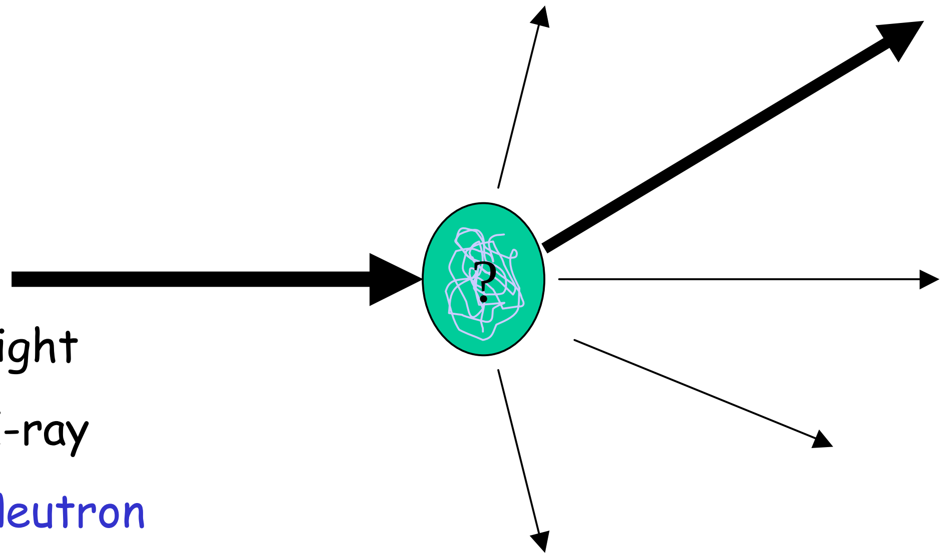
Scattering Experiment

$$k = \frac{2\pi}{\lambda}$$



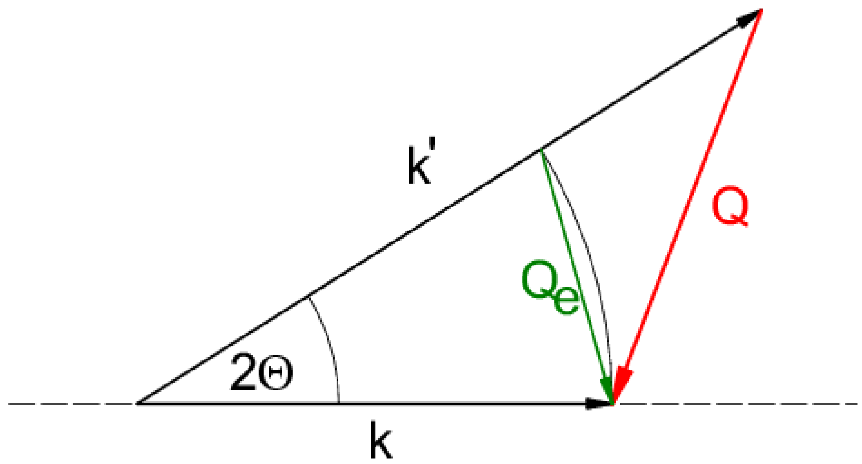
Light

X-ray

Neutron

……

Reveals structure and eventual Dynamics



Relations for neutrons

- $k = 2\pi / \lambda$ wavenumber → wavelength
- $k = 2\pi\, mv/h$ wavenumber → momentum
- $\lambda = h / mv$ wavelength → velocity
- $E = \frac{1}{2}\, mv^2$ energy → velocity
- $E = \frac{1}{2}\, h^2/m^2\lambda^2$ energy → wavelength
- ……

momentum transfer

$$\underline{Q} = \underline{k}_i - \underline{k}_f$$

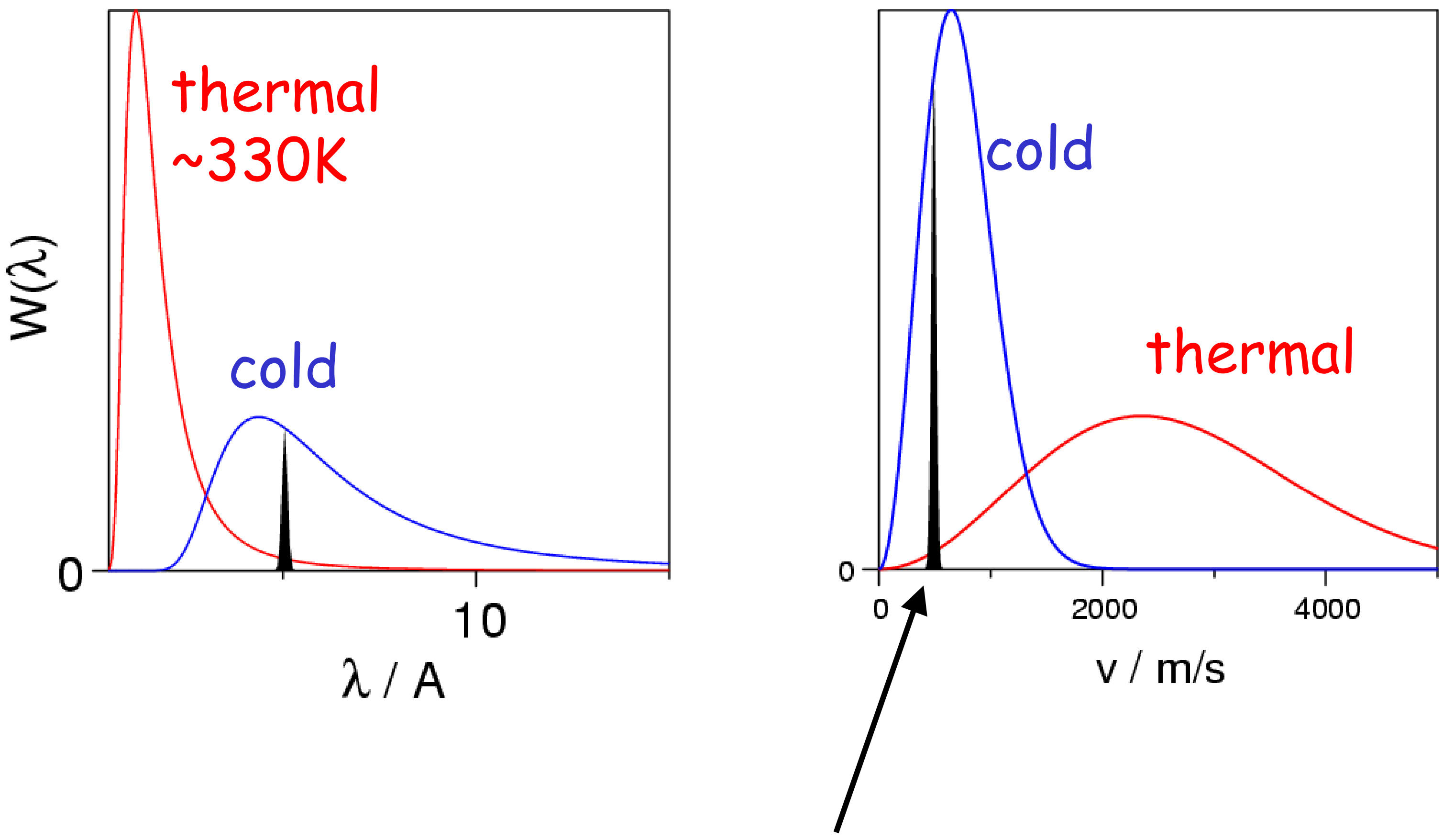
energy transfer

$$\Delta E = E_i - E_f = \hbar\omega$$

$$= \frac{1}{2}\, h^2/[m^2\ (\lambda^2_i - \lambda^2_f)]$$

$$= \frac{1}{2}\, m\ (v^2_i - v^2_f)$$

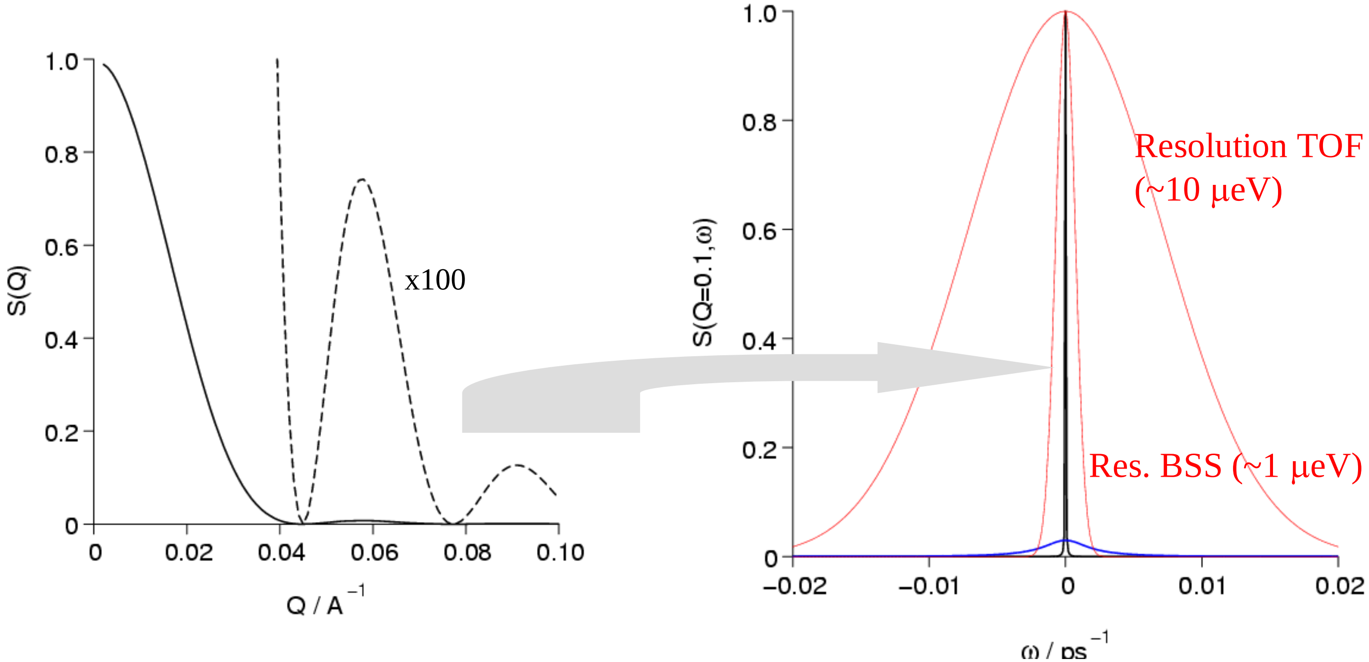
Neutron sources yield Maxwellian type spectra



E=1.3 meV → 2 x 10^{12} s^{-1}

Sphere R=100Å

Diffusion in “water”

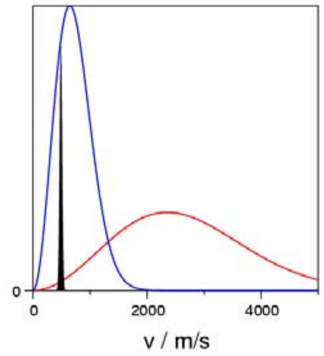


SANS

$\omega \sim \Delta v$

$\Delta v/v < 10^{-4}$

Need to detect Δv smaller than 10^{-4} v

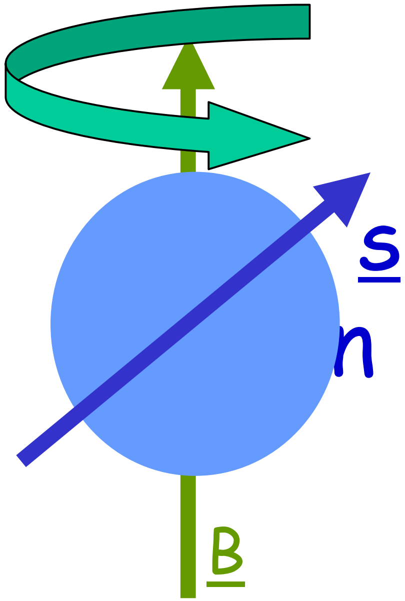


direct filter-filter

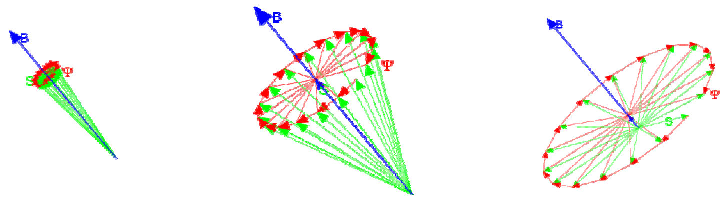
NO intensity !

