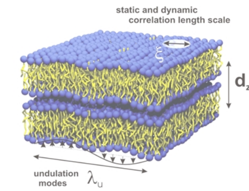
NEUTRONS FOR SCIENCE



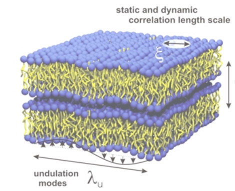
Exploring the collective dynamics of lipid membranes with inelastic neutron scattering

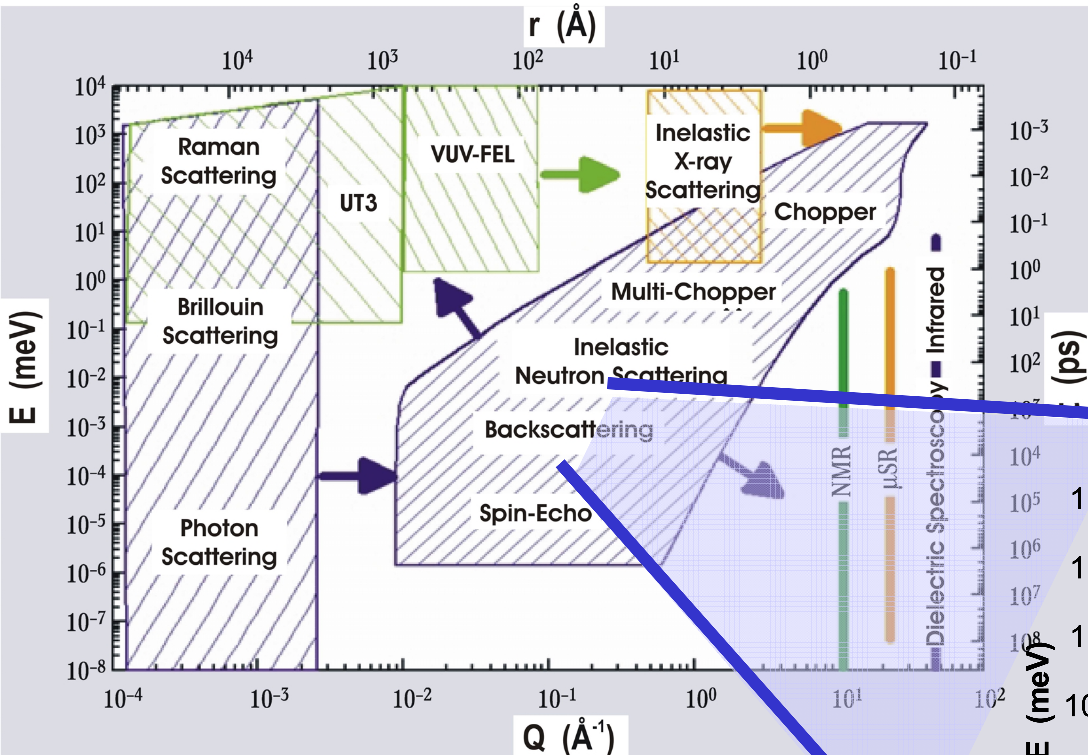
Maikel C. Rheinstädter
Institut Laue-Langevin, Grenoble, France

BioMaterials and Neutrons,
AVS Meeting Boston,
October 31 2005

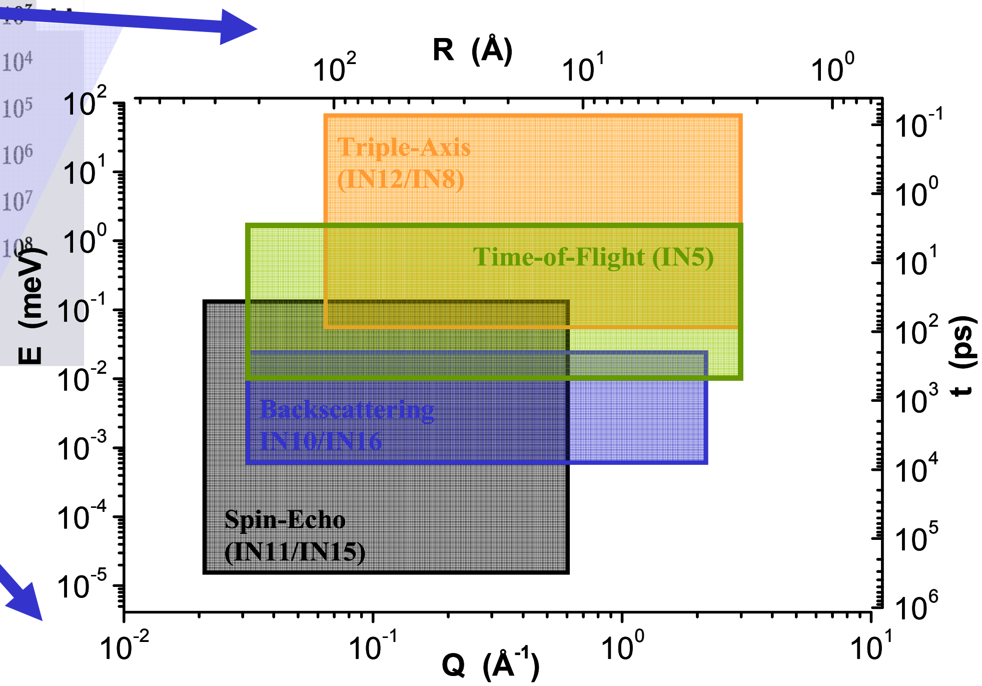
“Broadband” Neutron Spectroscopy

NEUTRONS FOR SCIENCE



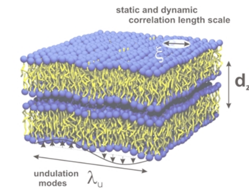


Inelastic neutron scattering gives wave vector resolved access to dynamics

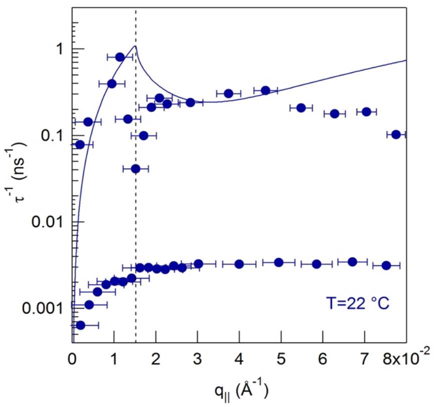


excitations
relaxations
⟷ specific motions

Mesoscopic Membrane Fluctuations



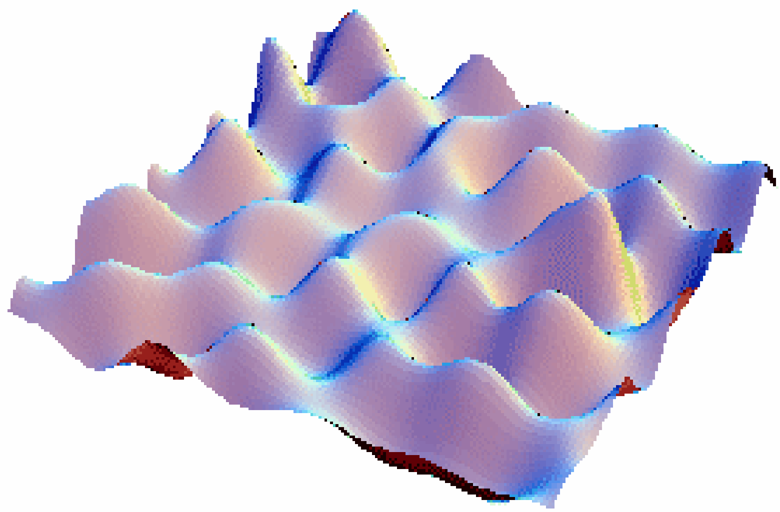
Dispersion relation

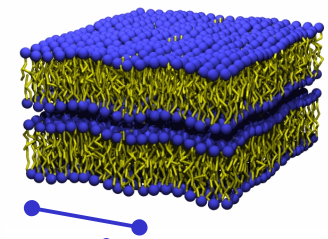


Contains 'dynamic' information

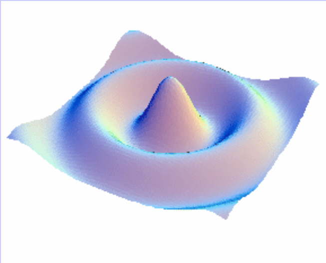
q-dependence of excitation frequencies and relaxation rates

