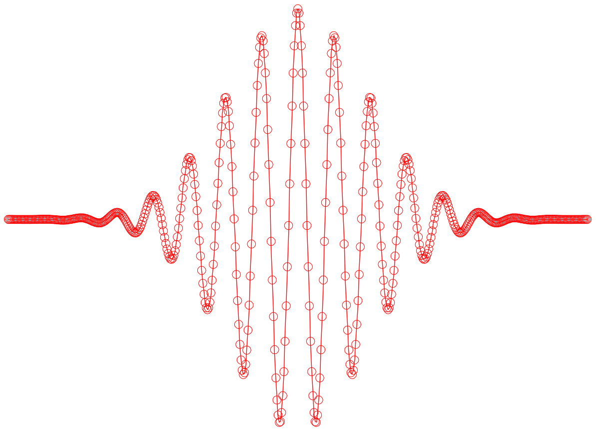


Shape variations of spherical shell microemulsion using Neutron Spin Echo

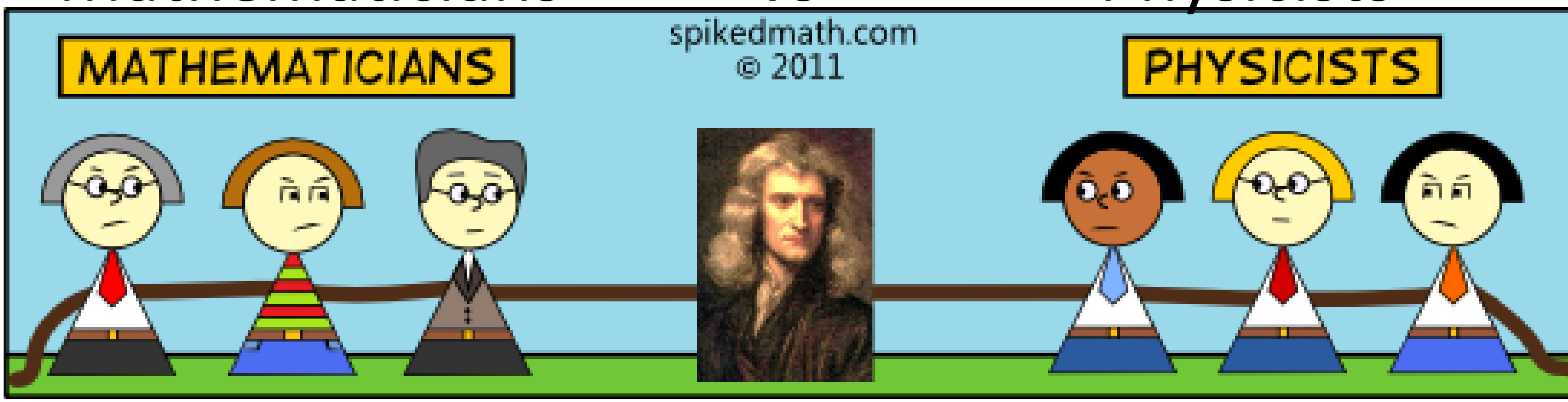
Brisa Arenas, Scott Danielsen, Joey Kim,
Jannatun Nayem, Yimin Wang,
Zhikun Cai, Namrata Salunke

Outline

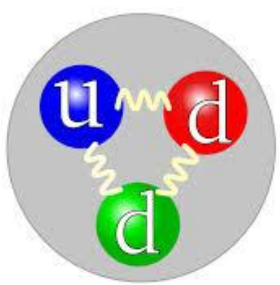
- Surfactants
- Why spin echo?
- Neutron Spin Echo
  - Principle
  - Instrumentation
- Data Reduction
- Data Analysis
- Summary