Spin-echo trick:

use precessing neutron spin as watch !



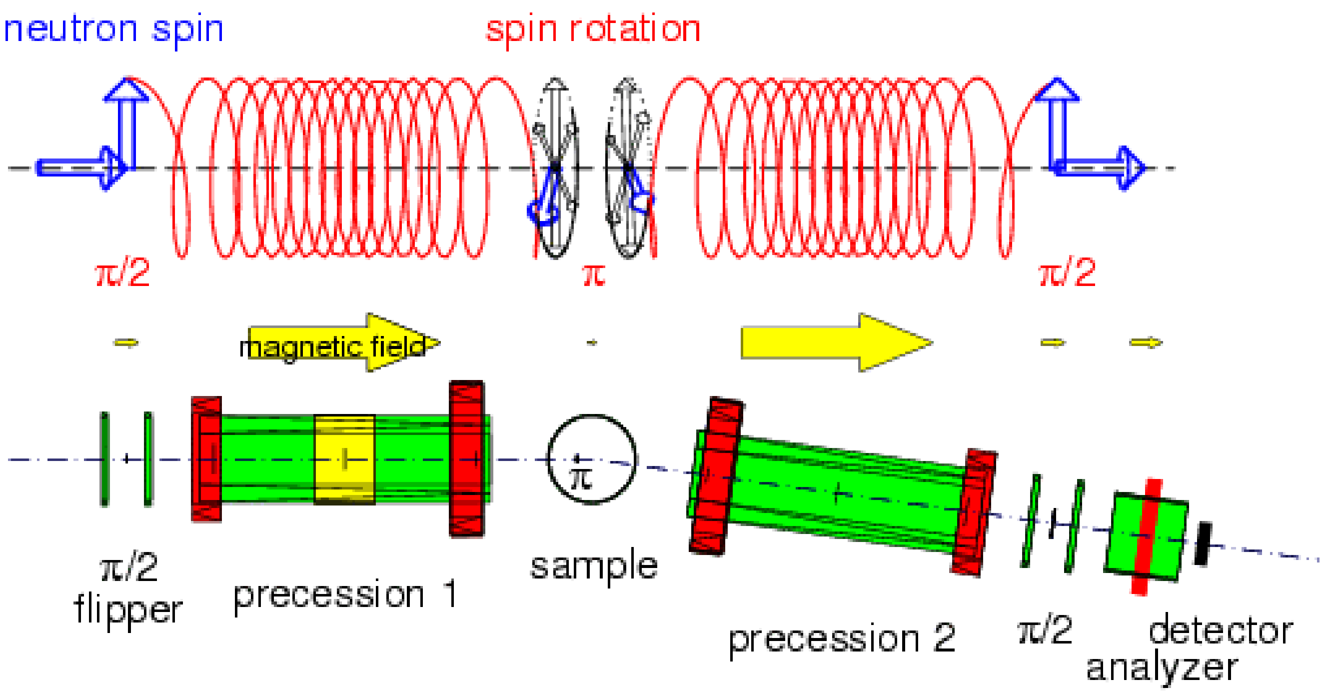
$$d\underline{s}/dt = \gamma\, \underline{s} \times \underline{B}$$