Thermal membrane fluctuations



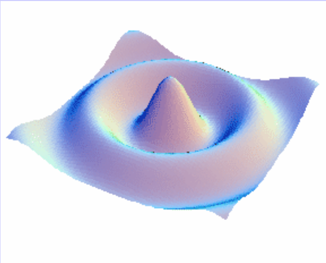


Elementary excitations



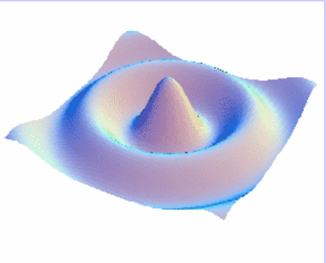
Propagating

\+



Oscillating

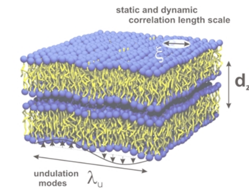
\+



Relaxating

Mode

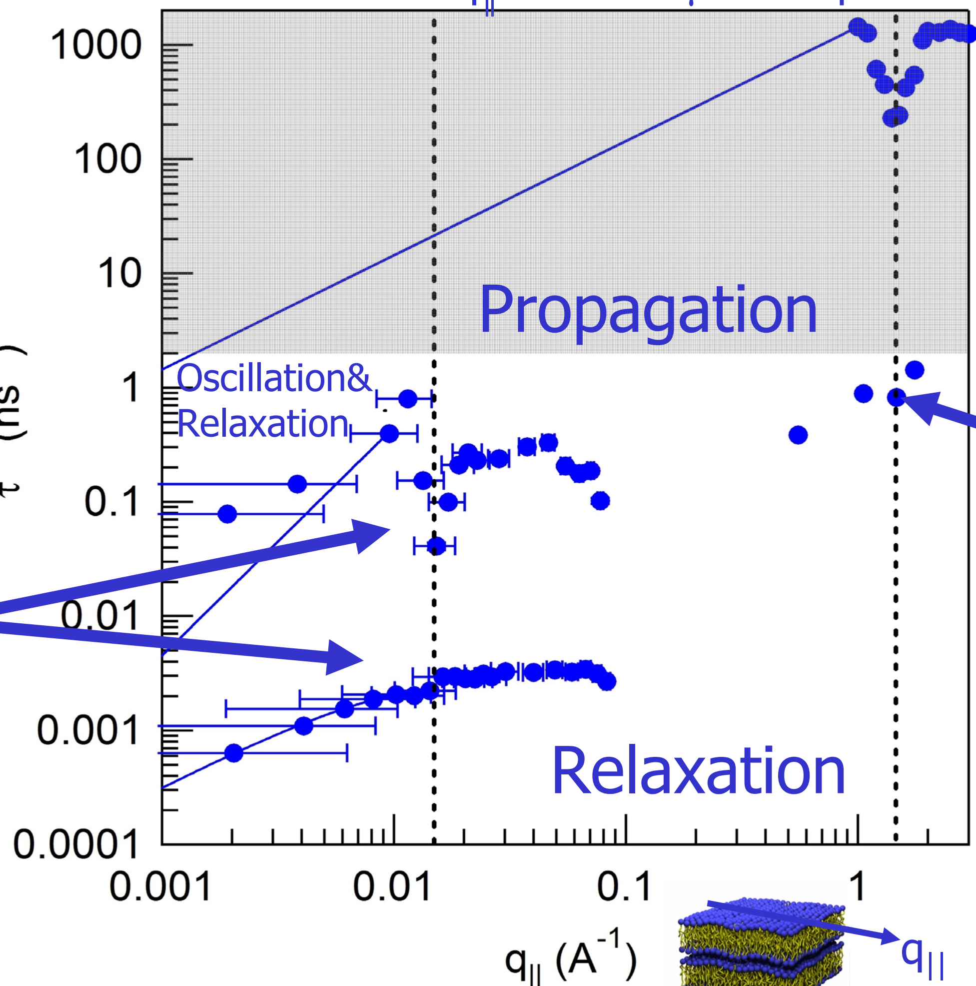
Collective Excitations in model membranes



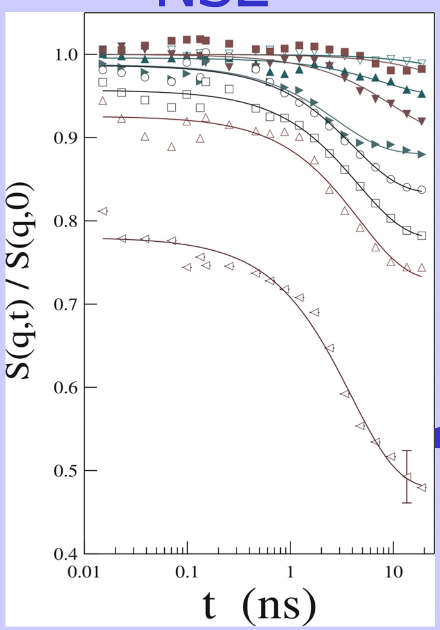
The 'Neutron Window'

DMPC –d54

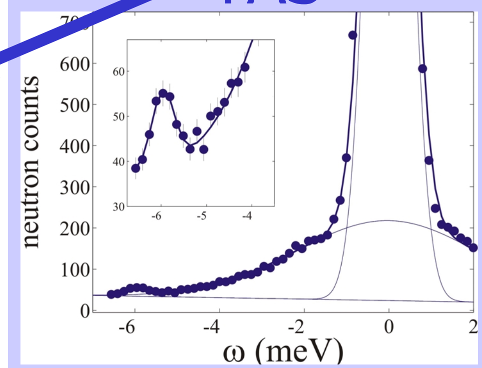
0.002Å^{-1}<$q_{||}$<3Å^{-1} & 1μs<τ<1ps



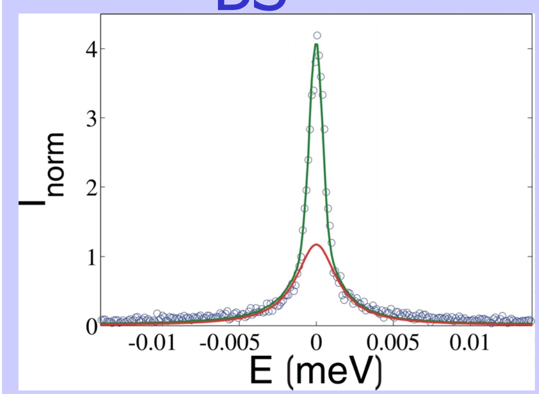
NSE



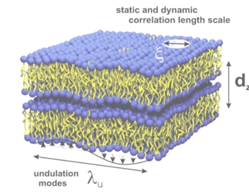
TAS



BS

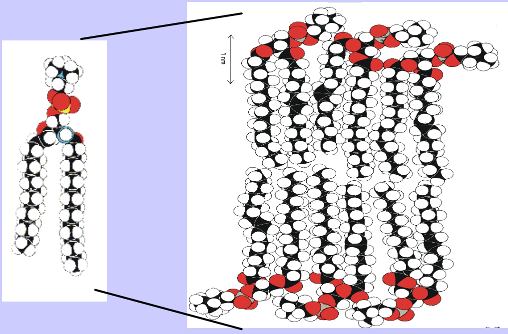


Outline



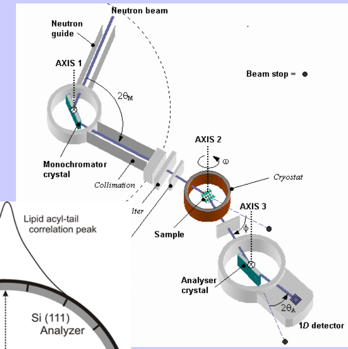
Lipids and Membranes

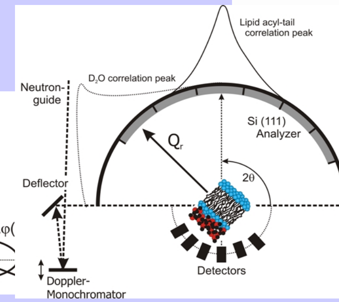
- Structures and Phases
- Sample Preparation

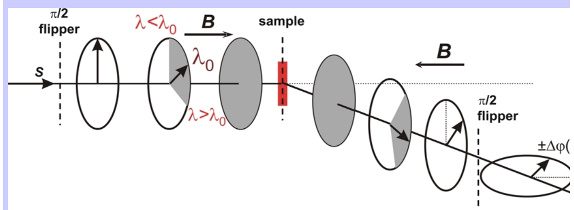


Quasielastic and Inelastic Neutron Scattering

- Three-Axes
- Spin-Echo
- (Backscattering)
  - spectrometers

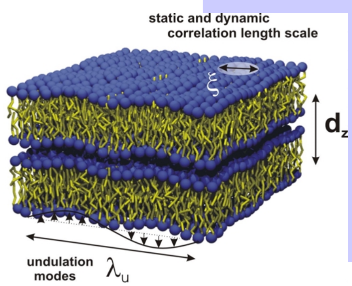




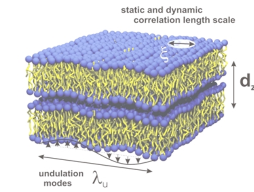


Collective Membrane Dynamics

- Short wavelength density fluctuations
  - -Dispersion relation in lipid bilayers on TAS
- Long wavelength undulation modes
  - -Dispersion relations on NSE
  - -Theoretical models
  - -Access to elasticity parameters
- (Q-dependent molecular mobility
  - Dynamics of lipids and membrane water)