Blind dates

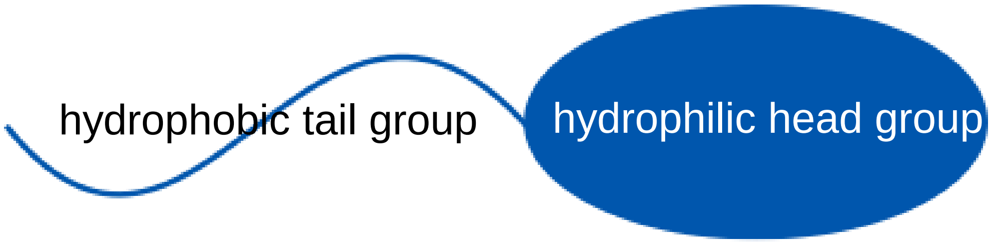
Mathematicians vs Physicists



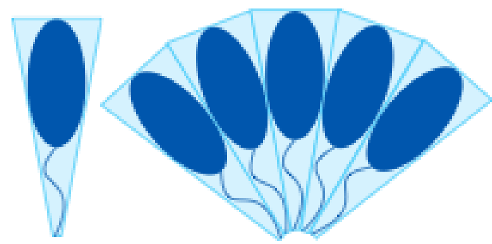
Neutrons vs X-Rays



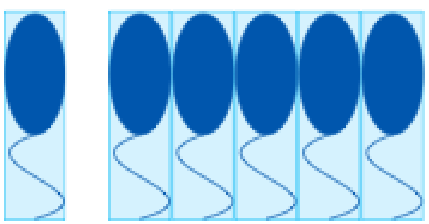
Surfactants – the molecular ice breaker



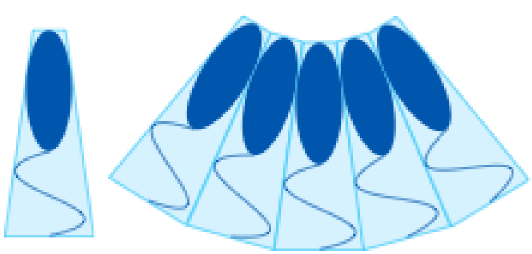
Reduces interfacial tension



micelles $c_0 > 0$



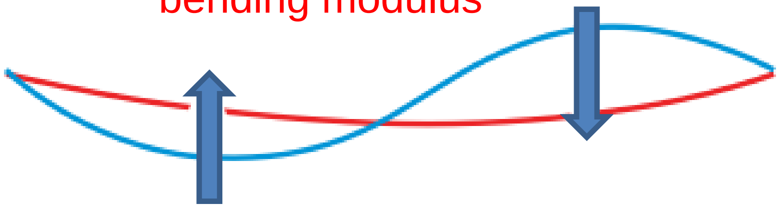
lamellae $c_0 = 0$



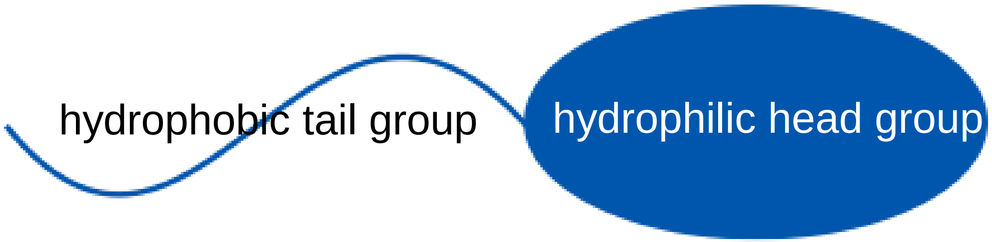
inverse micelles $c_0 < 0$

$$f_{bend} = 2\kappa\left(\frac{c_1 + c_2}{2} - c_0\right)^2$$

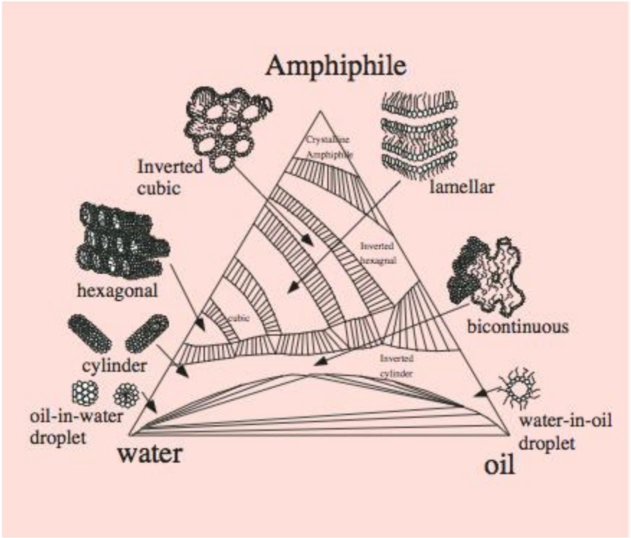
bending modulus

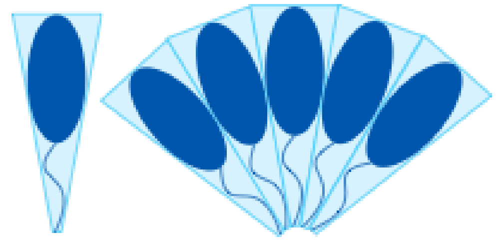


Surfactants – the molecular ice breaker

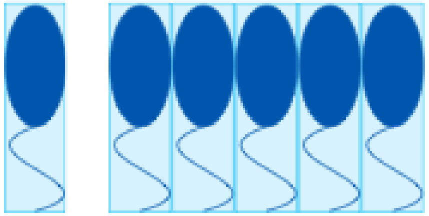


Reduces interfacial tension

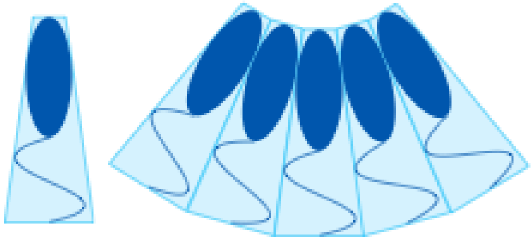




micelles $c_0 > 0$



lamellae $c_0 = 0$



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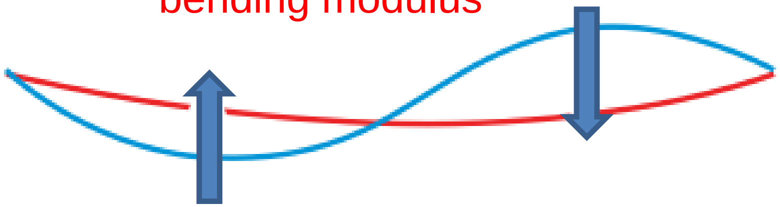
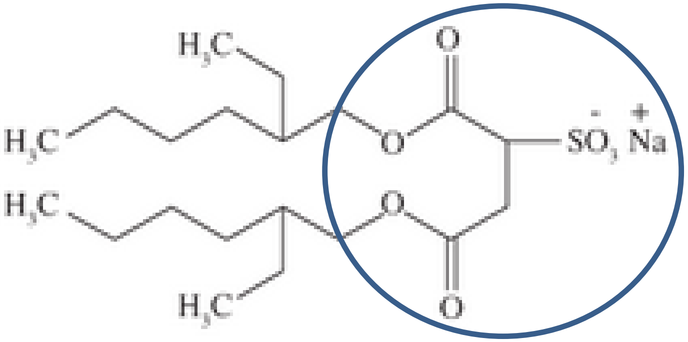
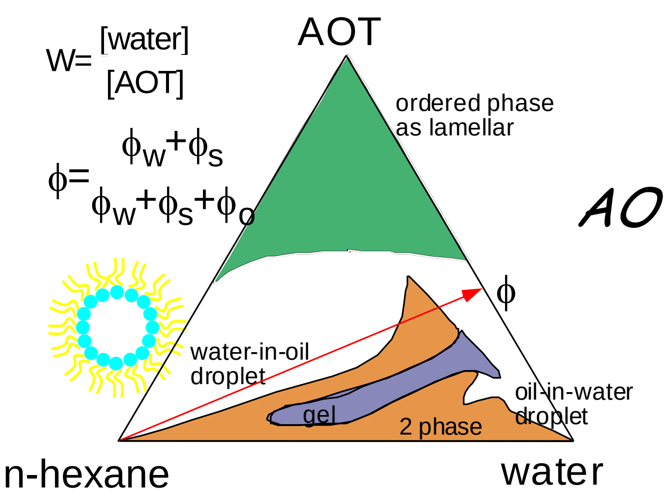