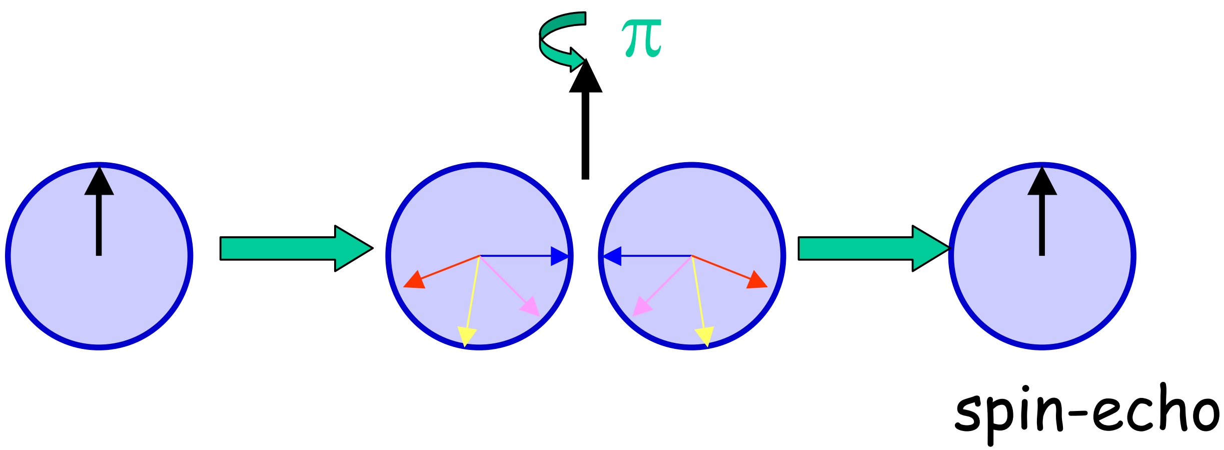


$$\Omega = \gamma\, B$$

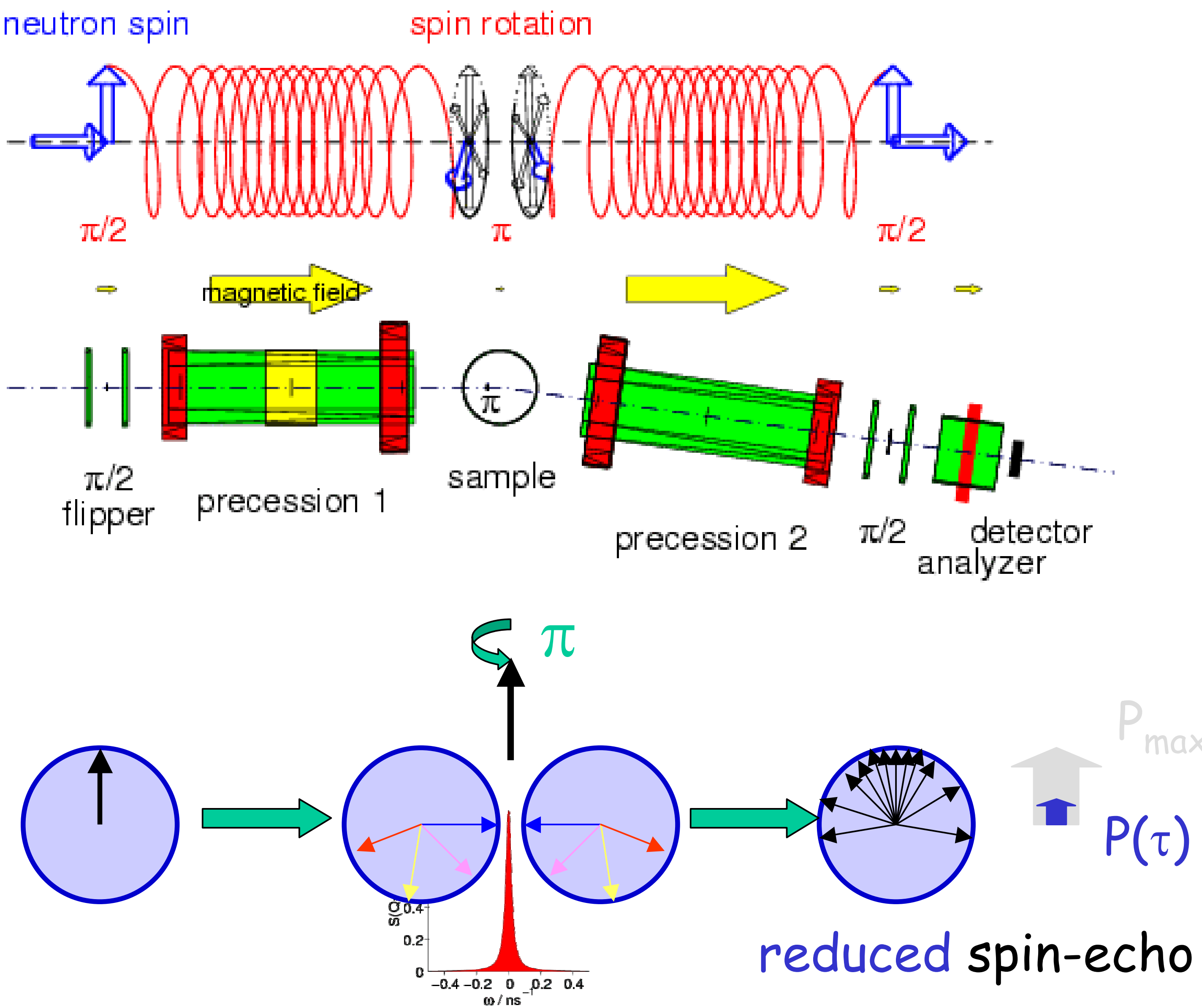
~3000 Hz at 1 Gauss

NSE spectrometer

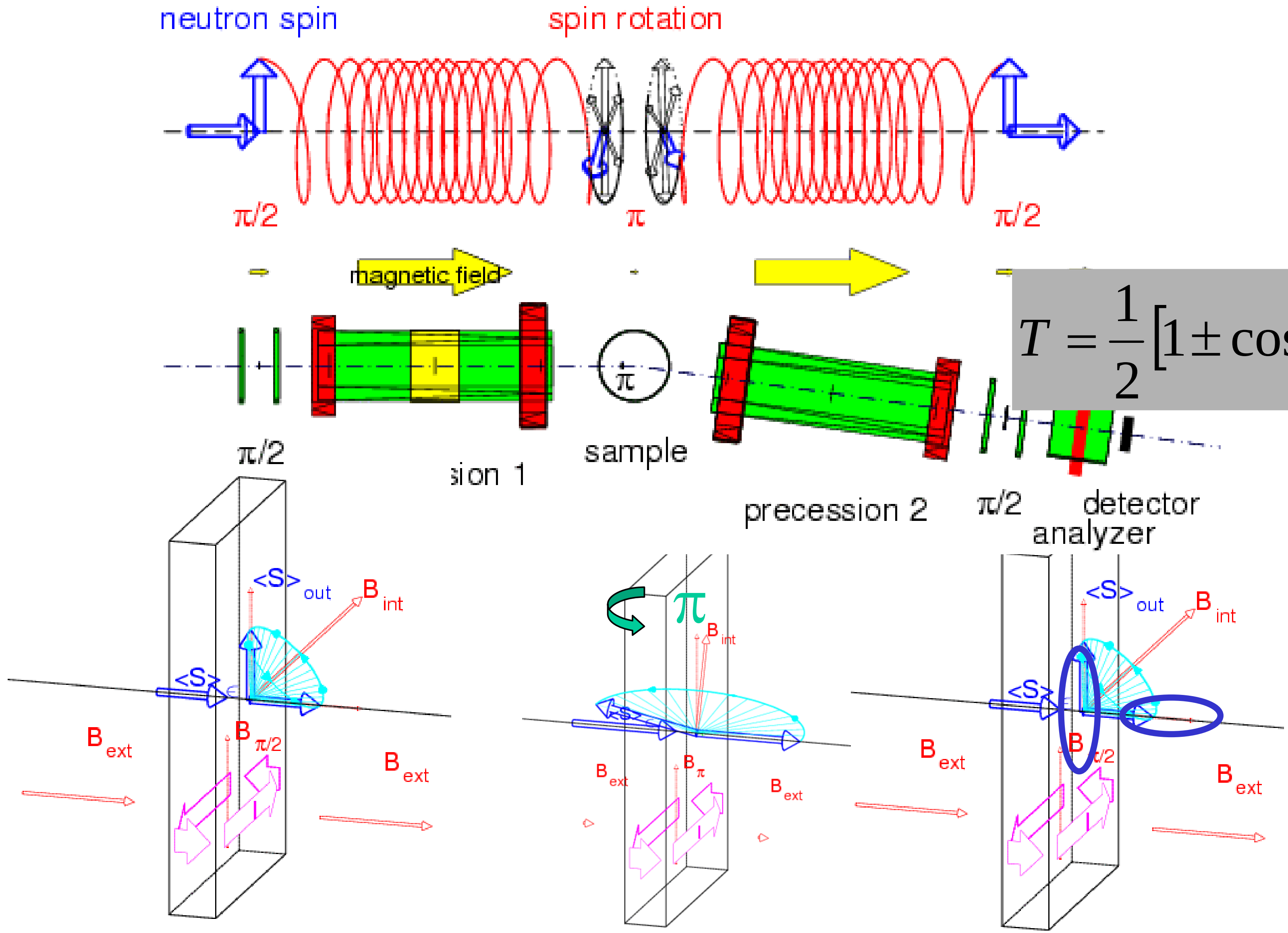




NSE spectrometer: (quasielastic scattering)



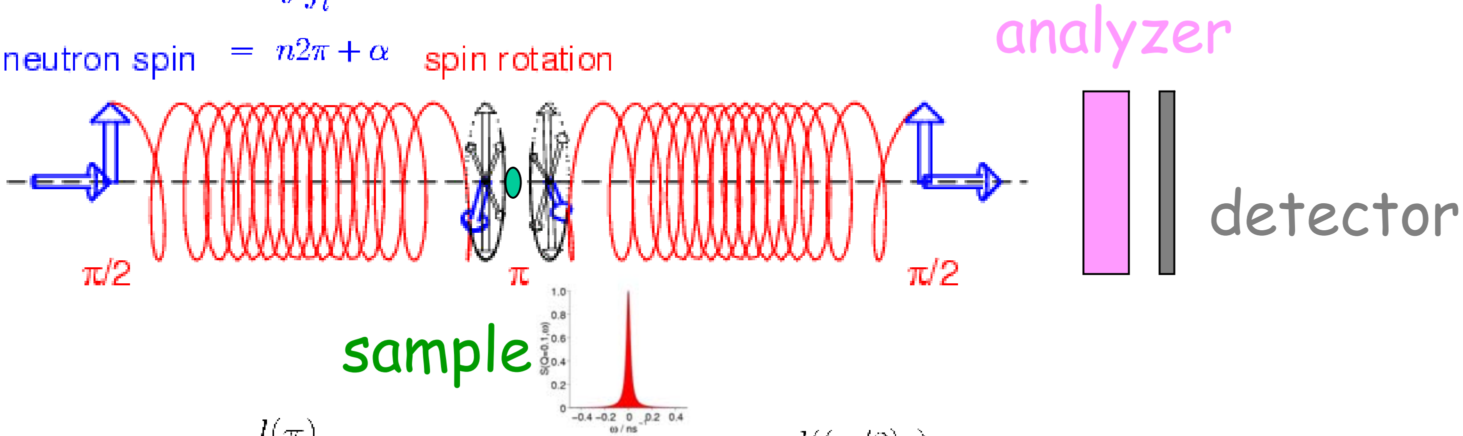
NSE spectrometer: technical aspects



$$T = \frac{1}{2}\left[1 \pm \cos(\psi)\right]$$

$$\Psi = \frac{\gamma}{v}\int_l |B| dl$$

neutron spin $= n 2\pi + \alpha$ spin rotation



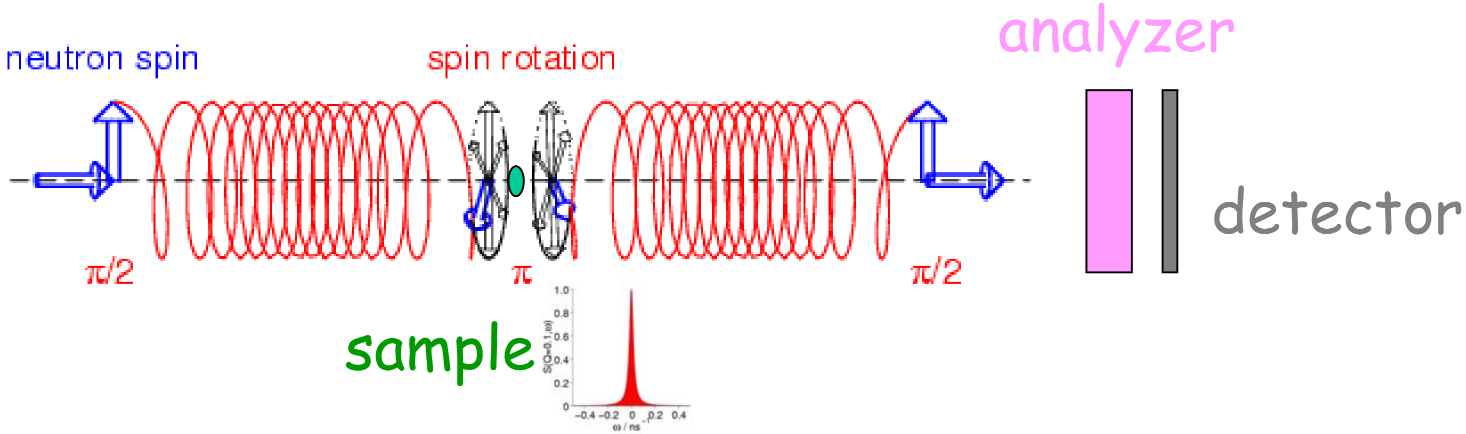
$$J_1 = \int_{l((\pi/2)_1)}^{l(\pi)} |B| dl \qquad J_2 = \int_{l(\pi)}^{l((\pi/2)_2)} |B| dl$$

$$\Psi_{1,2} = -\frac{\gamma J_1}{v} + \frac{\gamma J_2}{v + \Delta v} + 4n\pi$$

$$T_a = \frac{1}{2}\left[1 + \cos(\underbrace{-\frac{\gamma J_1}{v} + \frac{\gamma J_2}{v+\Delta v}}_{\Delta\Psi})\right]$$

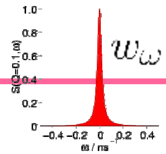
$$I = \eta S(Q) \iint \frac{1}{2}\left[1 \pm \cos(-\frac{\gamma J_1}{v} + \frac{\gamma J_2}{v+\Delta v})\right] w_\omega(\Delta v) w_\lambda(v)\, d\Delta v\, dv$$

NSE what do we measure ?



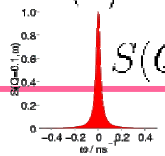
$$I = \eta S(Q)$$

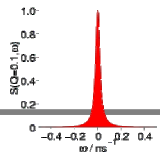
$$\iint \frac{1}{2}\left[1 \pm \cos\left(-\frac{\gamma J_1}{v} + \frac{\gamma J_2}{v + \Delta v}\right)\right] w_\omega(\Delta v) w_\lambda(v)\; d\Delta v\; dv$$



$$I = \eta/2$$

$$\iint \left[1 \pm \cos\left(-\frac{\gamma J_1}{(h/m_n)\lambda^{-1}} + \frac{\gamma J_2}{(h/m_n)\lambda^{-1} + \lambda\omega/2\pi}\right)\right] S(Q,\omega) w_\lambda(\lambda)\; d\omega\; d\lambda$$





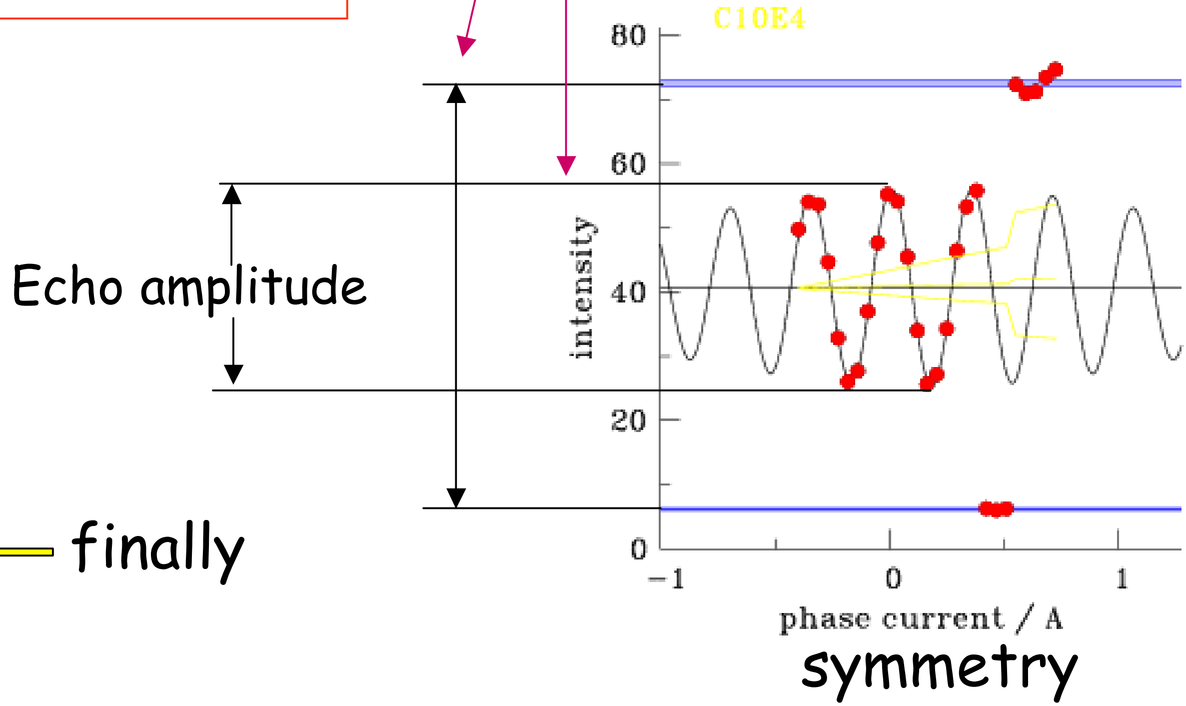
$$I = \eta \frac{1}{2}\left[S(Q) + \underbrace{\int \cos(\underbrace{\gamma J \frac{m_n^2}{h^2 2\pi}\lambda^3}_{t}\;\omega) S(Q,\omega) d\omega}_{S(Q,t)}\right]$$

The NSE signal, where is the information?