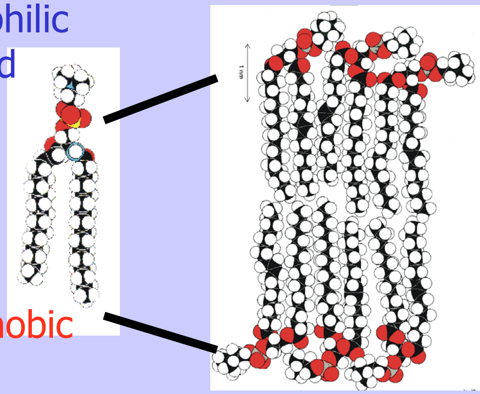


(Phospho-)Lipids and Membranes



Spontaneous aggregation to bilayers

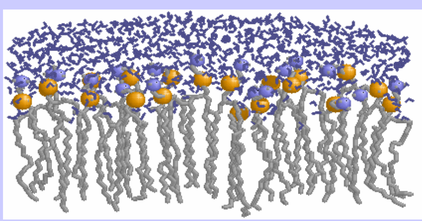
Hydrophilic head



Hydrophobic tail

„Main" transition

$P_{\beta'}$



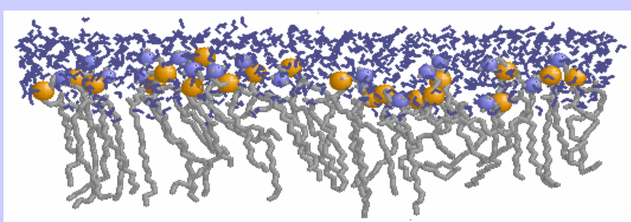
gel

DMPC –d54

T_c=21 °C

fluid

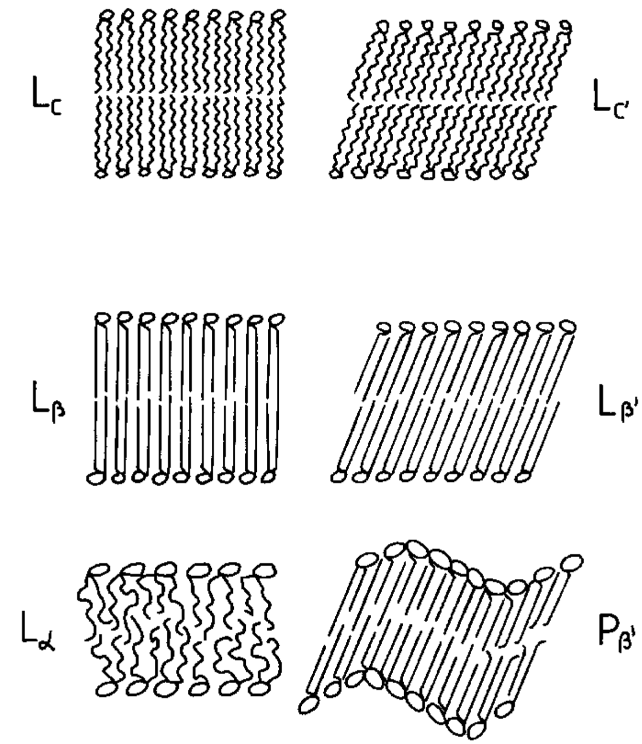
L_α



Molekulardynamik Heller et al., J-Phys.Chem 93

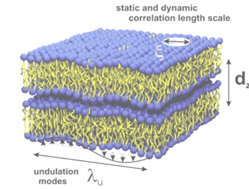
Lipid/Water Phases

Parameters: temperature + hydration

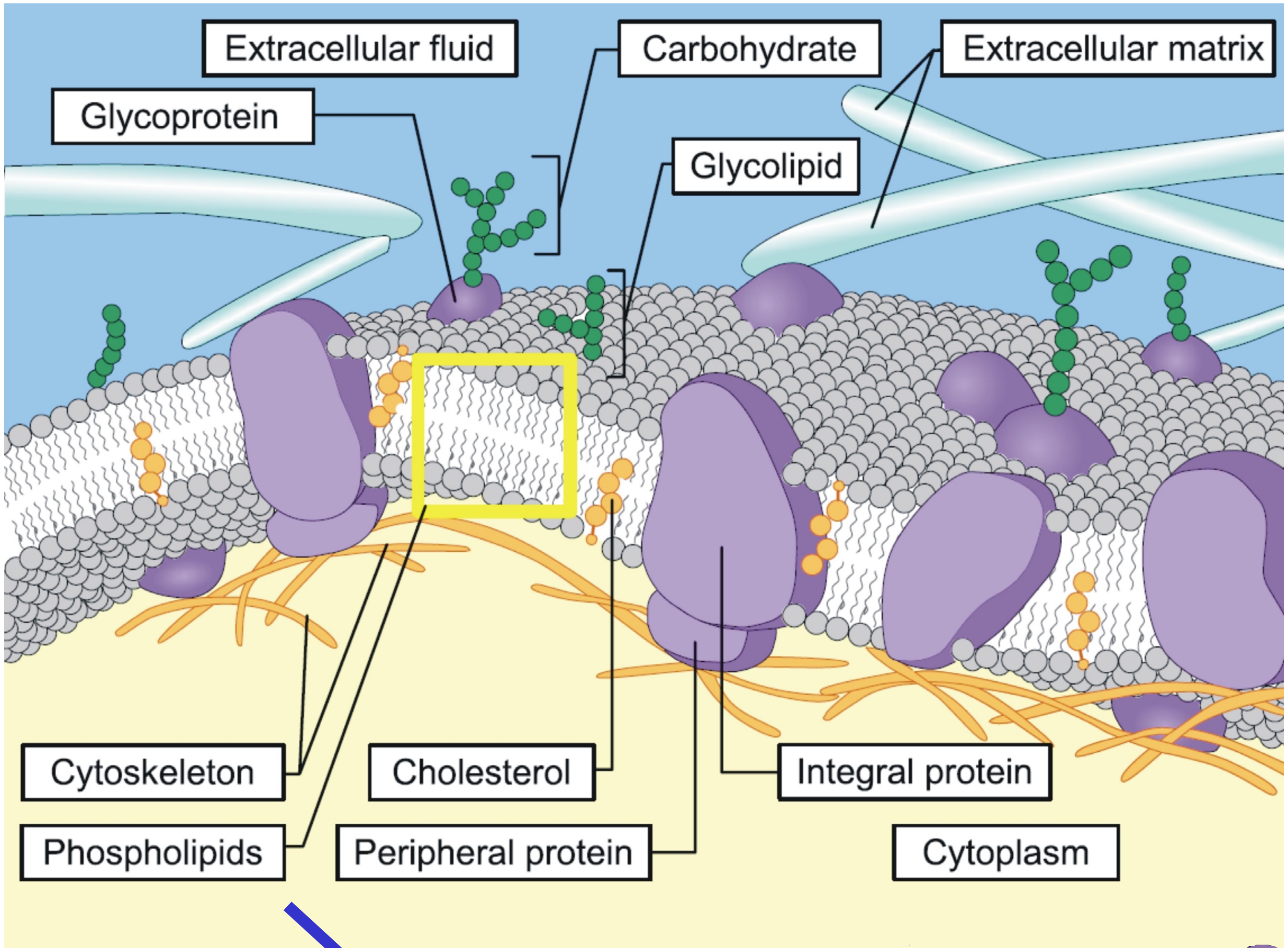


Handbook of Biological Physics

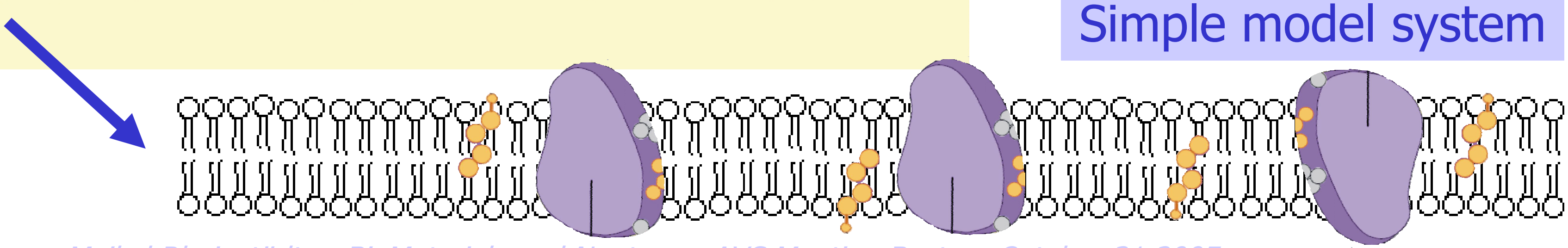
Functionality determined by structure and dynamics



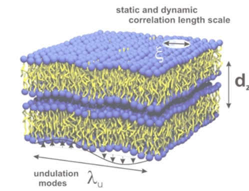
Towards biological membranes



Simple model system

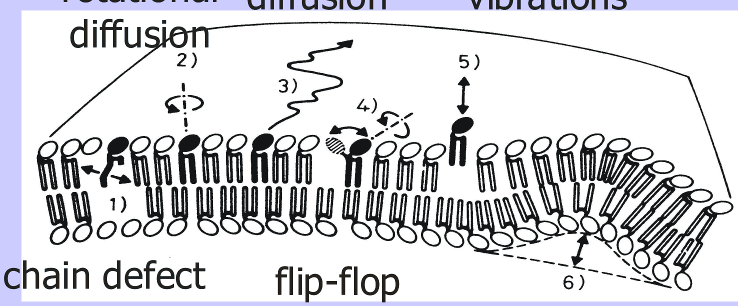


Membrane Dynamics



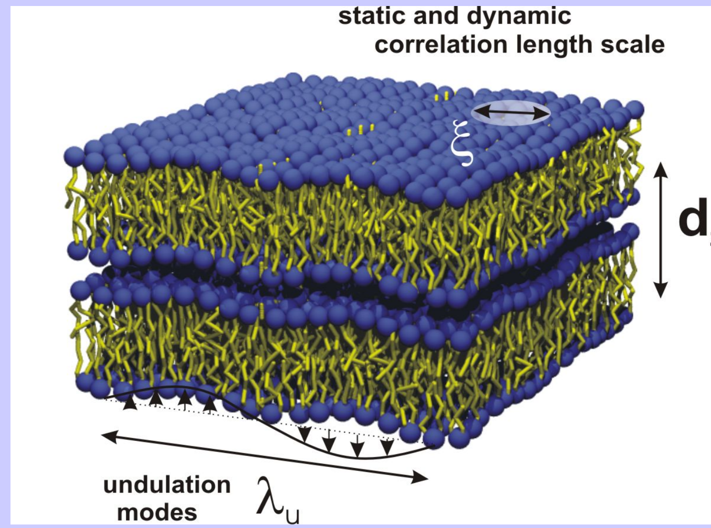
Local modes in bilayers

W. Pfeiffer *et al.*, EPL (1989)



- Incoherent inelastic neutron scattering
- NMR
- Dielectric spectroscopy

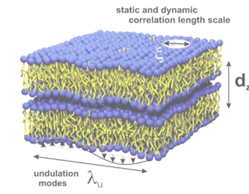
- Coherent in- and quasielastic neutron scattering
- Inelastic X-ray scattering



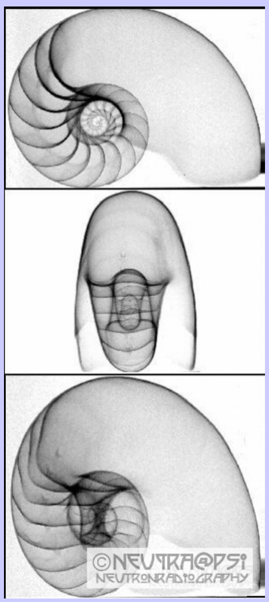
Collective excitations

Correlated molecular motions might be responsible for 'functionalities' of the membrane and structural changes

Why Neutrons?