The system of interest

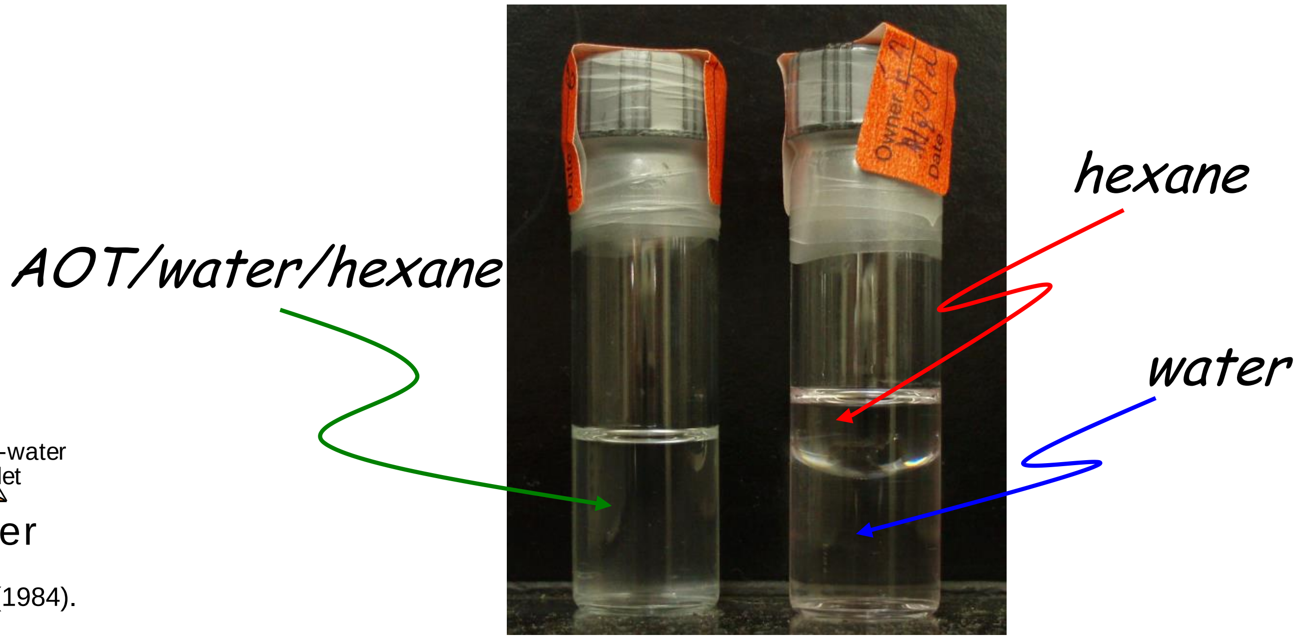


Dioctyl sodium sulfosuccinate (AOT)

AOT ($C_{20}H_{37}O_7SNa$): 5.1 vol.%
D_2O: 2.5 vol.%
d-hexane (C_6D_{14}): 92.4 vol.%

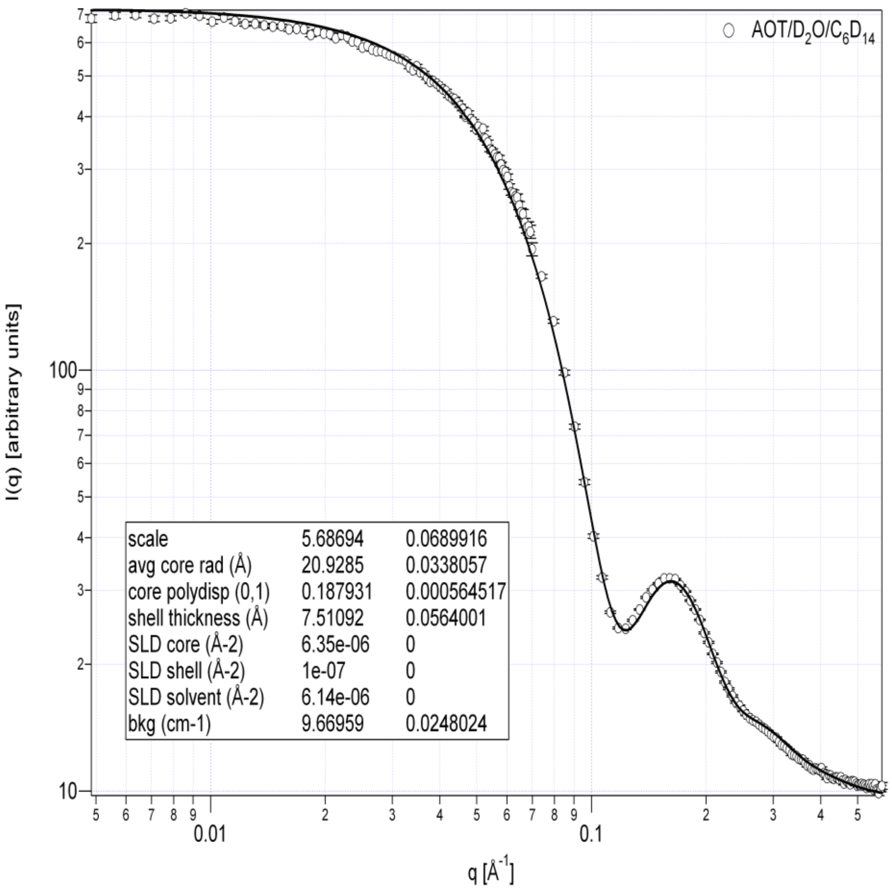


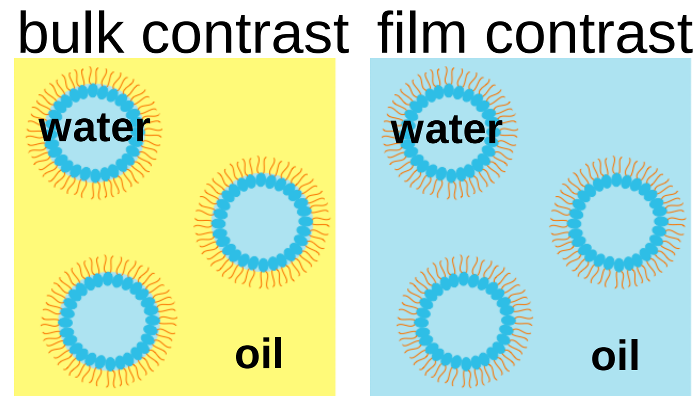
Kotlarchyk et al., *Phys. Rev. A* **29**, 2054 (1984).