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

$t \sim \lambda^3$!

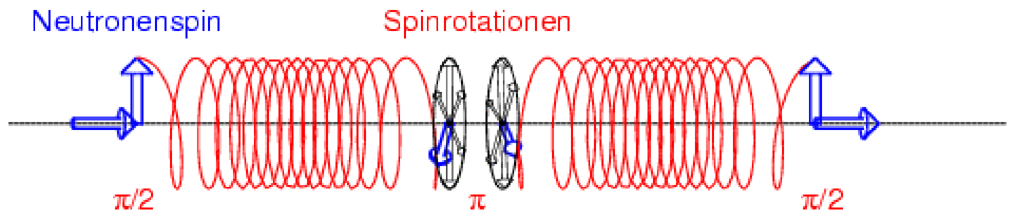
$$J_{\perp} = \int_{l((\pi/2)_{\perp})}^{l(\pi)} |B|\, dl$$

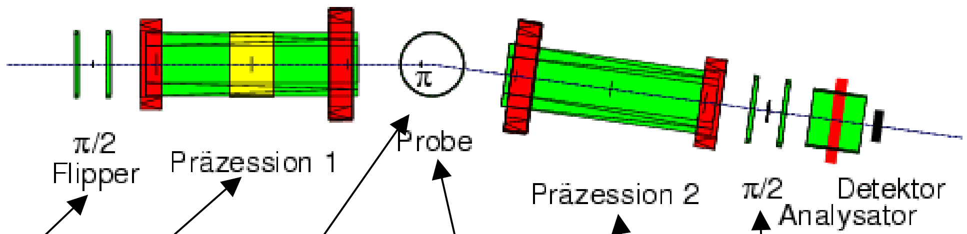


$$\frac{S(Q,t)}{S(Q)}$$ ⟸ finally

Principle of NSE : Summary

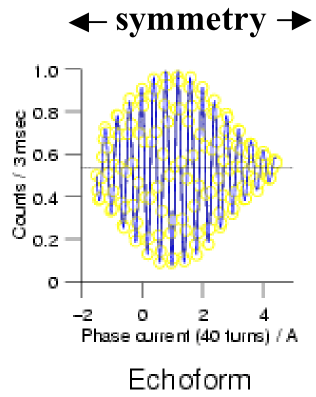
Polarized beam

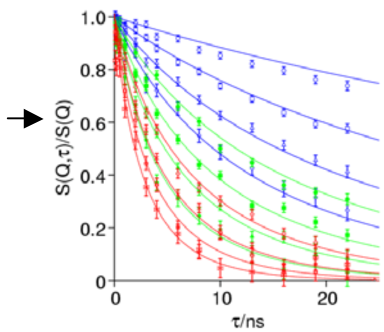




Start---run---timereversal---sample---run---Stop-readout

States of the indivdual spin-clocks





$$\tau \sim \lambda^3 BL$$

State of the art:

$\tau \sim \lambda^3$ **BL**

IN15

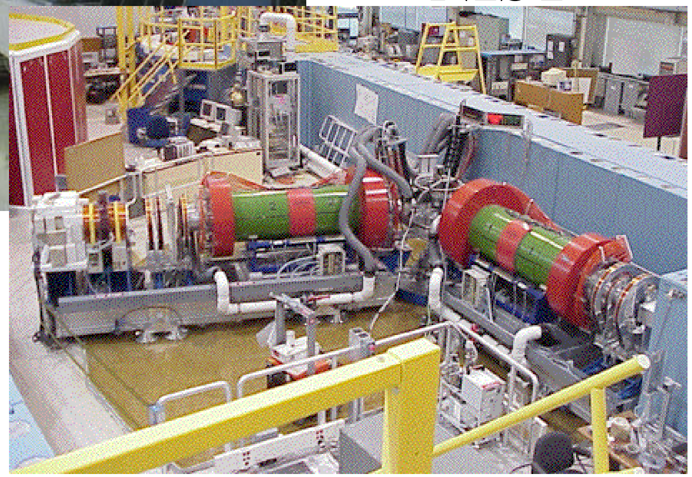
- t > 200 ns ! @ λ = 1.6 nm
- Very low Q option

FZJ-NSE

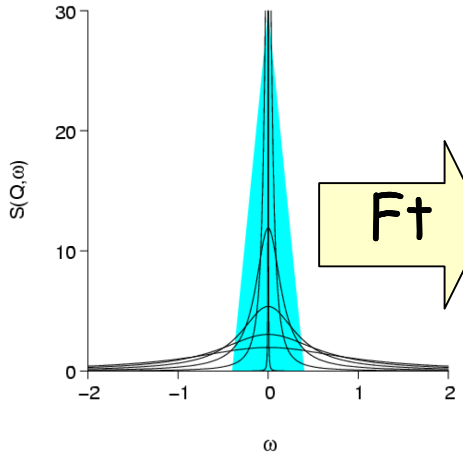
- compensated (low+high Q,stablility)
- solid angle (area detector)
- automatic setup
- t > 25 ns @ λ=0.8 nm

FZJ

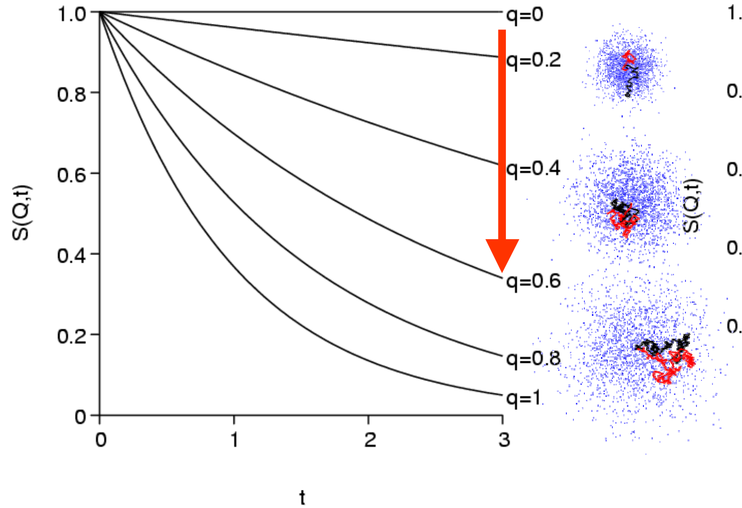
NIST

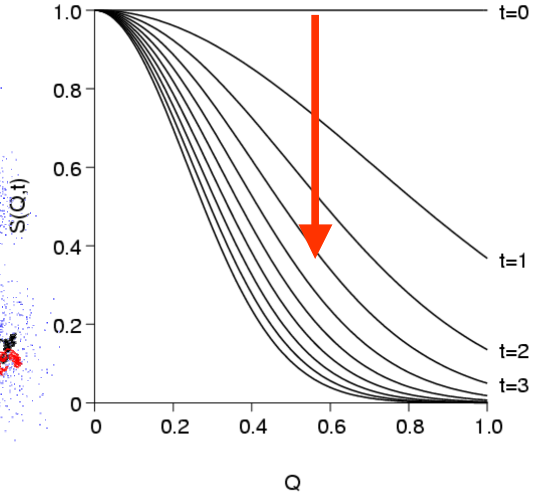


Intermediate scattering function S(Q,t):
Ex. simple diffusion



Ft



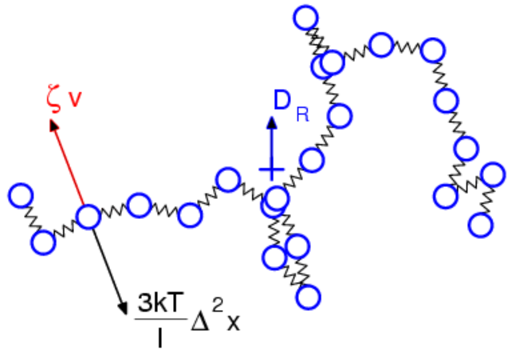


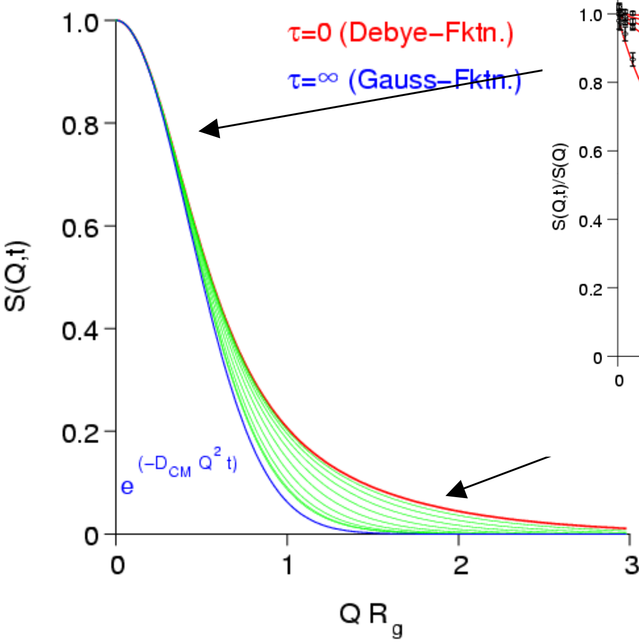
Ft(R,τ→Q,ω)

Ft(R→Q)

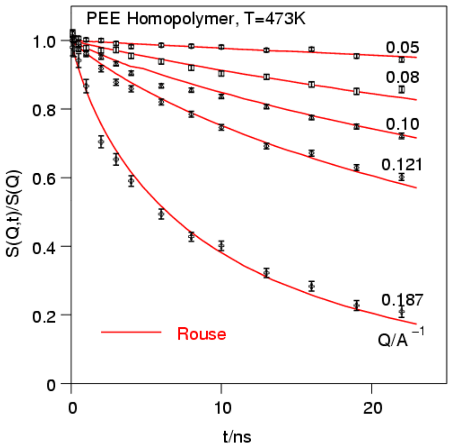
$$G(R,\tau) = \langle \rho(r+R,t+\tau)\rho(r,t) \rangle$$

