Triple-Axis Spectrometry

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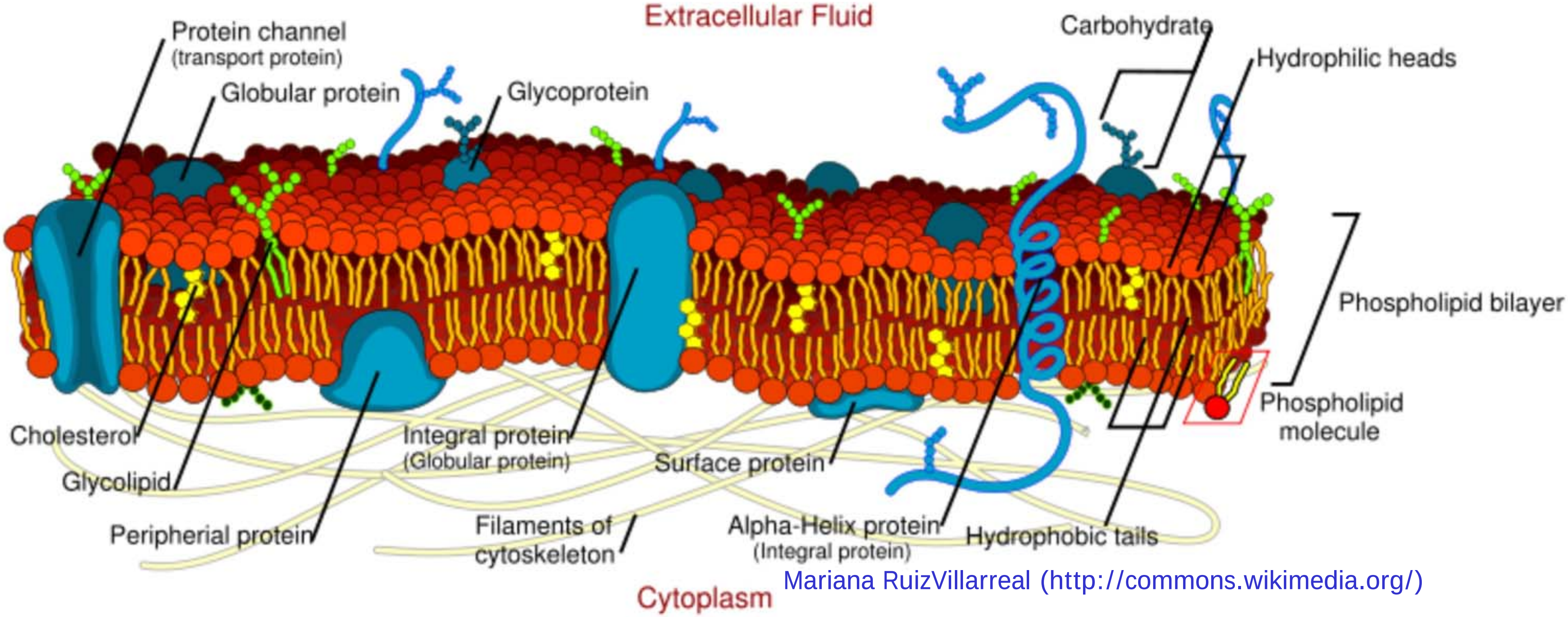
The Cell Membrane

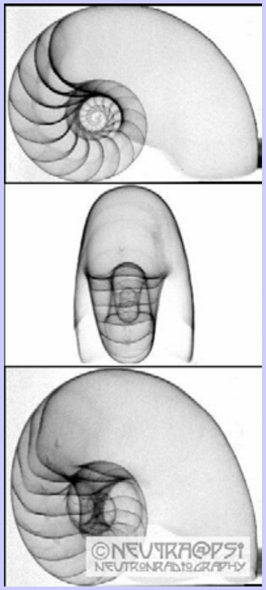


Mariana RuizVillarreal (http://commons.wikimedia.org/)