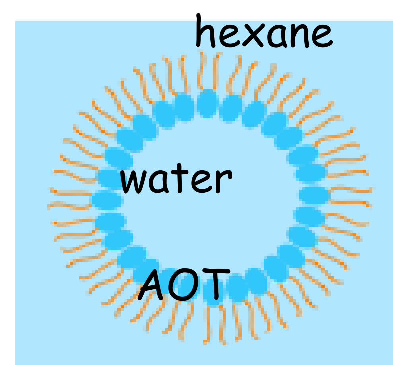


How to study microemulsions

static structure-from SANS







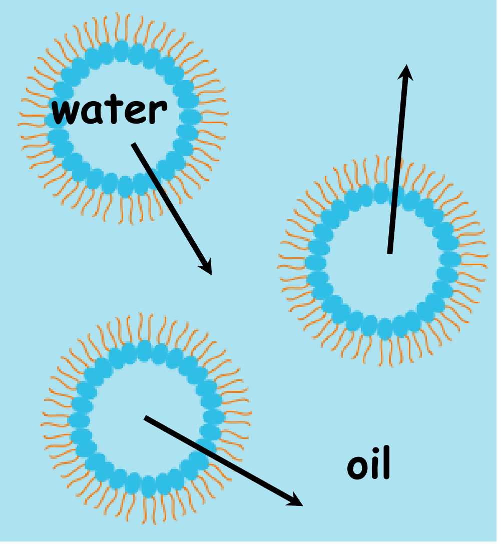
R_{core}=20.9Å

Shell thickness=7.5Å

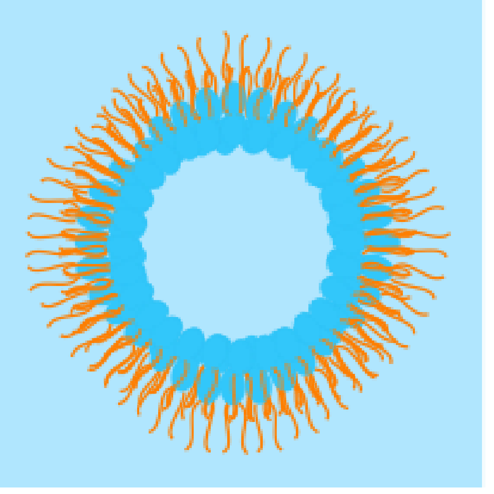
Core polydispersity=0.19

How to study microemulsions

Dynamic structure



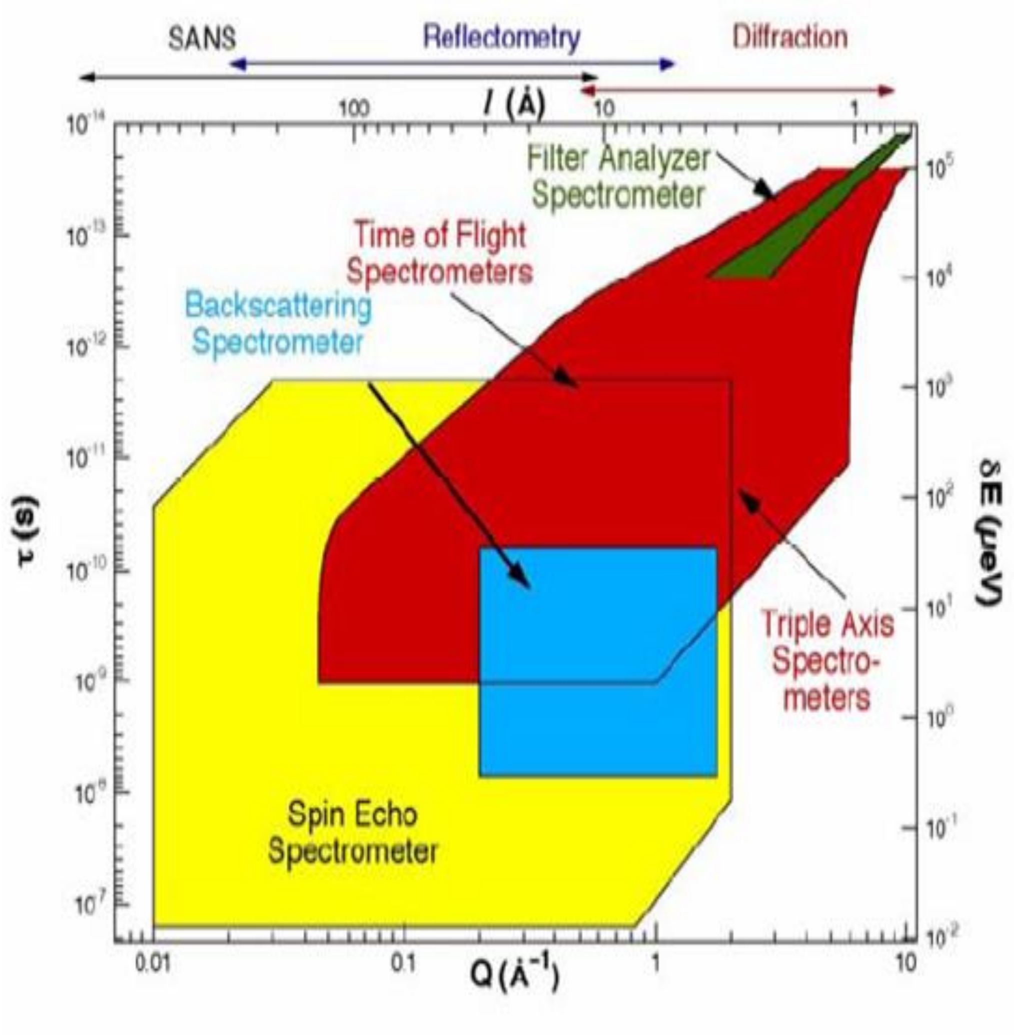
Translational diffusion



Shape fluctuation

So we need a technique that can measure both on length scale and time scale

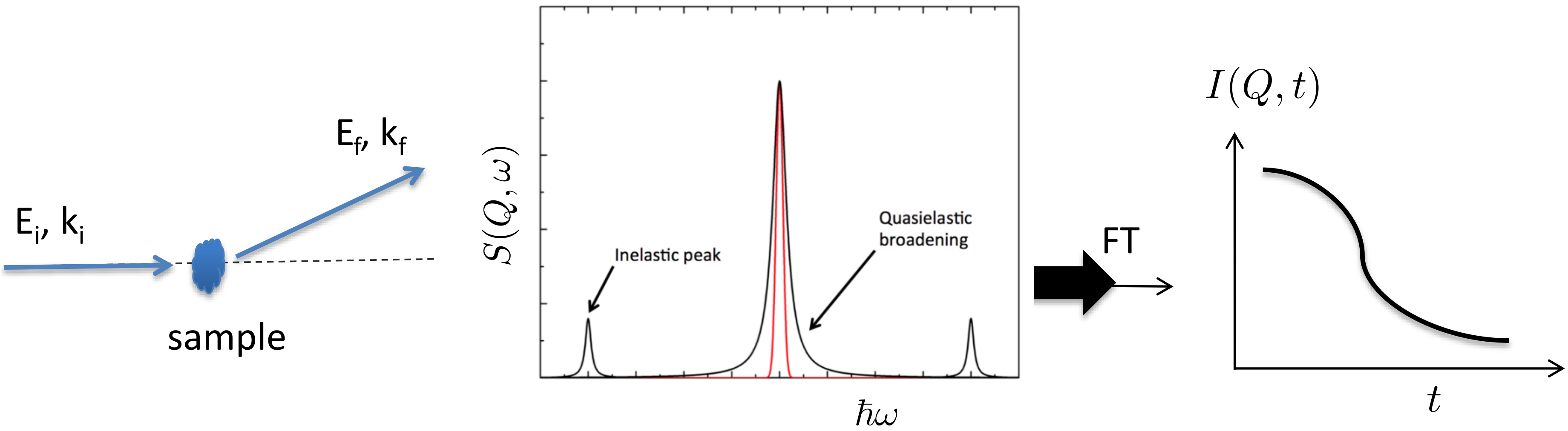
What are NSE advantages?