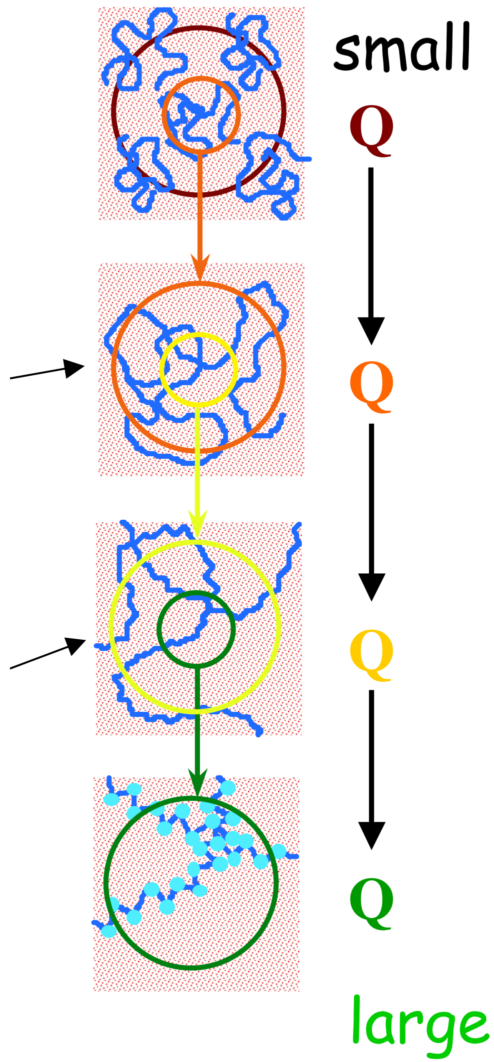
See the segmental dynamics of a linear polymer



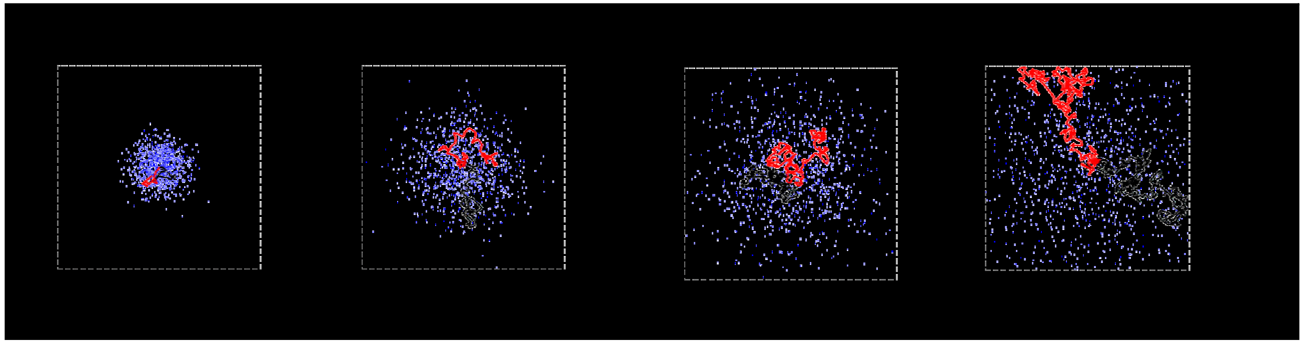


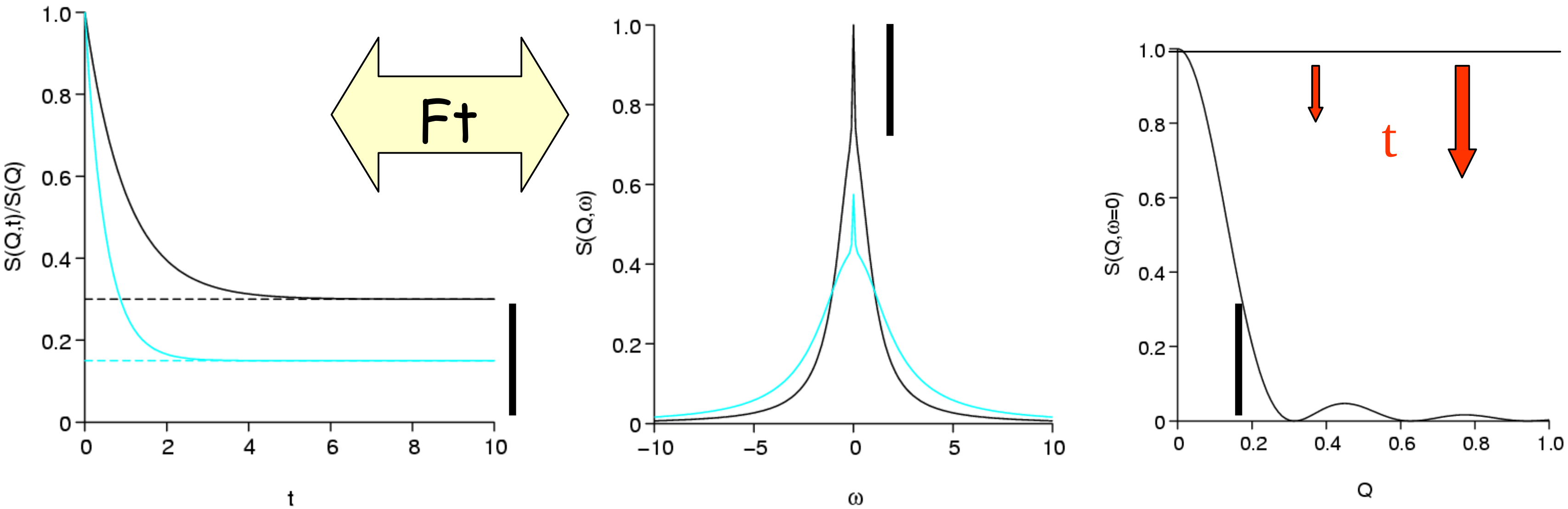
Rouse dynamics of a polymer coil





NSE (intermediate scattering function) and the EISF



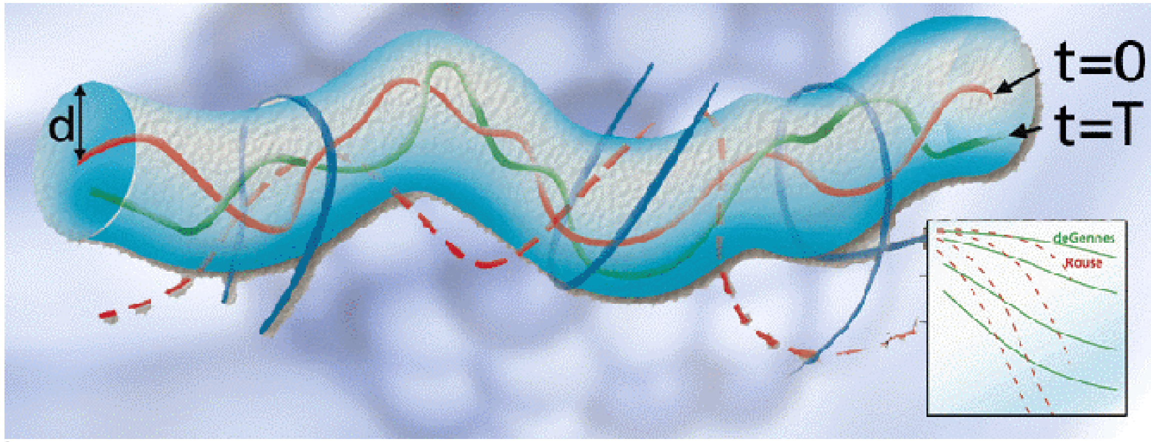


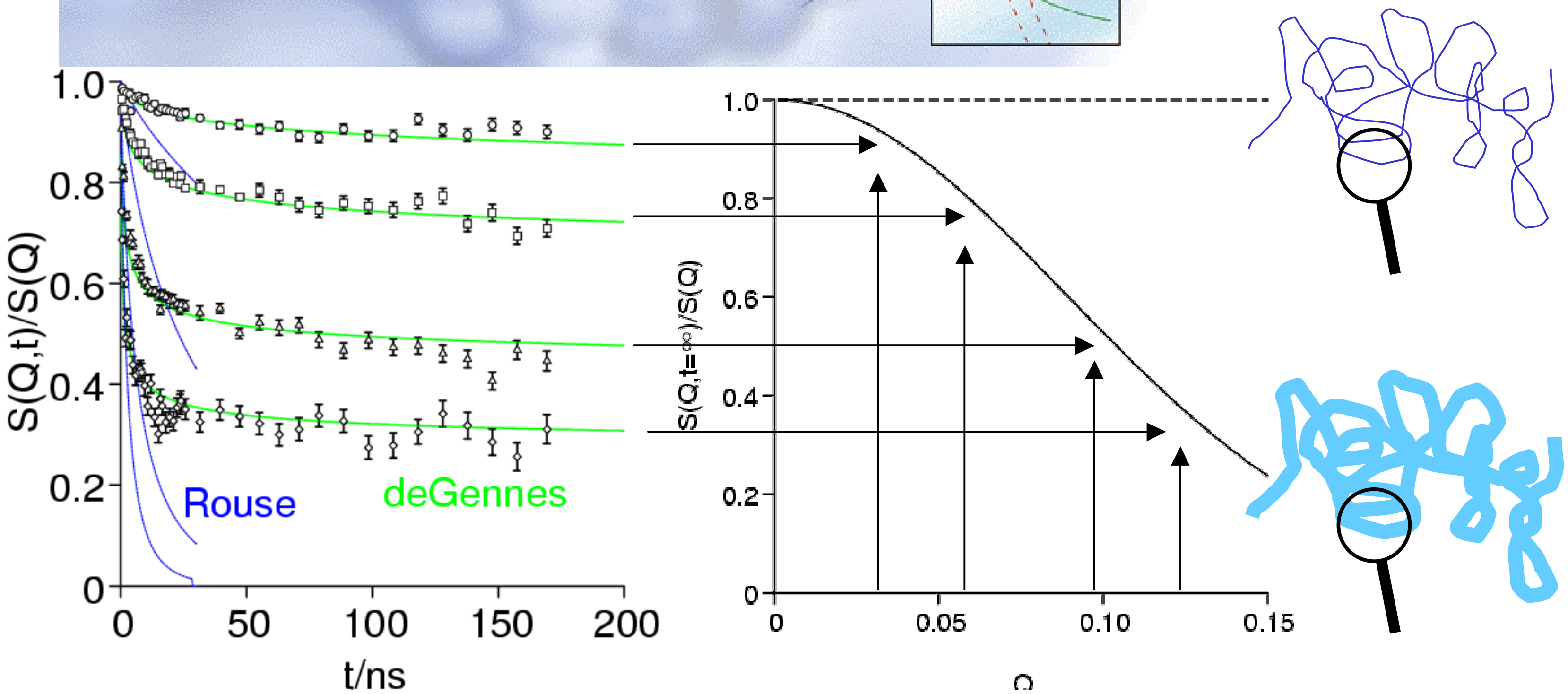
Reptation model (Edwards/deGennes)