Membrane is the primary site of (inter)action

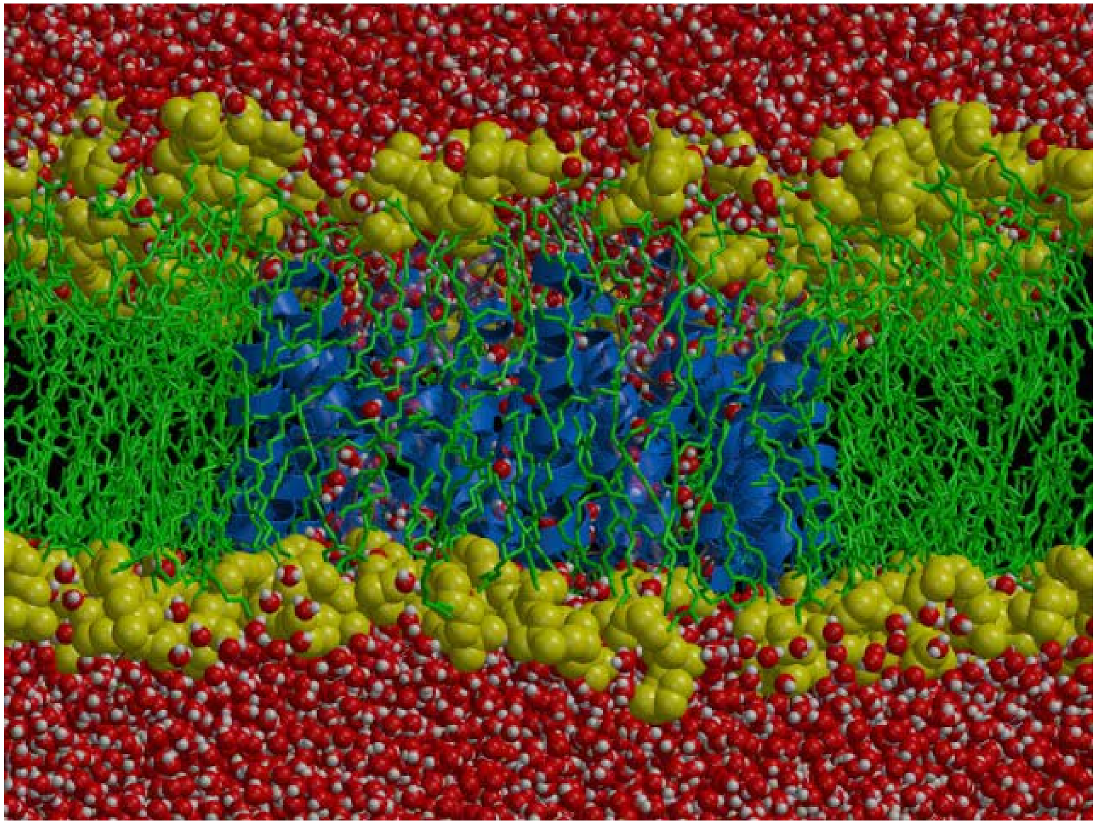
Why Neutrons?

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**

Membrane Dynamics



Bert L. de Groot, Rainer A. Böckmann, and Helmut Gruber

‘multi-scale’: relevant dynamics in a large range of length and time scales

missing or not well developed periodic **structure** (BZ concept)