Larger length scale

Larger time scale

The "Special" Instrument: Neutron Spin Echo



NSE directly measures the intermediate scattering function in time domain!

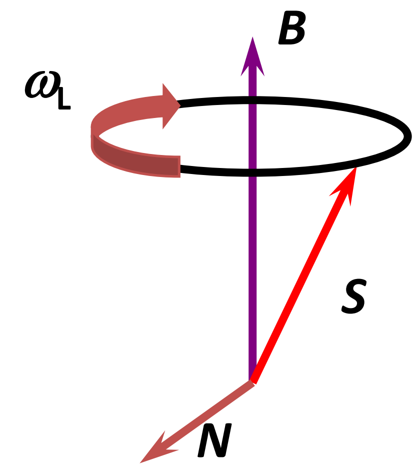
The Idea of NSE: Precession of Spin

Neutron Properties

- Spin, $S = 1/2\ \hbar$
- Gyromagnetic ratio $\gamma = g_n \mu_n / \hbar$

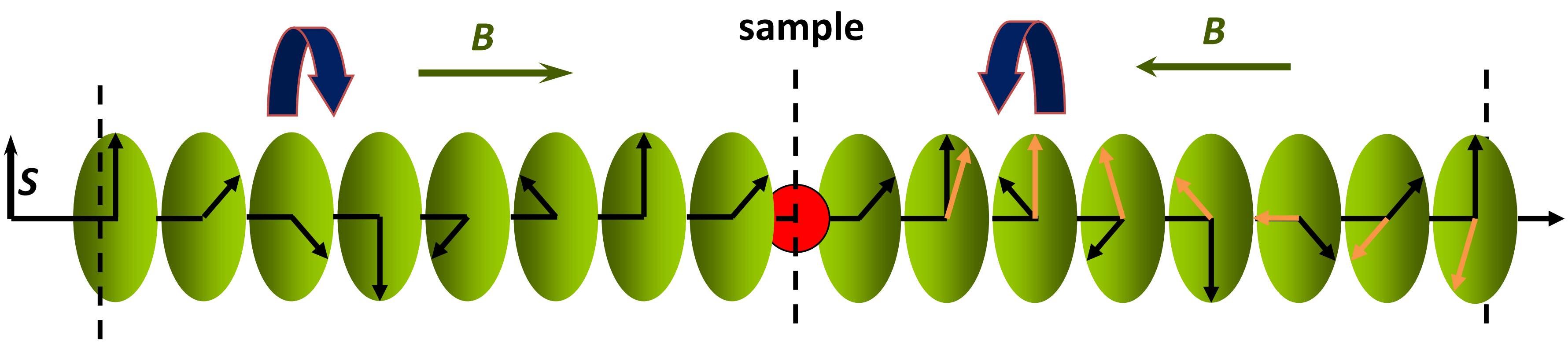
Torque in a magnetic field: $N = S´\ B$

Larmor Precession Frequency: $\omega_L = \gamma B$



Larmor Precession

- elastic scattering
- quasi-elastic scattering



Encoding neutron velocity (energy) into spin orientation!

I(Q, t) from Polarization Measurement

Quasi-Elastic scattering

Phase angle difference $$\varphi \approx \gamma \frac{m^2 \overline{\lambda}^3}{2\pi h^2} J_0 \omega + \gamma \frac{m}{h}(J_0 - J_1)\lambda$$

Polarization

$$P_x = \langle \cos(\varphi) \rangle = \int f(\lambda) \cos\left[\gamma \frac{m}{h}(J_0 - J_1)\lambda\right] d\lambda \times \int S(Q,\omega) \cos\left[\gamma \frac{m^2 \overline{\lambda}^3}{2\pi h^2} J_0 \omega\right] d\omega$$