Confinement in a tube seen by NSE

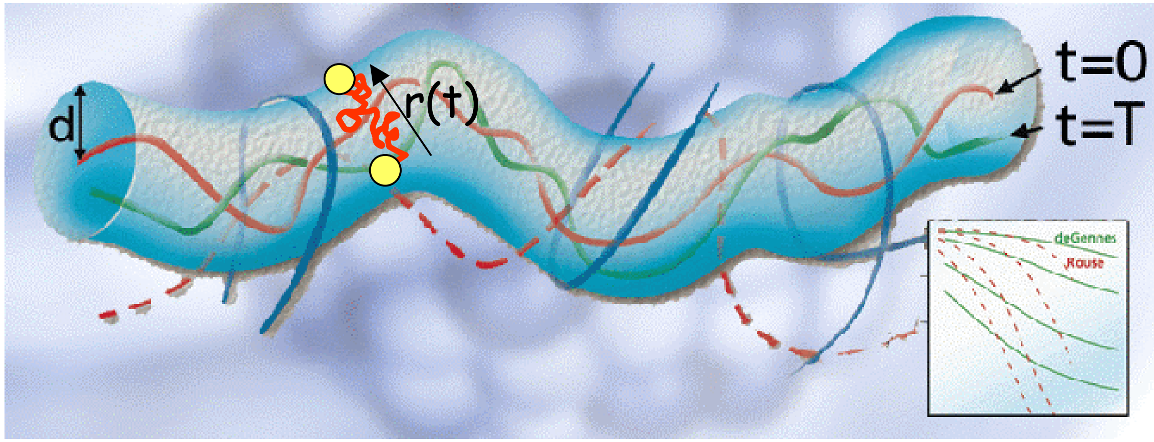
coherent scattering, labeled chain

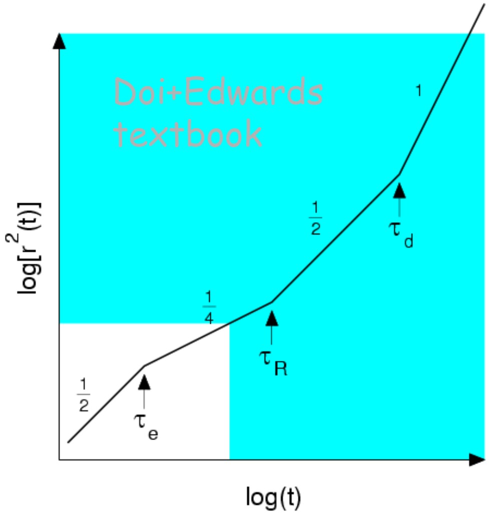
melt of long chain linear polyethylene

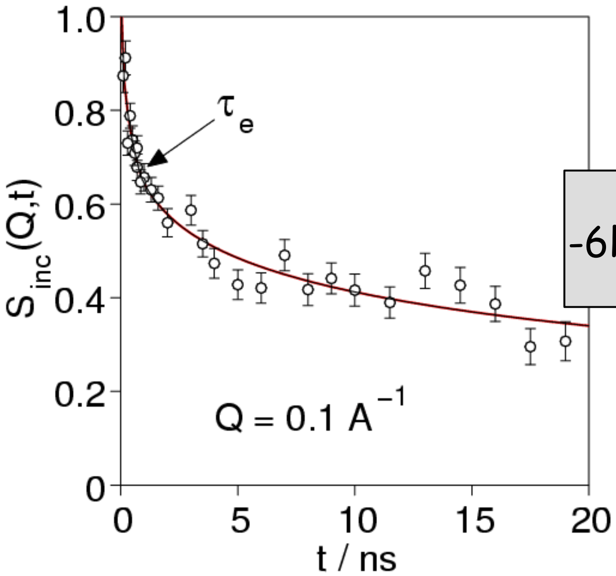




Segment displacement r(t) from incoherent scattering

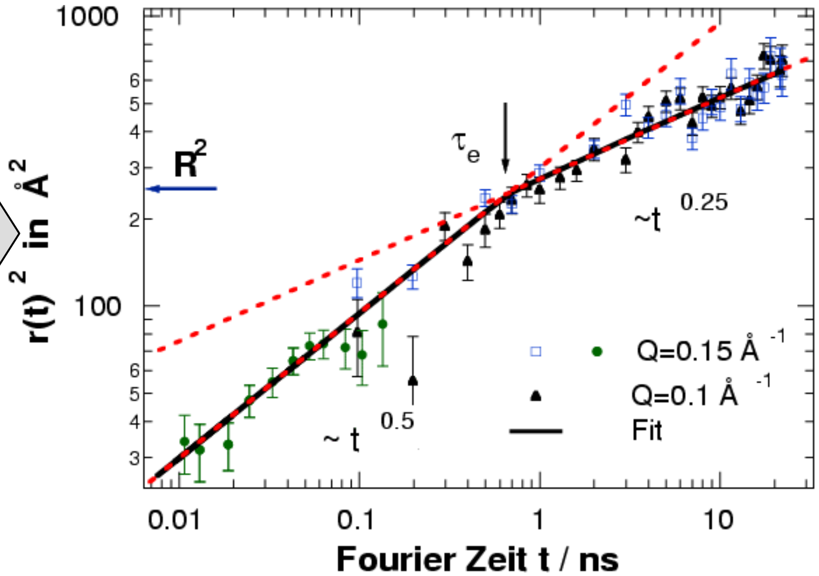






$-6\ln[S(Q,t)]/Q^2$

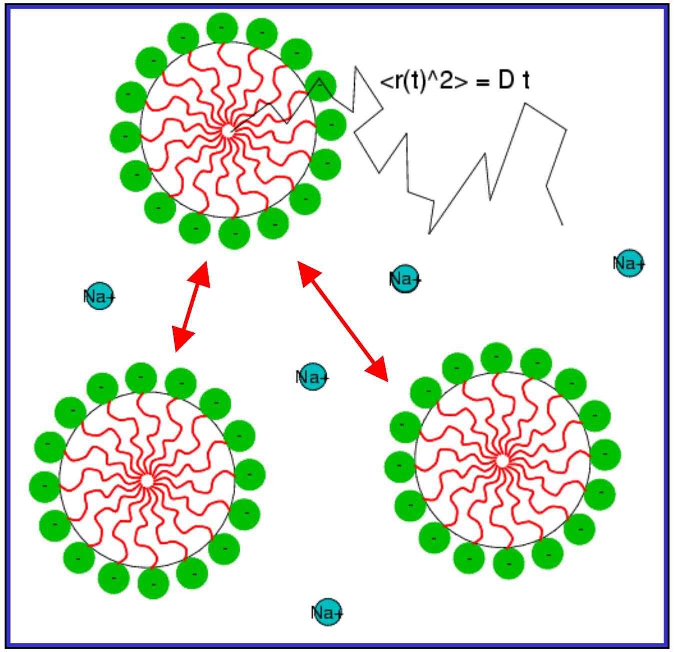
Caveat!

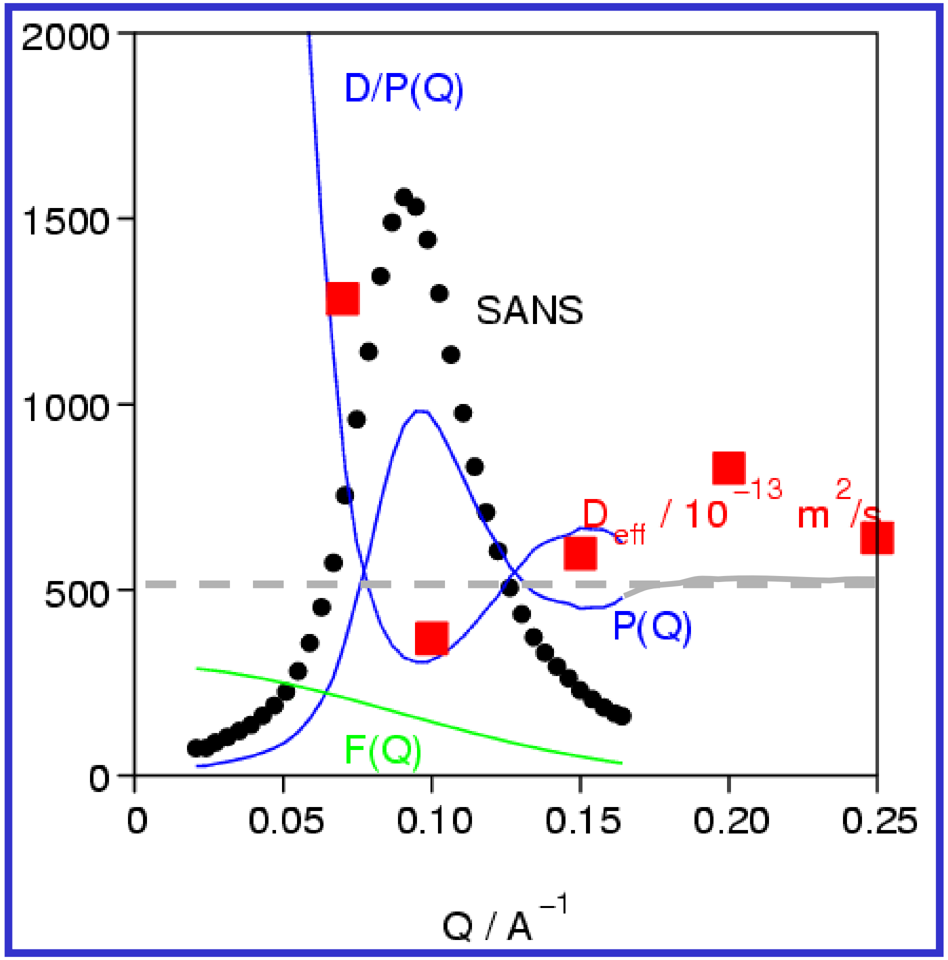


Modified diffusion → interactions

Example:

SDS micelles in D_2O





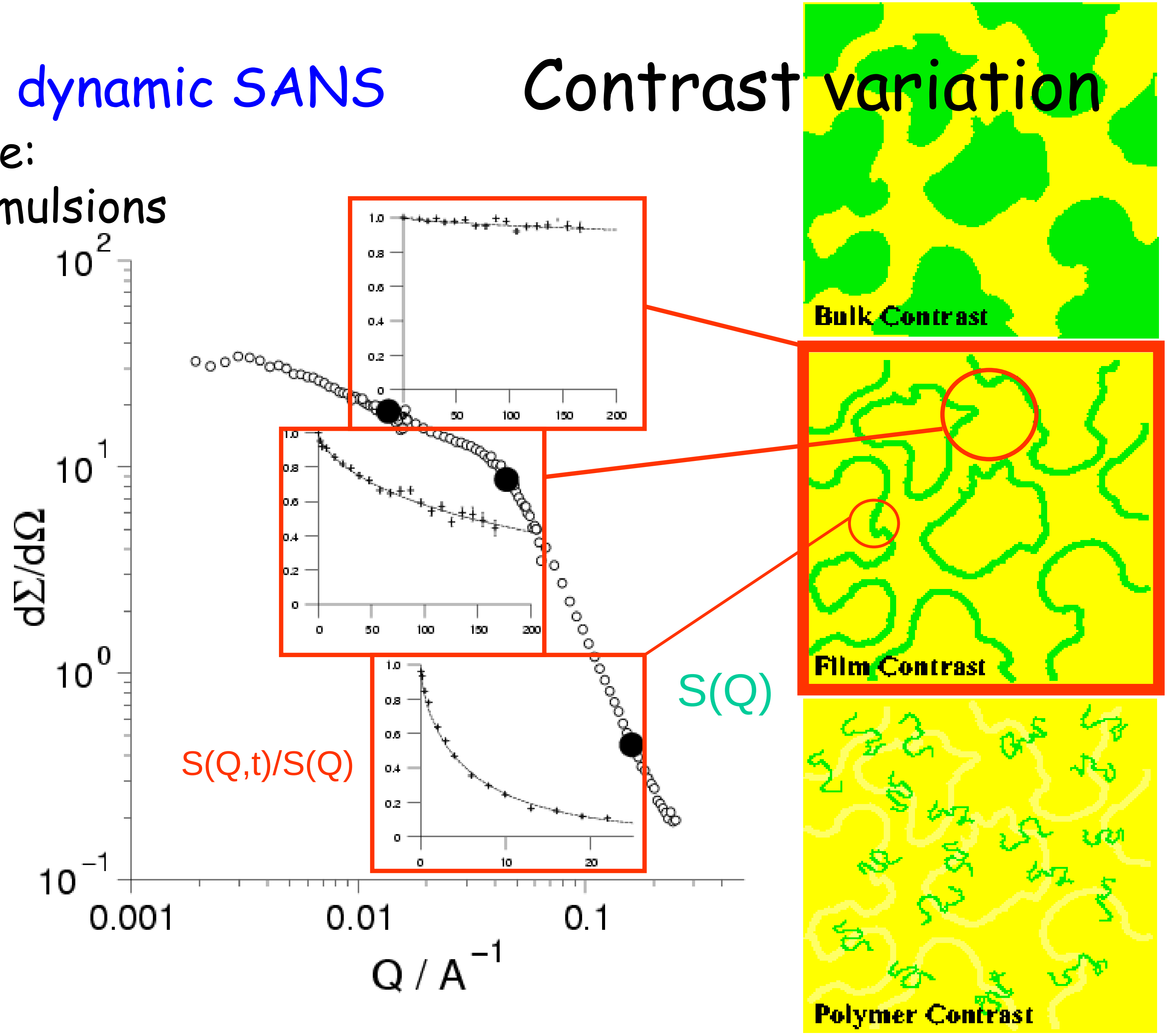
$$D_{eff} = D_0 \, H(q)/P(q)$$

Friction (ηr) x hydrodynamic interac. x susceptibility 1/P(Q)

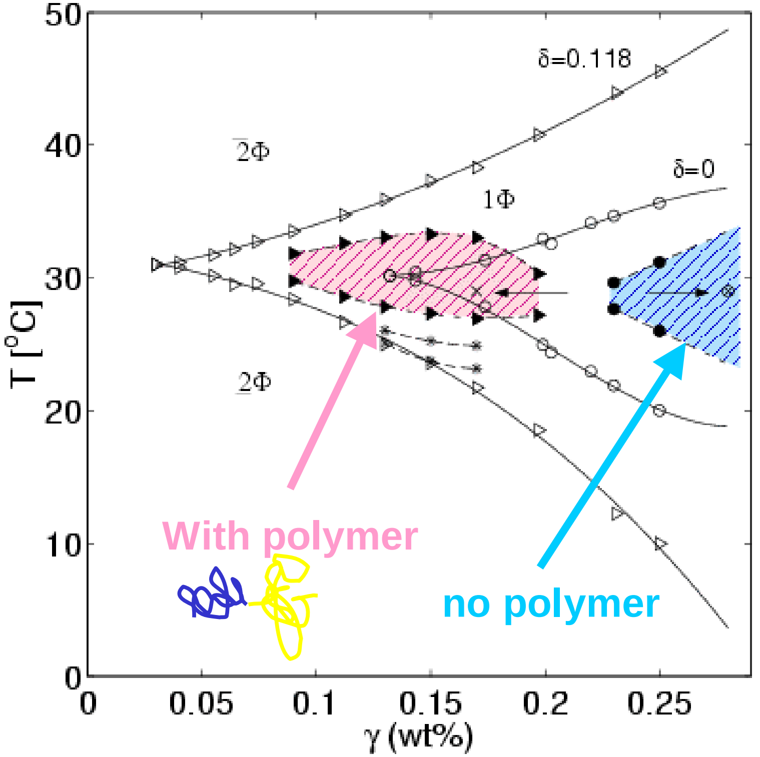
NSE => dynamic SANS

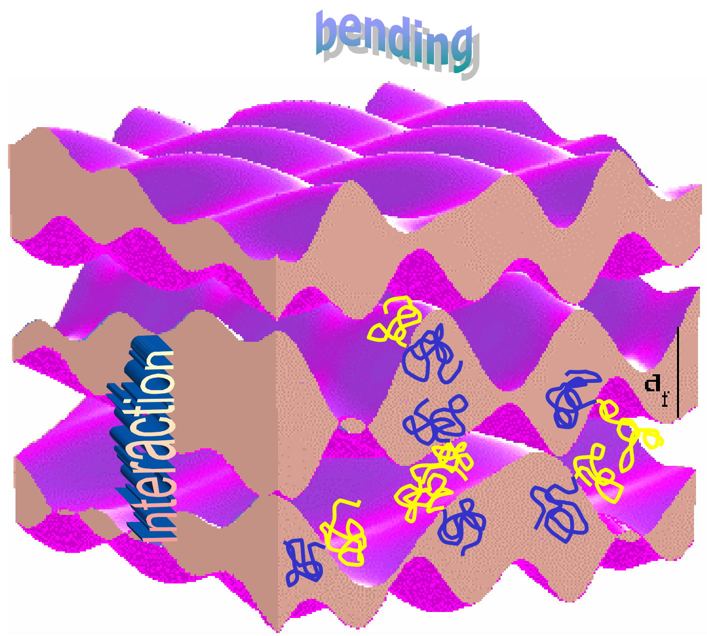
Contrast variation

Example:
microemulsions



Lamellar Phases

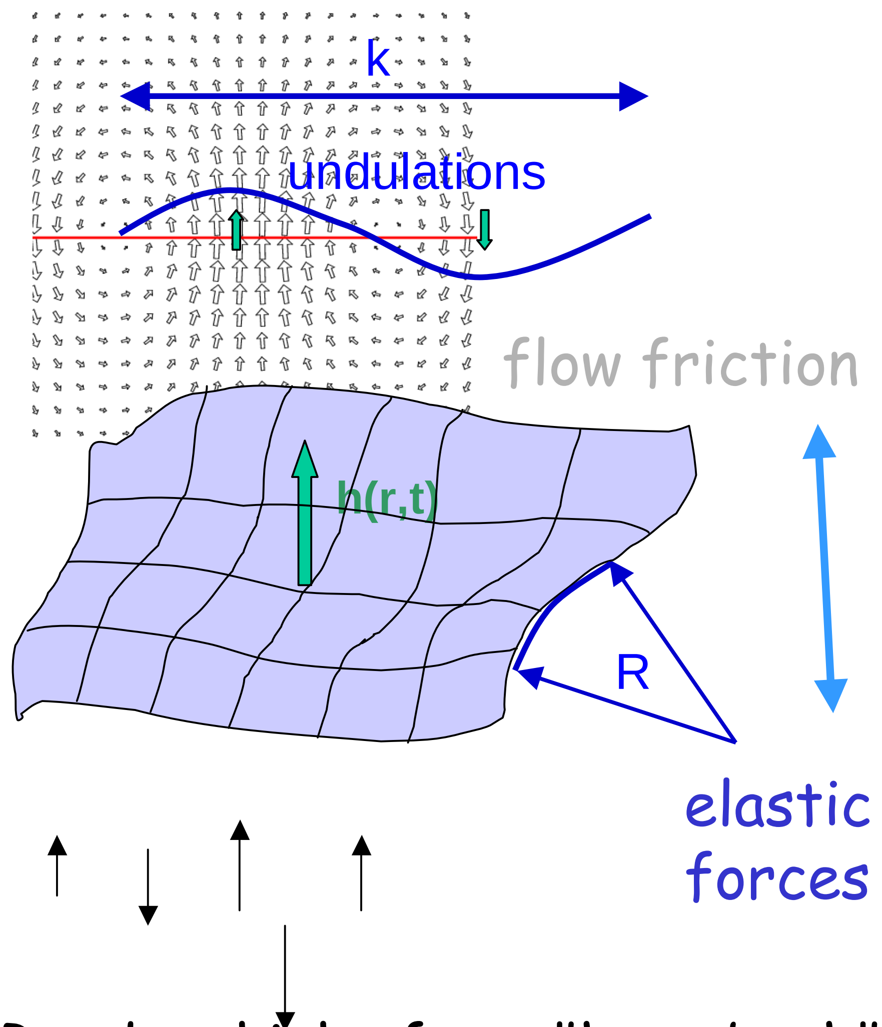


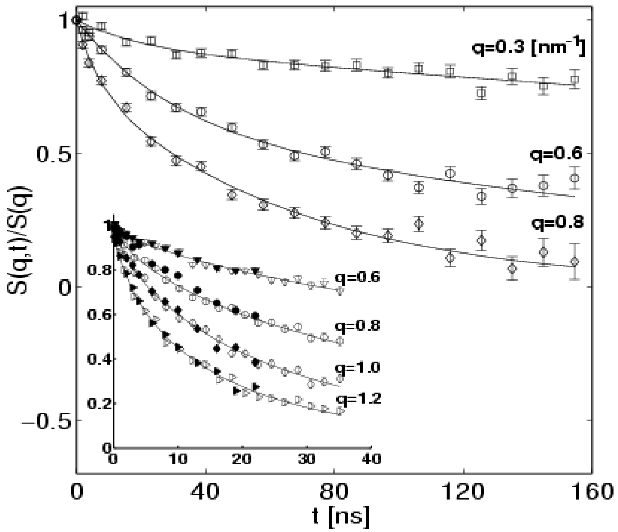


$$\left\langle \left| U_k \right|^2 \right\rangle = \frac{k_B T}{B k_z^2 + \kappa_c k_\perp^4}$$