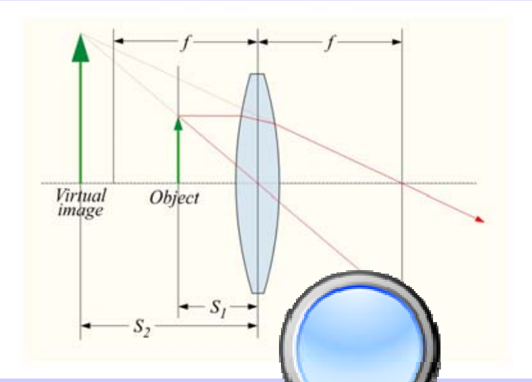
high ‘intrinsic’ background

- different molecular components
- single and collective molecular motions

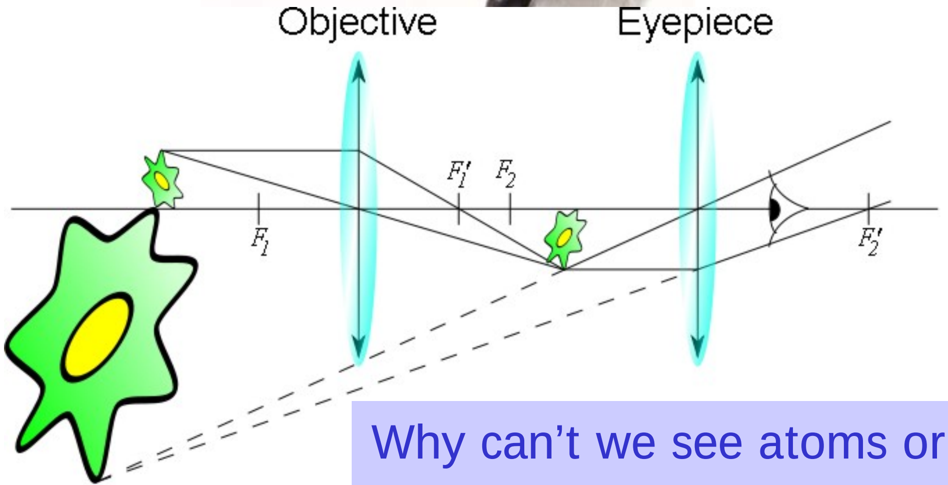
Optical Techniques

Laboratory for Membrane and Protein Dynamics

Magnifying Glass



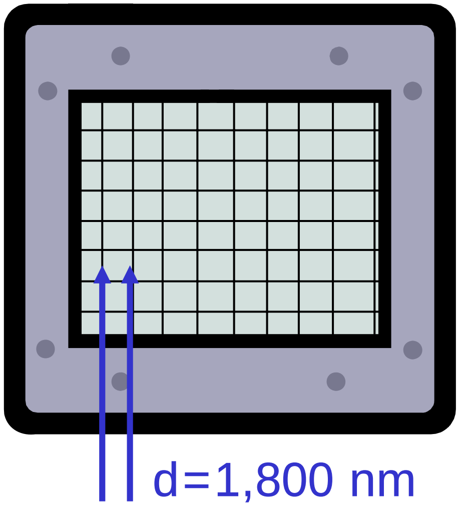
Optical Microscope



Why can't we see atoms or molecules?
-> neutron scattering

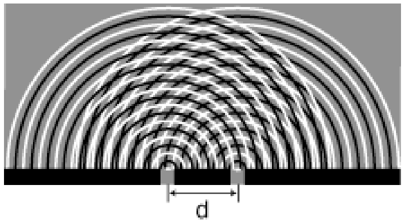
Wave Properties

Diffraction grating



Grating: 13,500 lines/inch

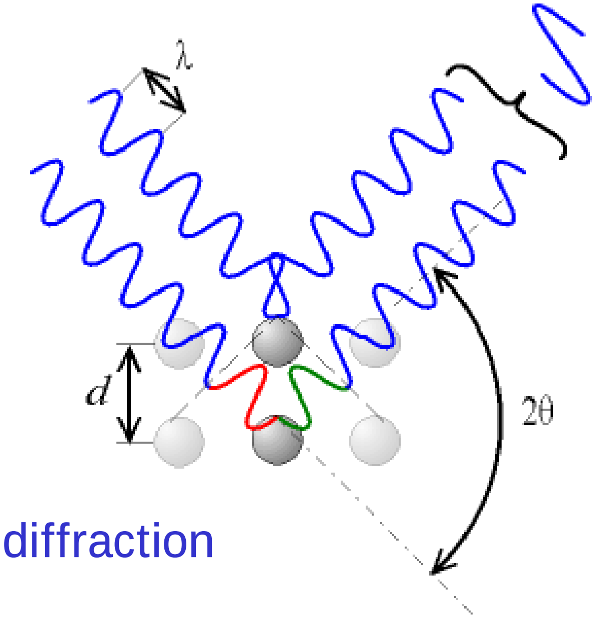
Green Laser: 532 nm



Wave character becomes important when things get ‘small’

‘Diffraction limit’ when wavelength meets object size:
Limit for optical techniques
=> Neutrons and X-rays

Scattering-Reciprocal Space

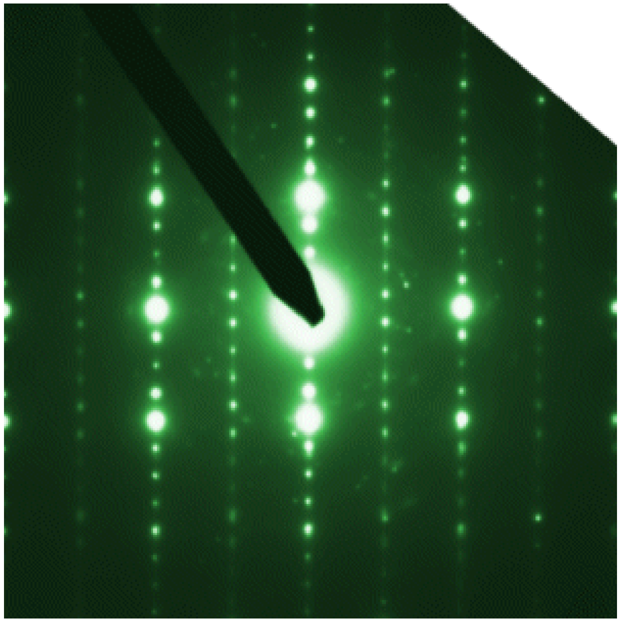


diffraction

"…where the atoms are and how they move."