FT of the wavelength distribution

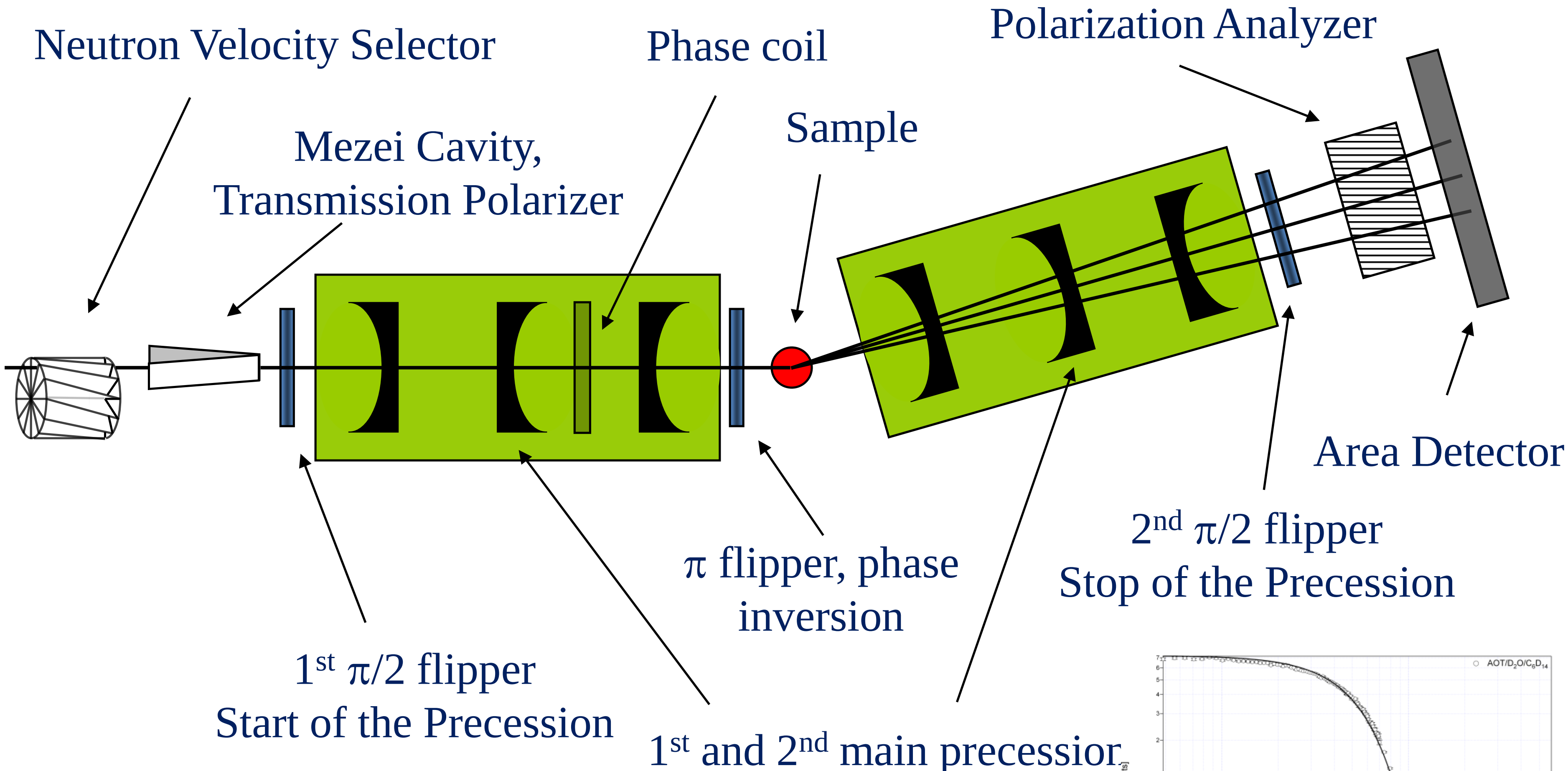
FT of the Dynamic Structure Factor

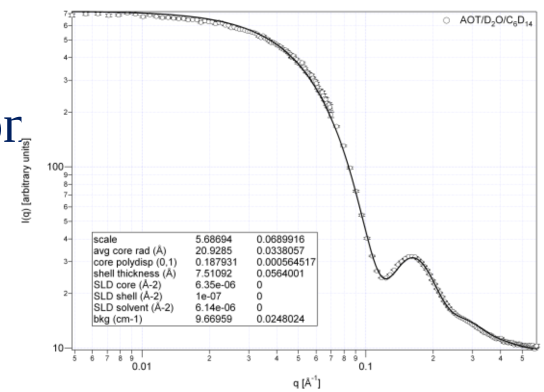
Fourier time $$t = \gamma \frac{m^2}{2\pi h^2} J_0 \overline{\lambda}^3$$

$$P_x\left(\Delta J^{ph_i}, Q, t\right) = P_s\left(\Delta J^{ph_i}\right) \int S(Q,\omega) \cos[\omega t]\, d\omega = P_s\left(\Delta J^{ph_i}\right) I(Q,t)$$

NSE measures the Fourier Transform of the Dynamic Structure Factor, namely, the Intermediate Scattering Function.