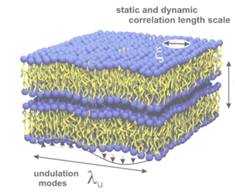


Neutrons and Biology

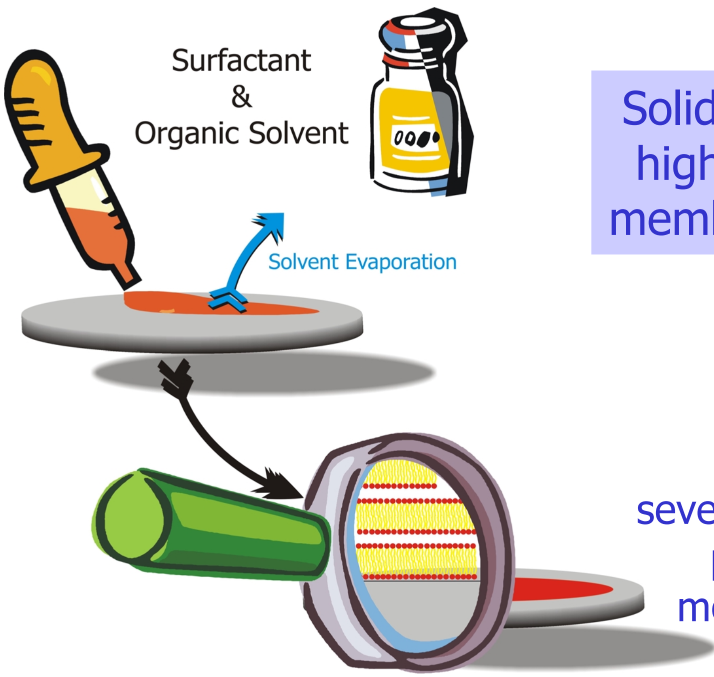


- **Neutrons are (coherently) scattered equally well by light and heavy atoms**
- **Neutrons penetrate deeply into matter (little absorption by sample and substrate)**
- **H and D scatter very differently (selective deuteration)**
- **Neutrons are gentle, causing little or no damage to delicate systems**
- **Incident energy of the neutrons in the range of the excitations -> good energy resolution**

Stacked Planar Membranes

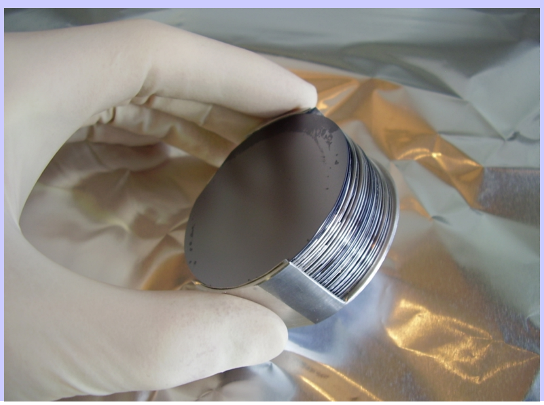


Sample Preparation



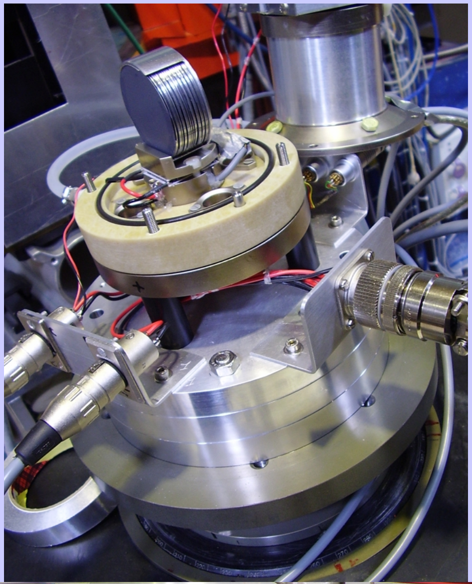
Solid supported, highly oriented membrane stacks

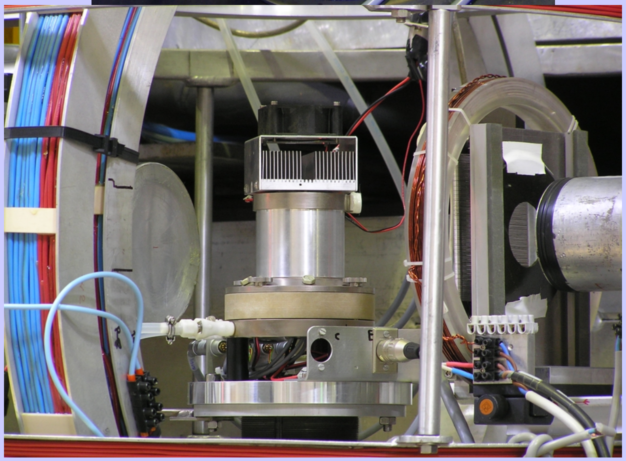
several 1000 bilayers per Si-wafer, mosaicity ~ 0.5°



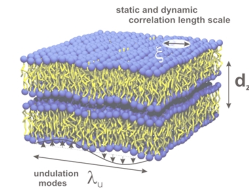
„Sandwich-sample“ with 500 mg of deuterated DMPC

“Humidity Chamber”