Membrane fluctuations

$$\frac{S(q,t)}{S(q)} = \exp[\,-\{\Gamma(q)\,t\}^{\beta(q)}\,]$$



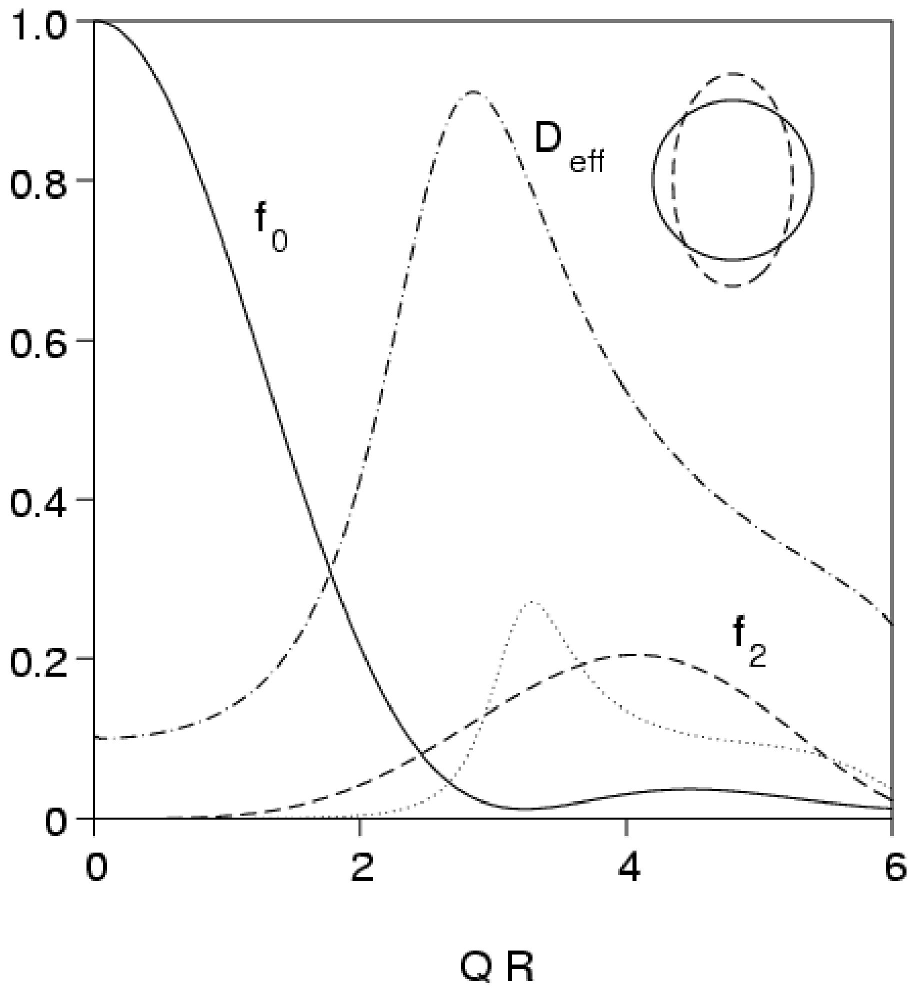


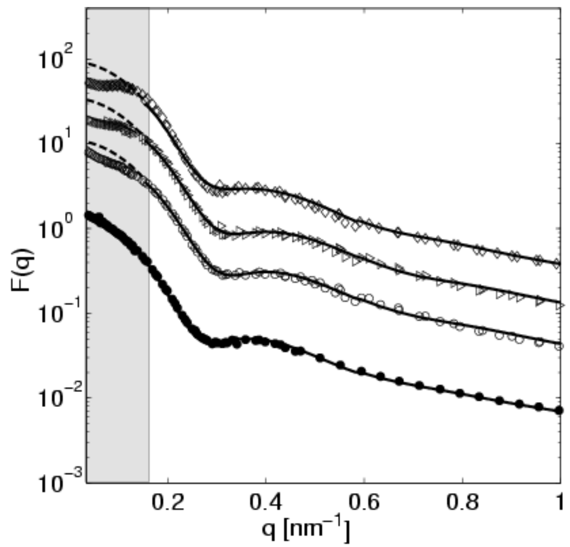
balance→relaxations time

elastic restoring forces

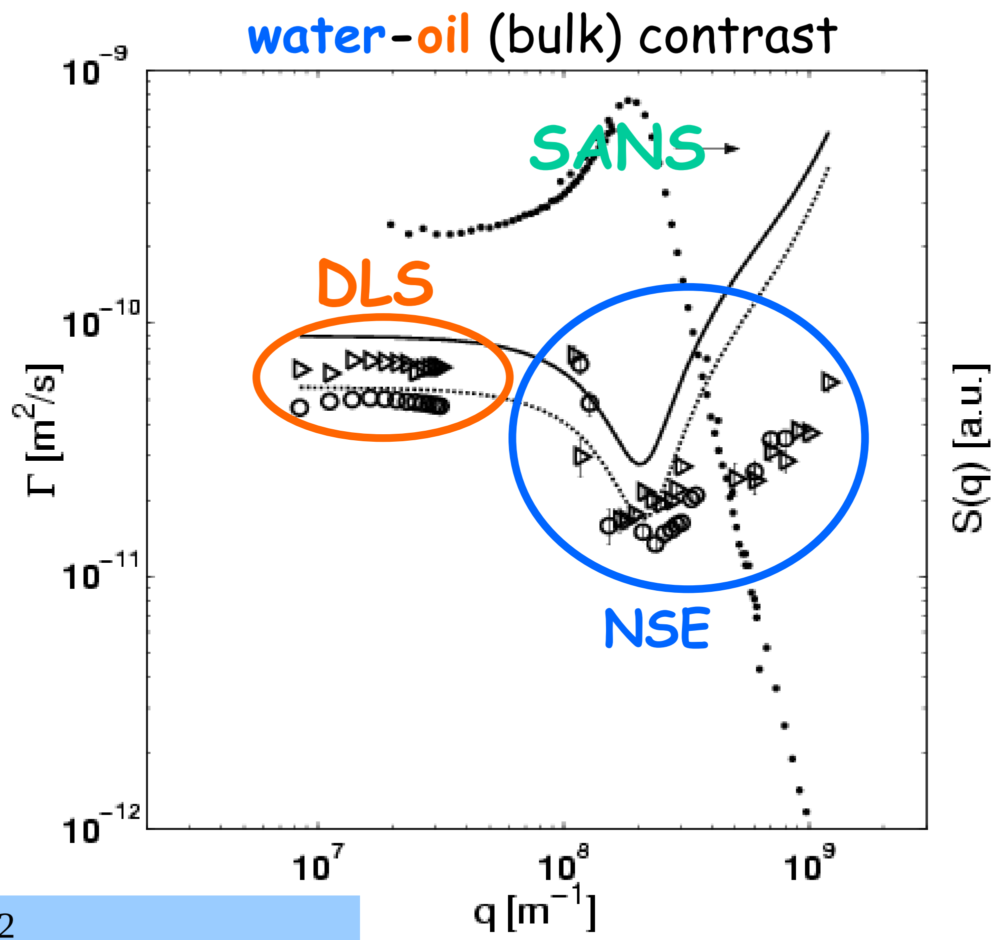
Random kicks from "heat bath" drive fluctuations (Brownian motions)

Shape fluctuations: e.g. microemulsion droplets

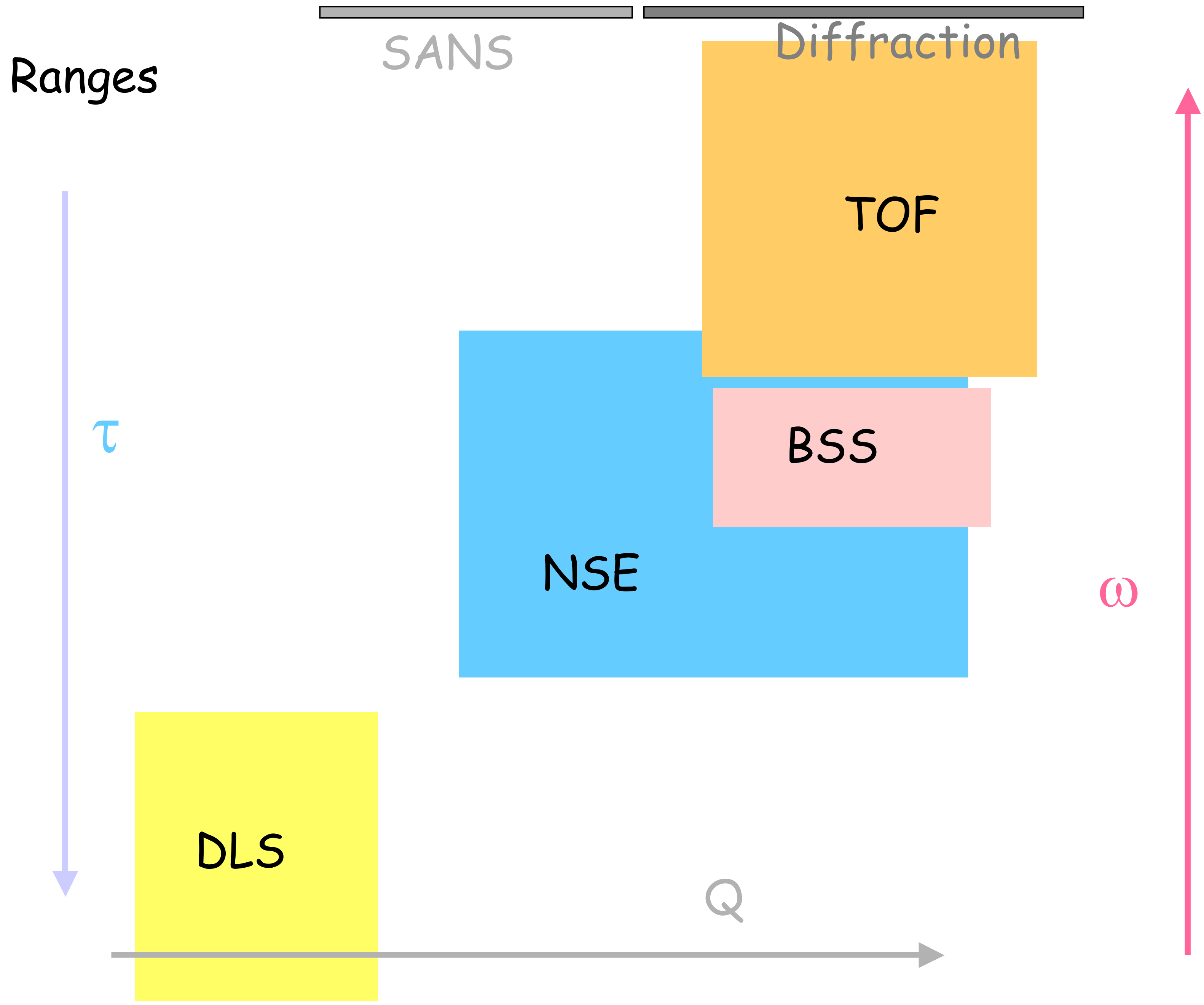




Connection to light scattering (DLS)



$$\Gamma(q) = \frac{\Gamma_b q^2}{S_b(q)} + D(q) q^2$$



Ranges
SANS
Diffraction
TOF
τ
BSS
NSE
ω
DLS
Q

Summary

- NSE is a high resolution neutron spectroscopy
- NSE yields the intermediate scattering function S(Q,t)
- NSE is opens a dynamic view into the SANS regime
- neutron scattering length labeling can "stain" objects
- sees: Diffusion
- sees: Chain and membrane fluctuations
- sees: shape fluctuations (rotations)
- in all kinds of complex liquids (incl. gels...).