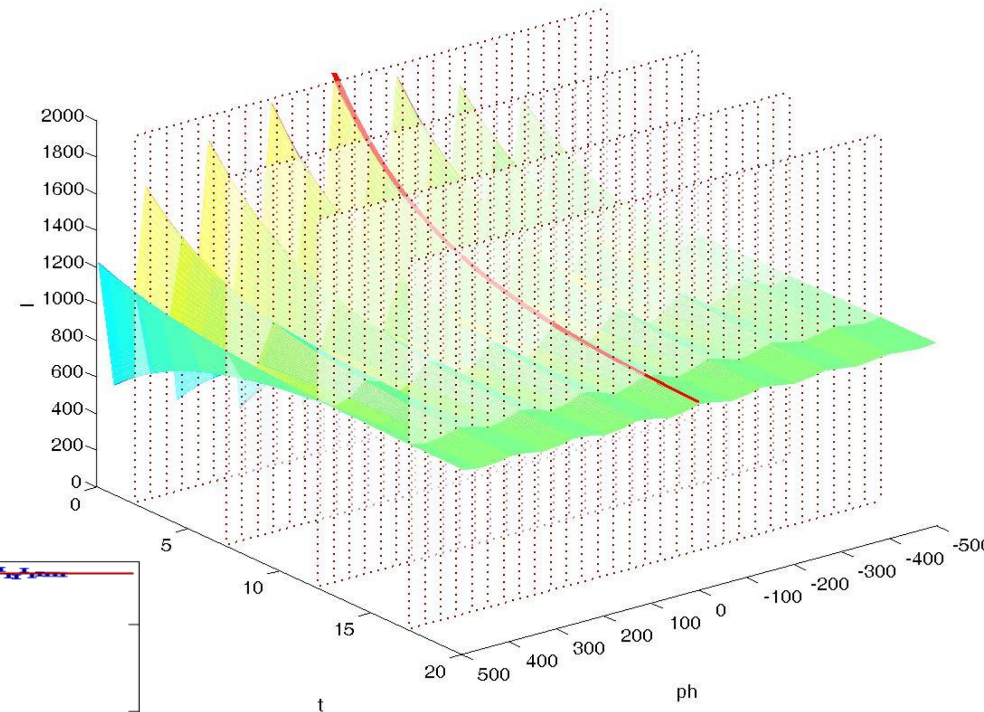
NSE: Instrumental Setup

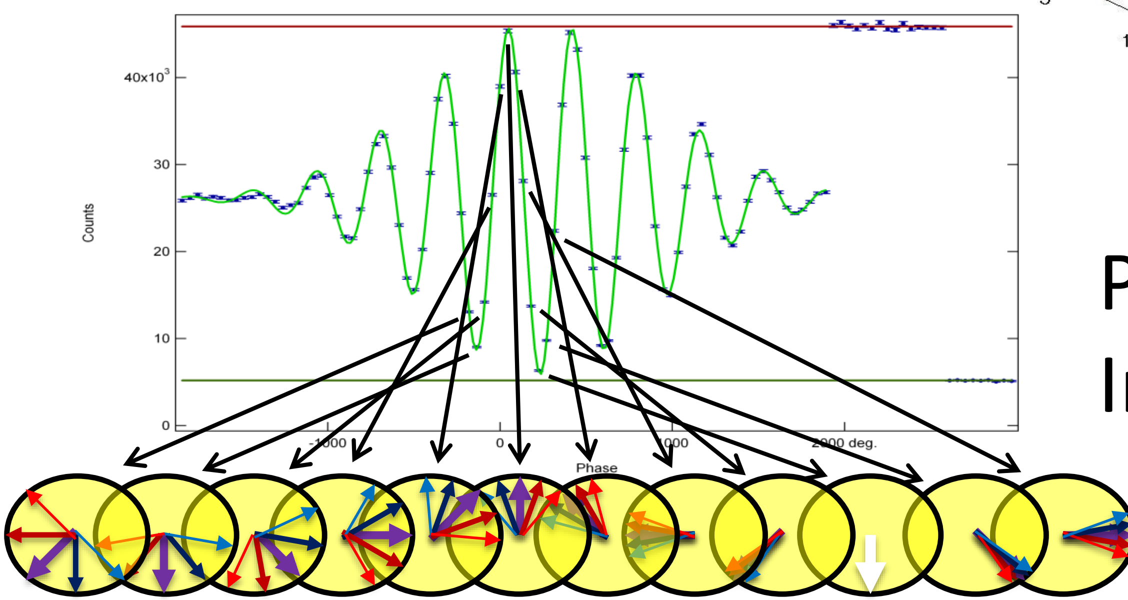




Polarization & Phase
for Range of Q and Fourier Time

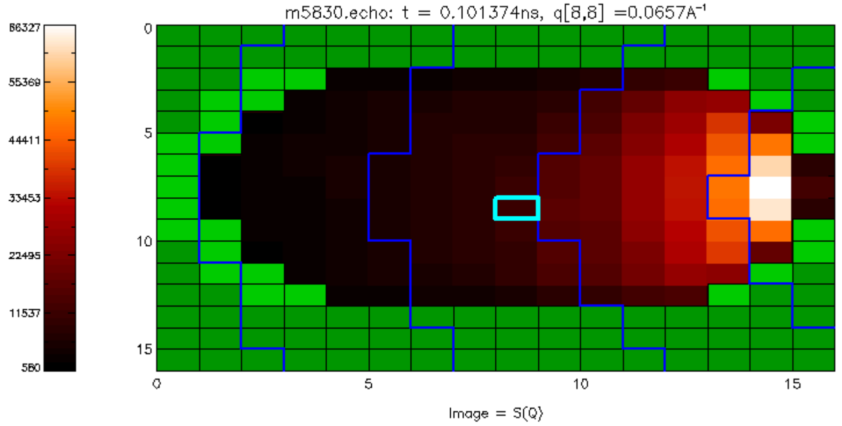
Polarization
Intensity vs. Phase
vs. Fourier Time

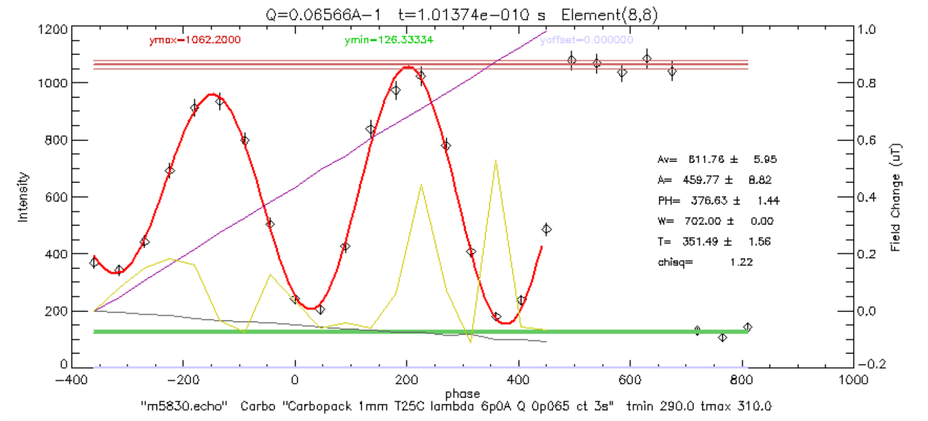




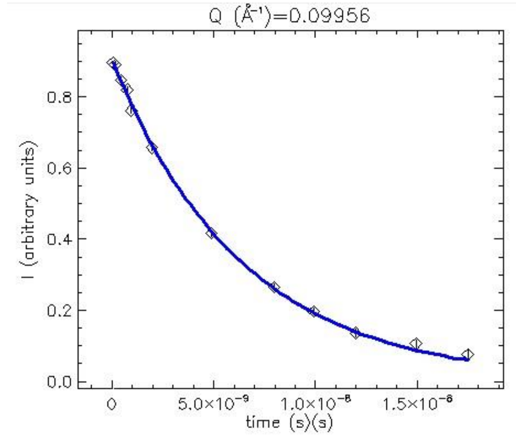
Polarization
Intensity vs. Phase

Physical Information
Embedded in 2D Detector





- 2D Detector
- Each pixel encodes an echo
- I(Q,t) calculated pixel by pixel and averaged by Q value



$$\frac{I(Q,t)}{I(Q)} = \frac{2\left[A-(1-\phi)\frac{T}{T^{BKG}}A^{BKG}\right] \Big/ \left[(Up-Dwn)-(1-\phi)\frac{T}{T^{BKG}}\left(Up^{BKG}-Dwn^{BKG}\right)\right]}{2A^{R}\Big/\left(Up^{R}-Dwn^{R}\right)}$$

Data Analysis

Full Cumulant Expansion

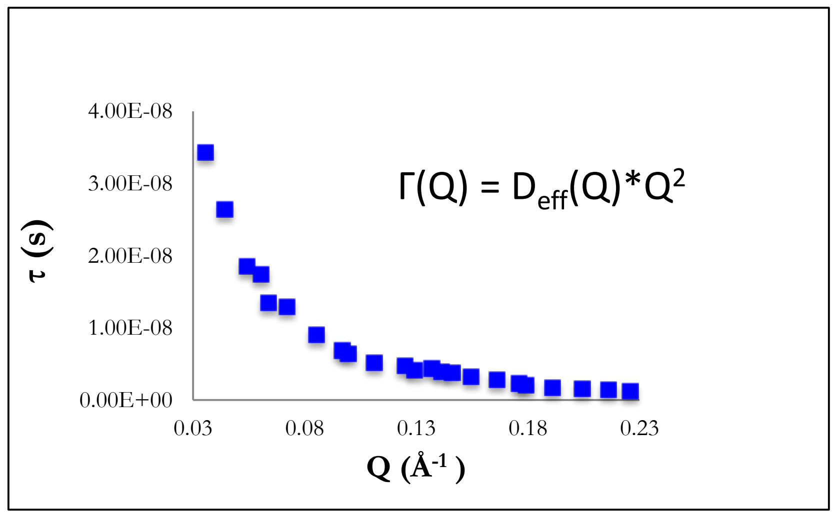
$$\frac{I(Q,t)}{I(Q,0)} = \exp\left[-\left(c_1(Q)\,t + \frac{c_2(Q)\,t^2}{2!} + \frac{c_3(Q)\,t^3}{3!} \ldots \right) \right]$$