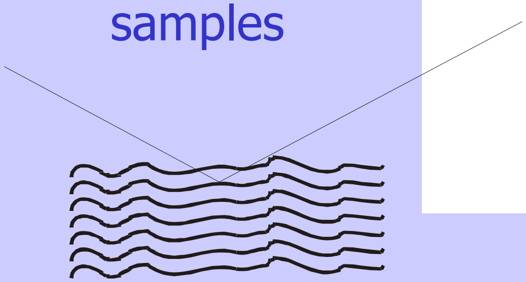


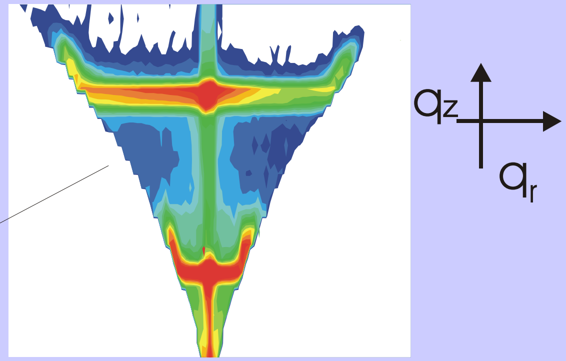


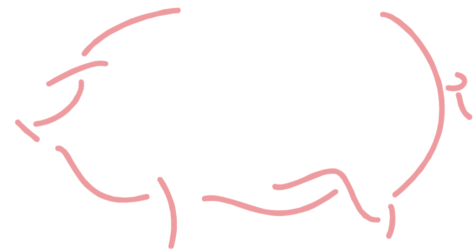
Scattering from aligned phases

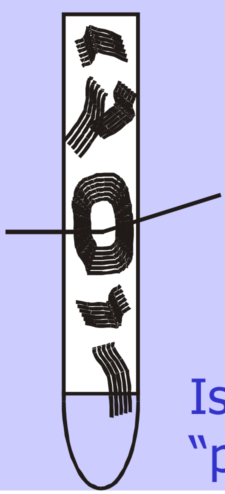


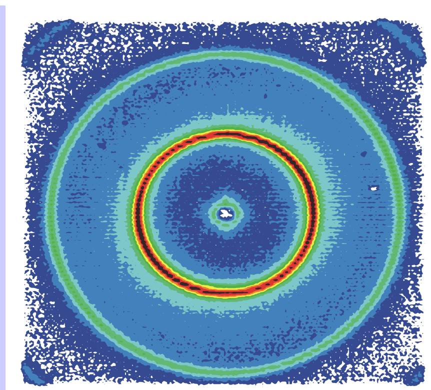
Highly oriented samples



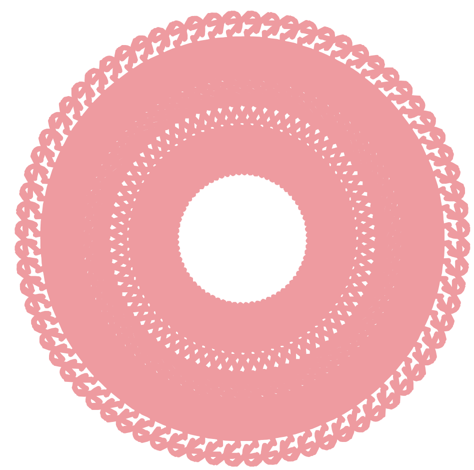


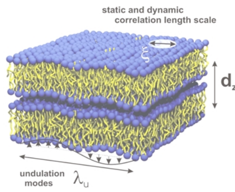




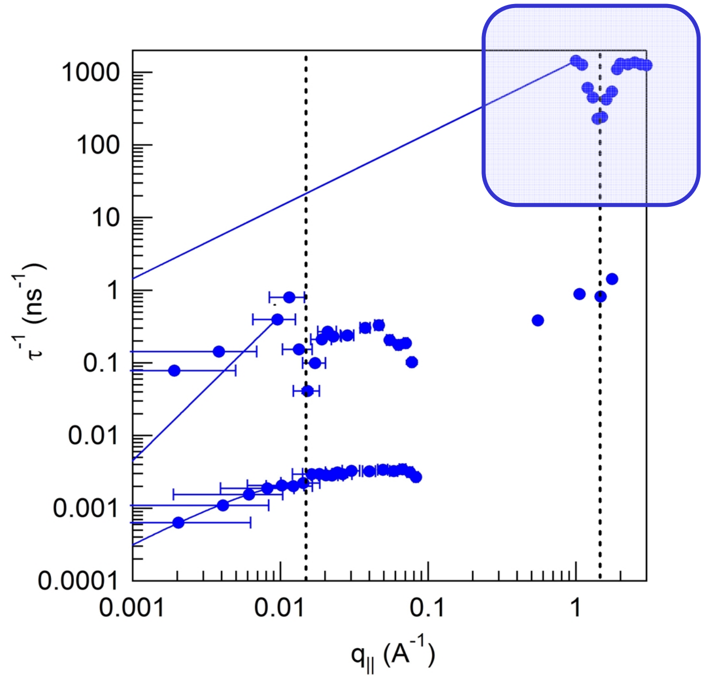


Isotropic solution
“powder”

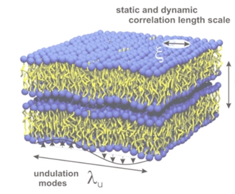


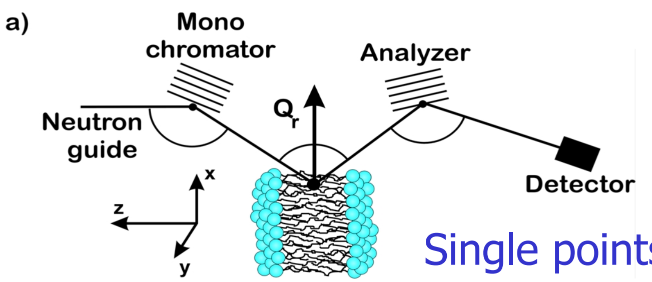


Neutron Three-Axes to measure the short wavelength fluctuations



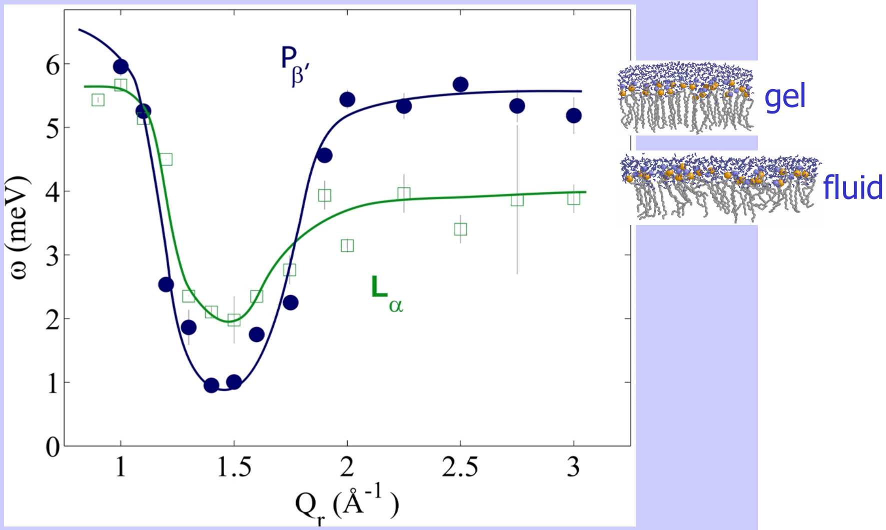
Short-Range Dispersion Relation on TAS





Single points in S(Q,ω)

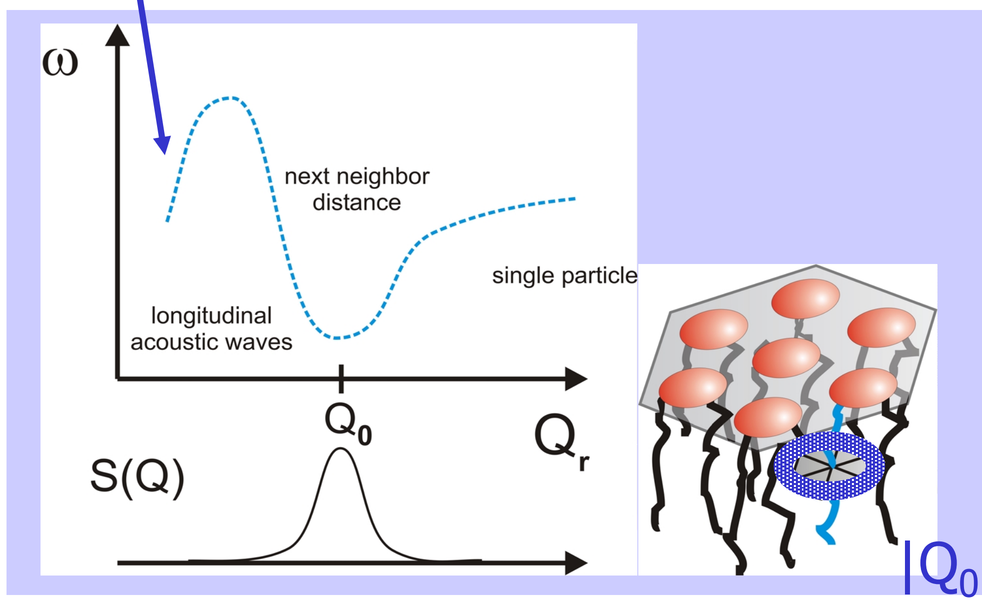
Dispersion relations in the gel- and the fluid phase of the DMPC model membrane.



Rheinstädter *et al.*, PRL (2004)

Dispersion relation as found in ideal liquids as liquid argon or liquid helium
→ c-atoms of the acyl-chains behave "quasi liquid"

Low-Q range difficult to access for neutrons (and X-rays)



$2\pi/Q_0$ defines quasi „Brillouin-zone"

Due to the large density of states, the fluctuations might trigger the phase transition to weakly 1st order
→weak crystallization scenario

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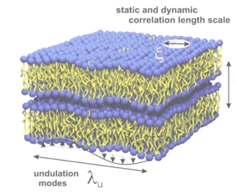
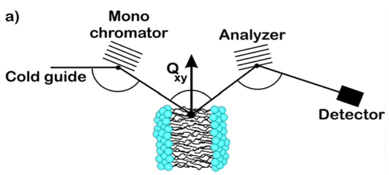
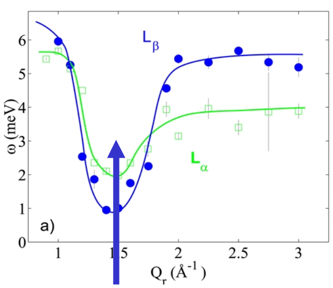
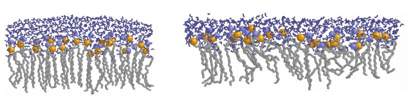
Coexistence of Gel and Fluid Phase





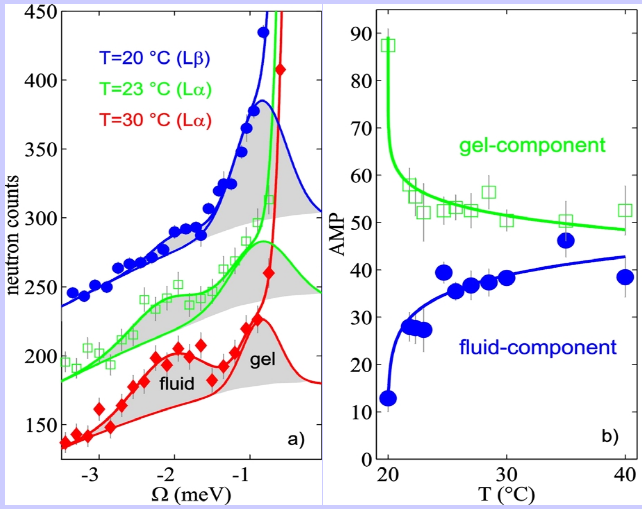




gel-phase fluid-phase

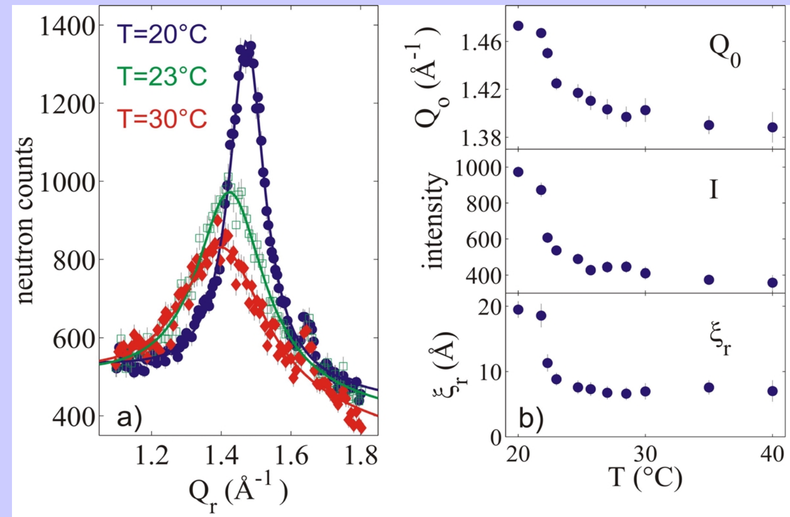
Dynamics:

Coexistence of gel and fluid excitations



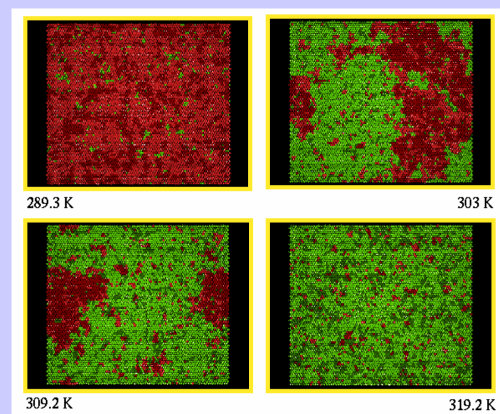
Neutron diffraction:

Continuous transition from gel to fluid



Micro-domain model

gel

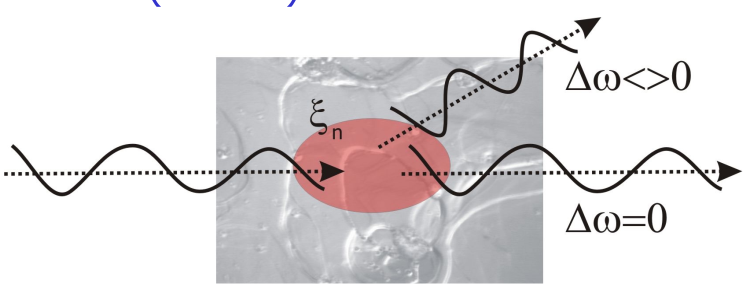


fluid

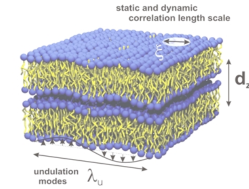
Hac et al, (2003)

Domain size smaller than neutron coherence length ξ_n (~100 Å)