First Cumulant Expansion

$$\frac{I(Q,t)}{I(Q,0)} = \exp\left[-D_{eff}(Q)\,Q^2 t \right]$$

$$D_{eff}(Q) = D_0 \frac{1}{S(Q)}$$

T	298	K
K_B	1.38E-23	m^2kg/s^2K
p	0.188	
η	0.31	cP
η'	1.096	cP
R_0	26.8	Å



Data Analysis

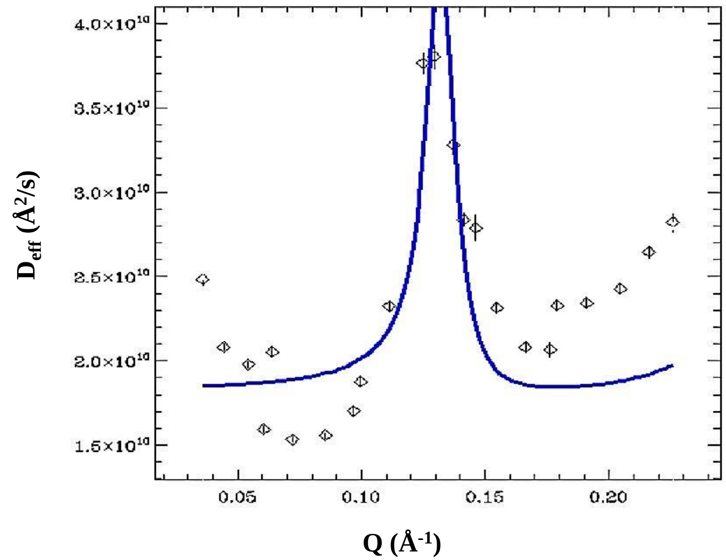
Effective Diffusion Coefficient = D_{eff}

$$D_{def}(Q) = \frac{5\lambda_2 f_2(QR_0)\langle |a_2|^2 \rangle}{Q^2\left\{4\pi\left[j_0(QR_0)\right]^2 + 5 f_2(QR_0)\langle |a_2|^2 \rangle\right\}}$$

$D_{eff} = D_{tr} + D_{def}$

Hydrodynamic Limit: (Q→0): $D_{eff} = D_{tr}$

λ_2	4.39E+08	s-1
D_0	1.84E+10	Å^2/s
R_0	23.4	Å



Stokes-Einstein Equation

$$D_0 = \frac{k_B T}{6\pi\eta R_H}$$

$R_H = 38.17$ Å

$\frac{R_H}{R_g}$	Theoretical Value	Experimental Value
	1.29	1.42

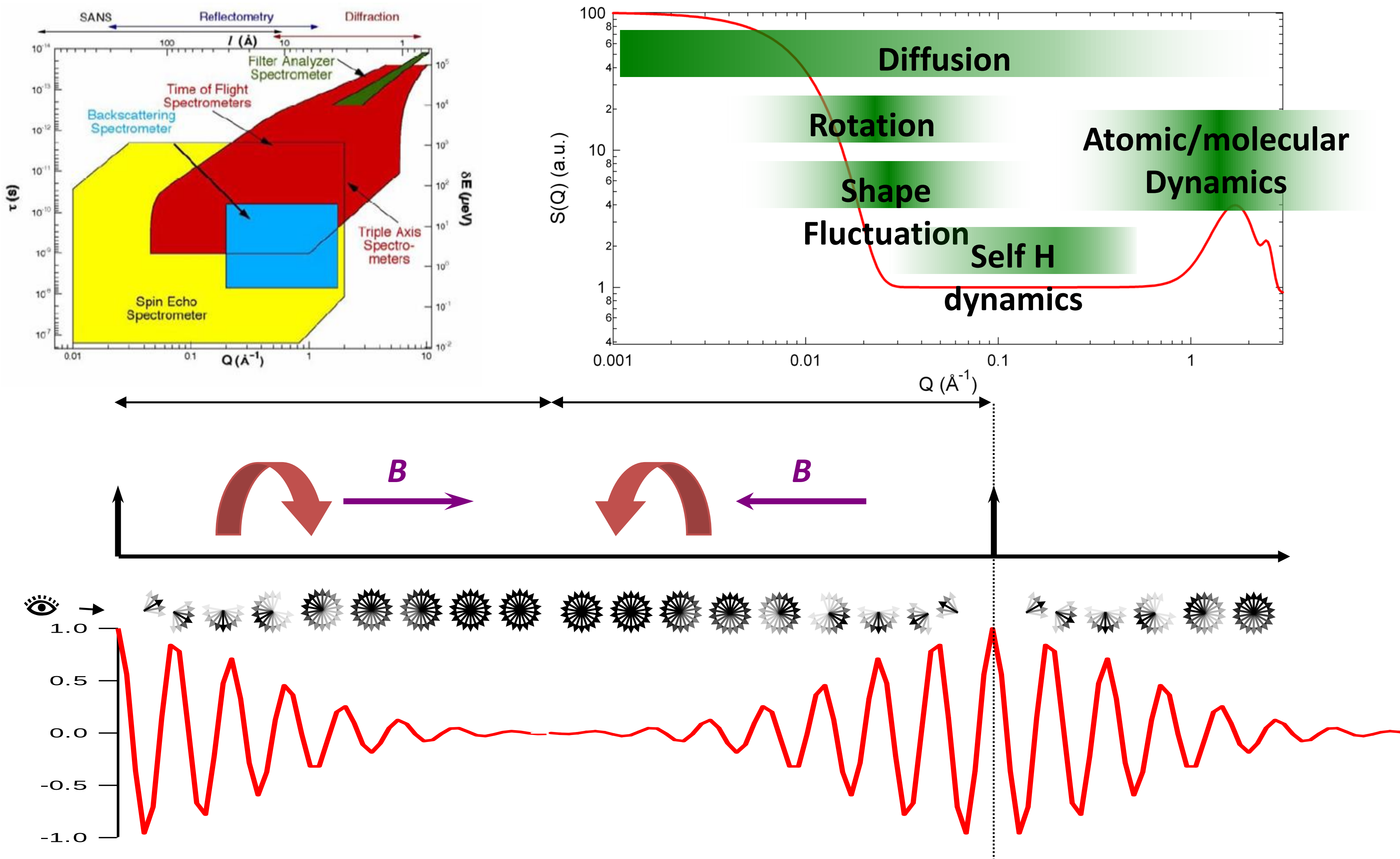
Bending Modulus of Elasticity

$$k = \frac{1}{48}\left[\frac{k_B T}{\pi p^2} + \lambda_2 \eta R_0^3 \frac{23\eta' + 32\eta}{3\eta}\right]$$

$k = 0.69\ K_B T$

Thermally Active

Summary



SANS
Reflectometry
Diffraction
Filter Analyzer Spectrometer
Time of Flight Spectrometers
Backscattering Spectrometer
Triple Axis Spectro-meters
Spin Echo Spectrometer
τ (s)
δE (μeV)
Q (Å⁻¹)
Diffusion
Rotation
Shape
Fluctuation
Self H
dynamics
Atomic/molecular Dynamics
S(Q) (a.u.)
Q (Å⁻¹)
B
B
1.0
0.5
0.0
-0.5
-1.0

Thank You!