No interference for inelastic scattering

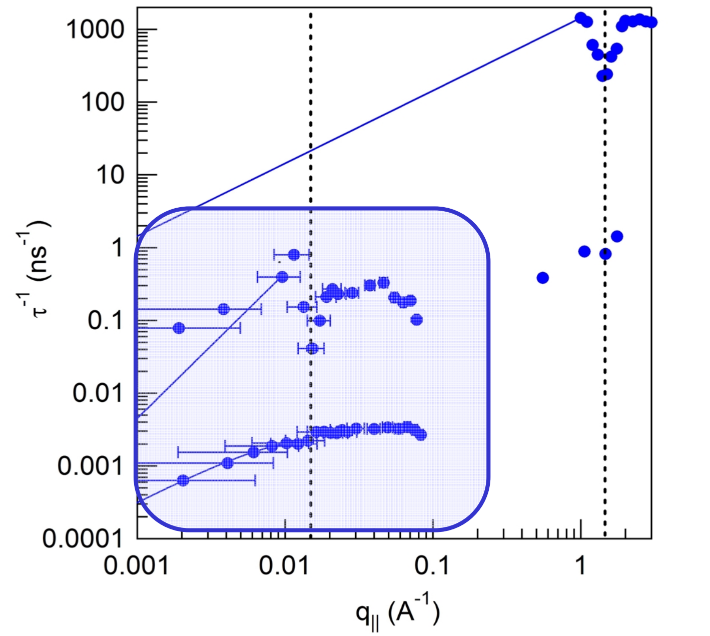


Elastically scattered waves interfere

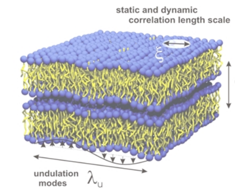


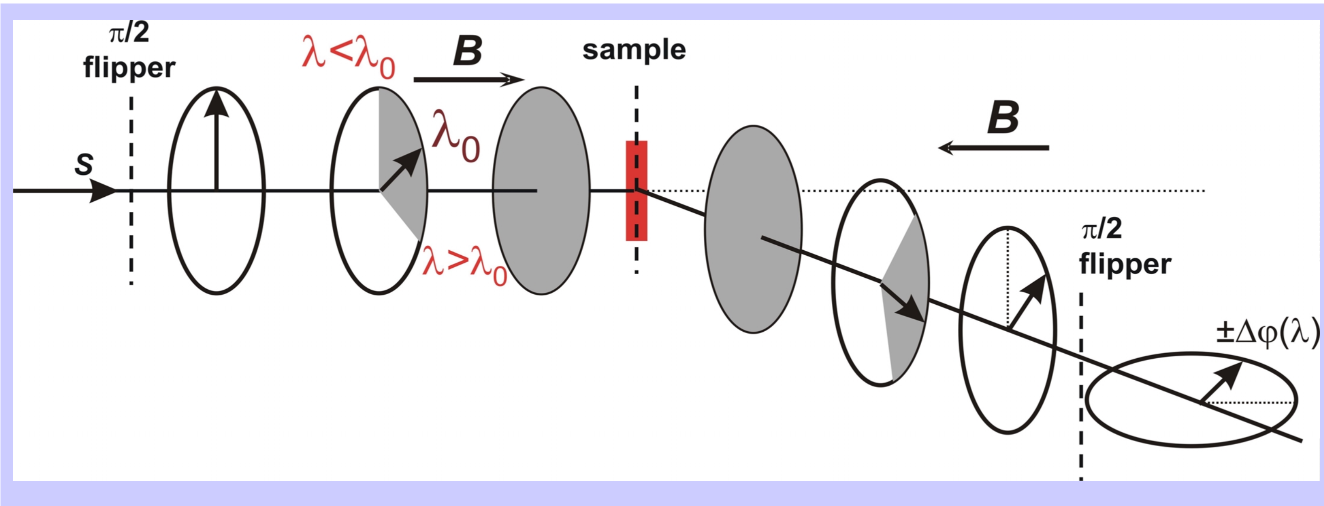
NSE

Neutron Spin-Echo to measure long wavelength undulations

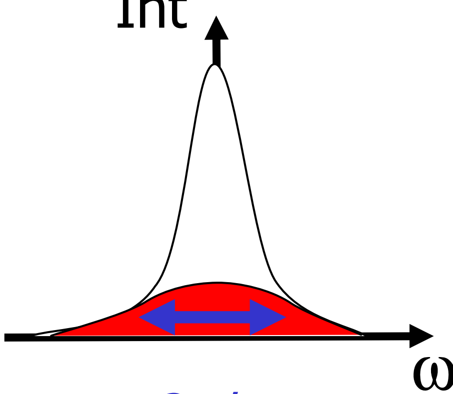


Spin-Echo Technique

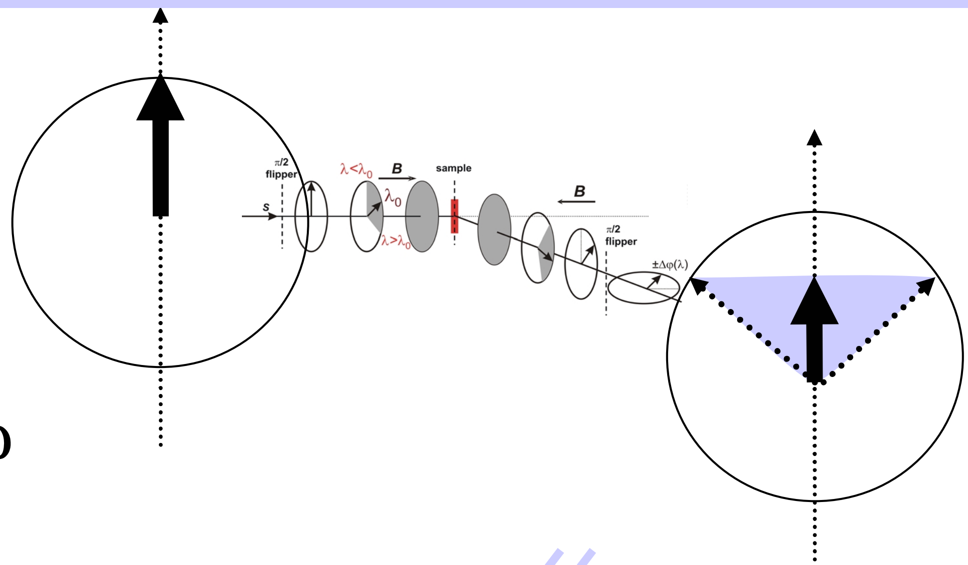


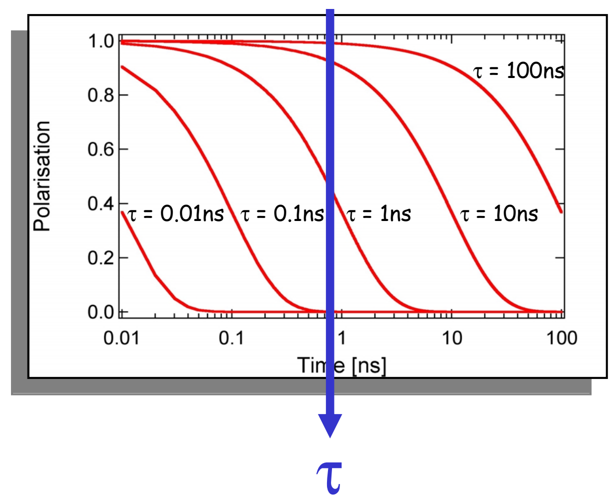


$\Delta\lambda/\lambda \cong 15\%$



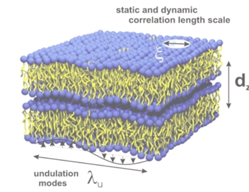
$\tau = 2\pi/\Delta\omega$

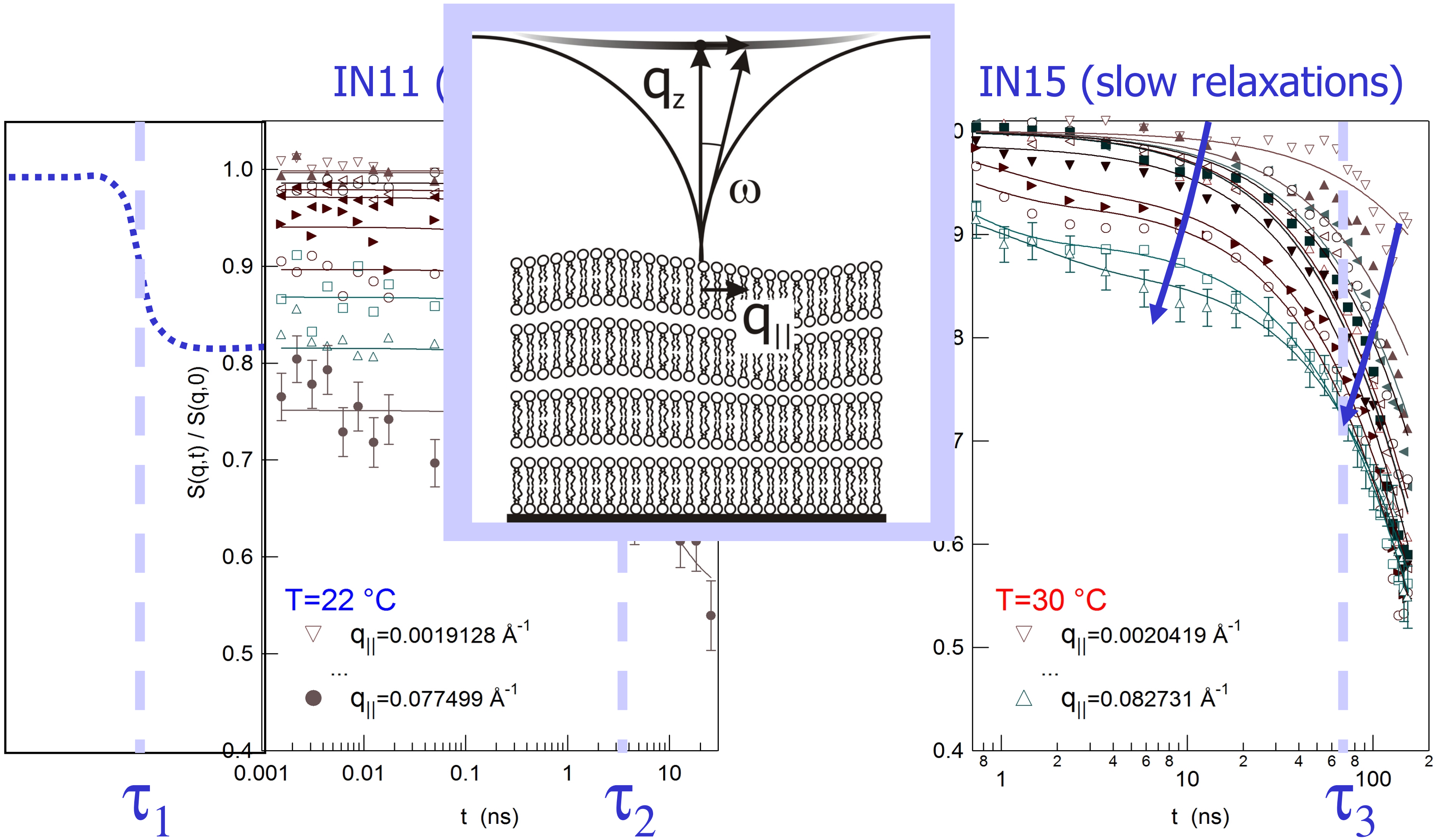




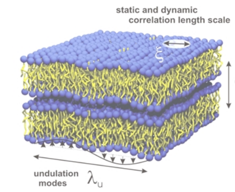
good monochromatization ⇹ good energy resolution

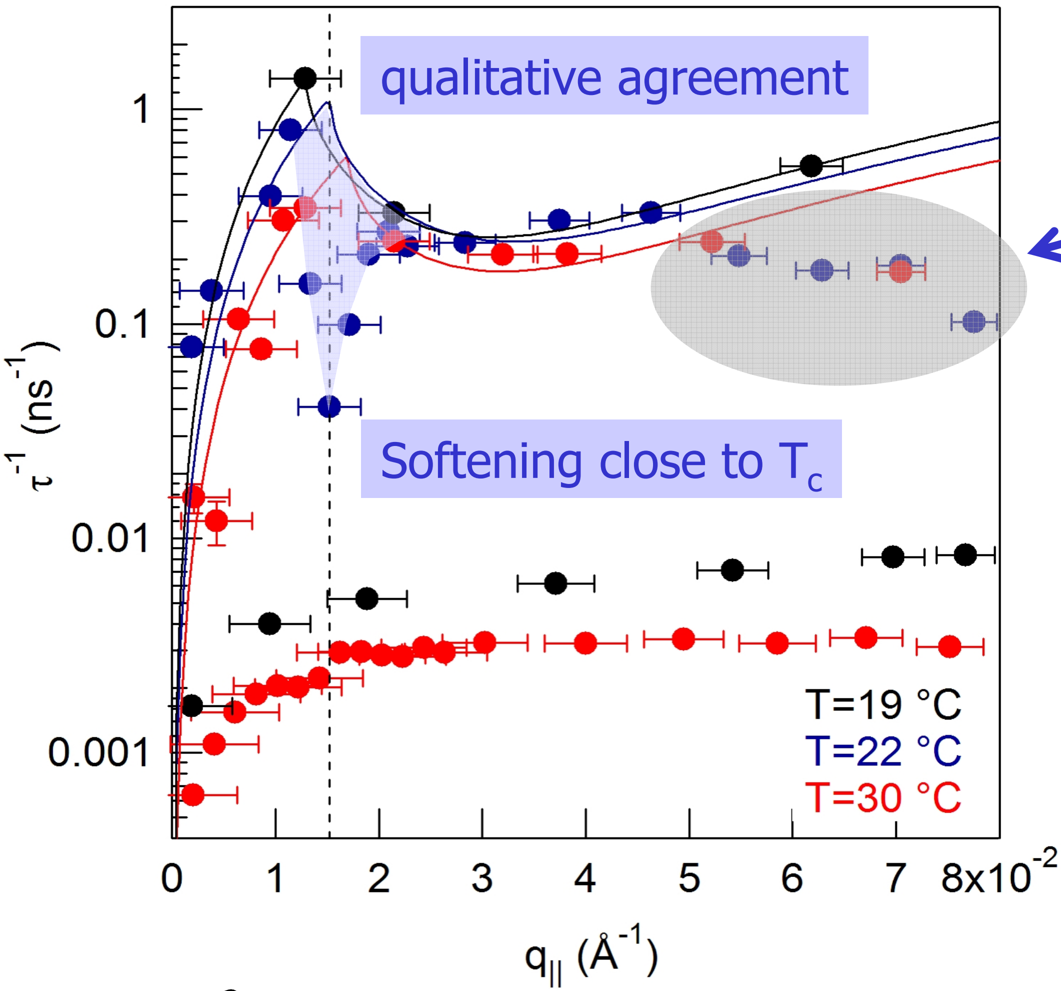
Spin-Echo Measurements



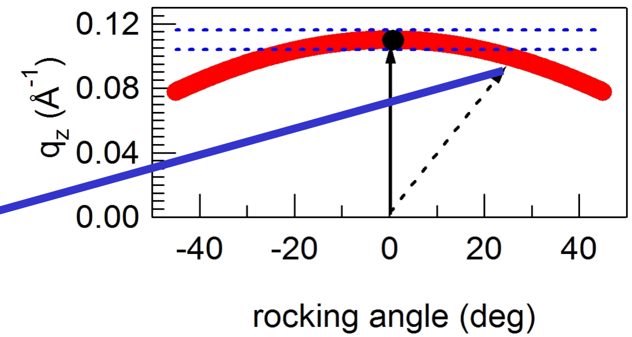


Undulation “Dispersion” Relations

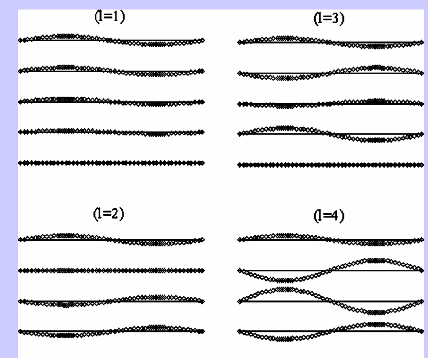




Not well described by present theories

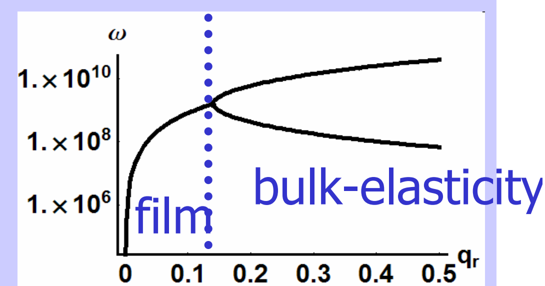


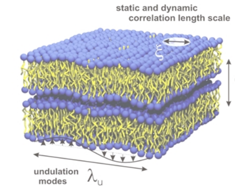
Theory



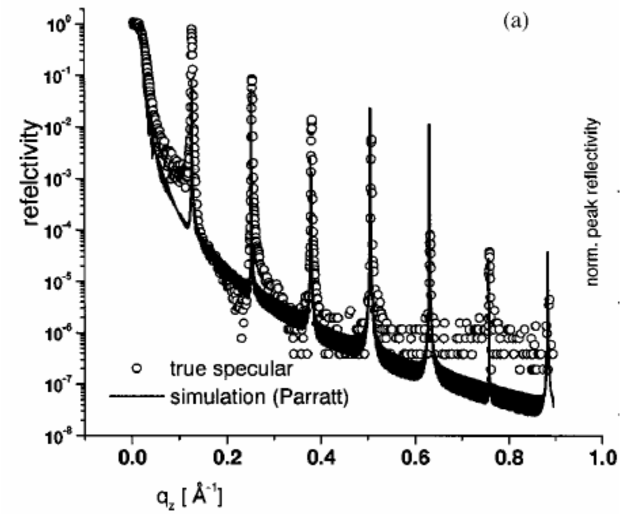
Romanov and Ul’yanov, PRE 66, 061701 (2002)

Relaxation

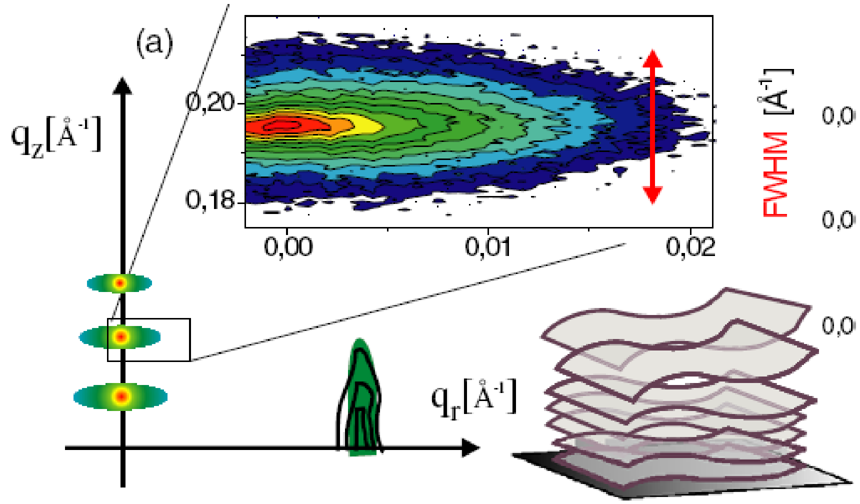




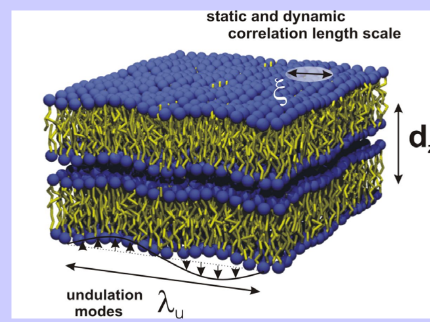
Neutron and X-ray Reflectometry



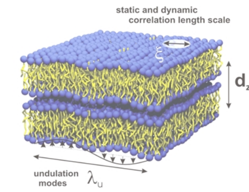
Knowledge about mesoscopic fluctuations in membranes mainly stems from diffuse reflectivity scattering and line shape analysis



Quasi- and inelastic measurements important to probe and improve theoretical membrane models



Elasticity parameters K and B from advanced (smectic) theory



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- Giovanna Fragneto, ILL, D17
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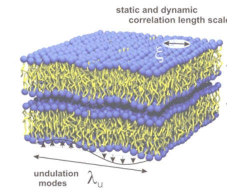
- Franz Demmel, ILL, IN3
- Arno Hiess, ILL, IN8
- Tilo Seydel, IN10/IN16
- Fanni Juranyi, FOCUS, PSI
- Dieter Richter, FZ-Jülich

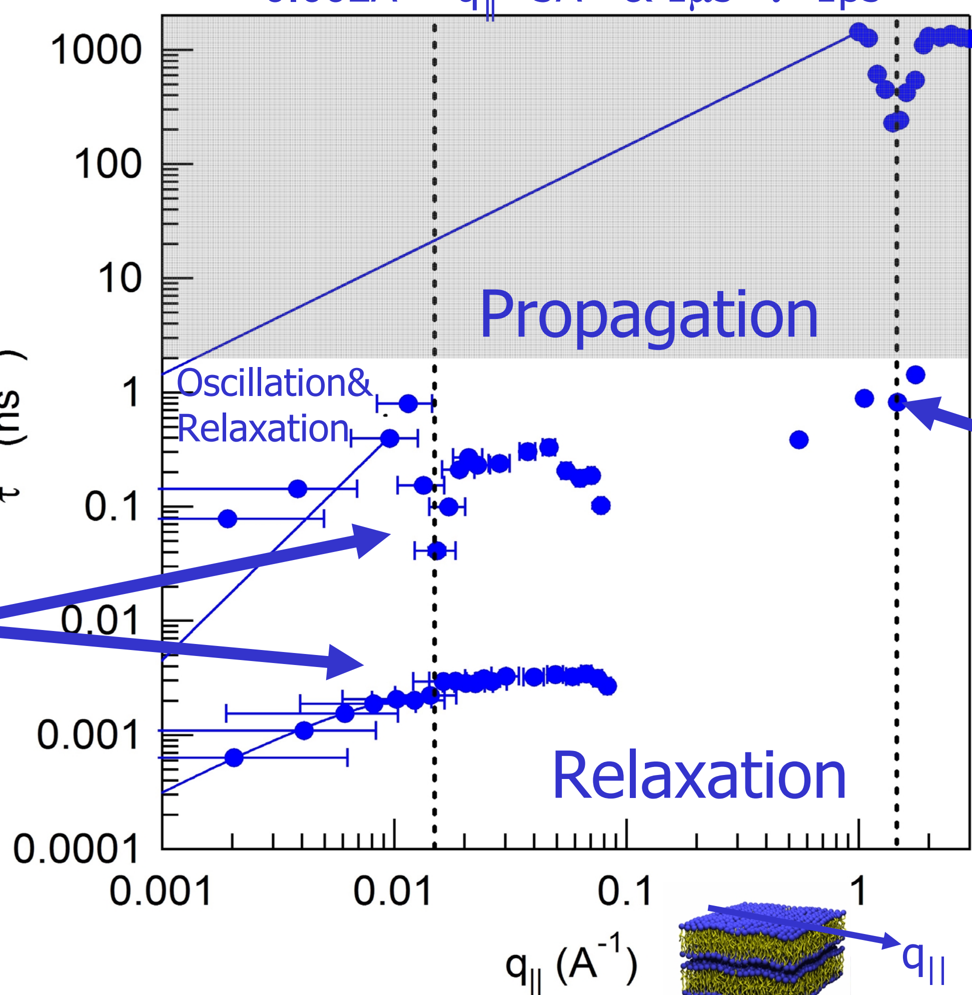
Collective Excitations in model membranes



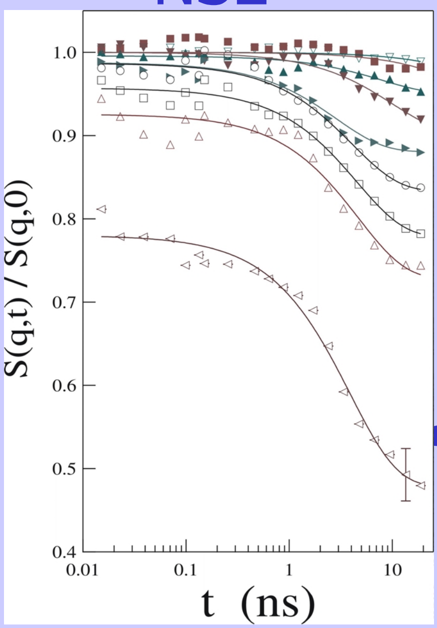
The 'Neutron Window'

DMPC –d54

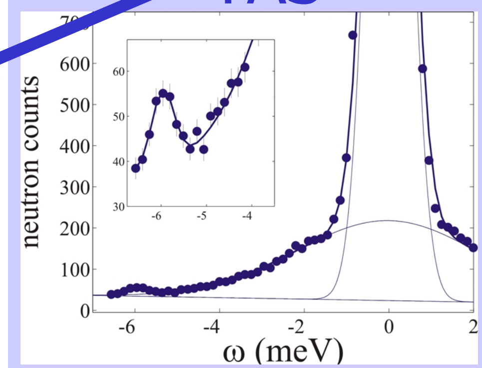
$0.002Å^{-1}<q_{\|}<3Å^{-1}$ & $1\mu s<\tau<1ps$



NSE



TAS



BS