Scattering vector

$$q = \frac{4\pi \sin\theta}{\lambda} = \frac{2\pi}{d}$$



Fourier Transformation

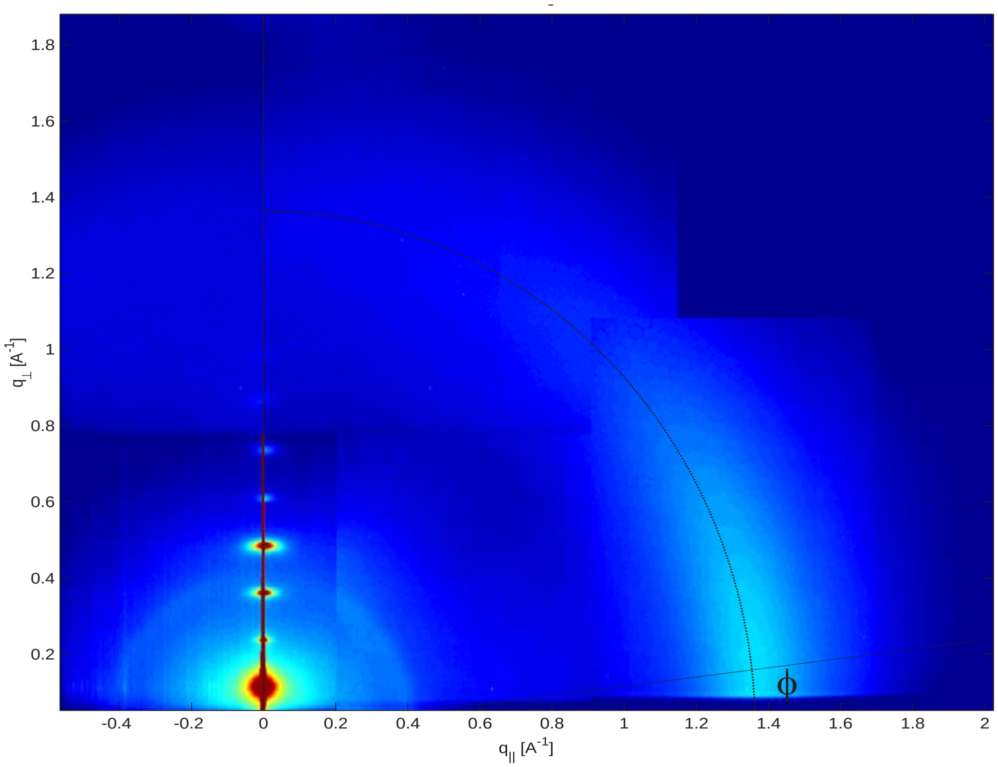
'real space' ⟷ *'reciprocal space'*

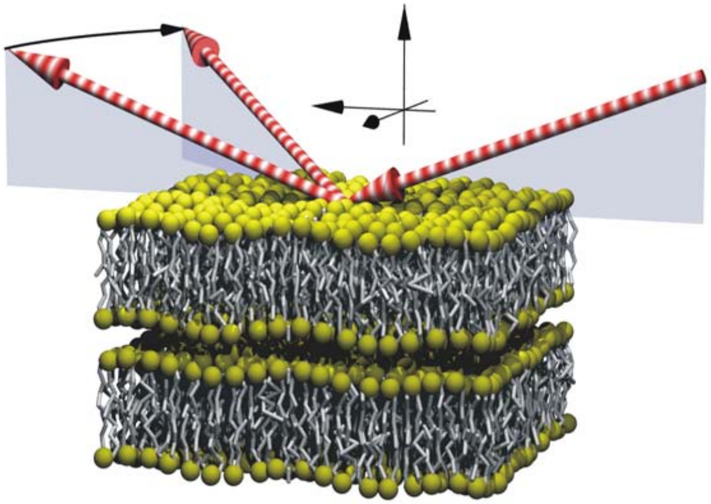
Scattering laws

momentum $\vec{q} = \frac{m}{\hbar}(\vec{v}_1 - \vec{v}_2)$

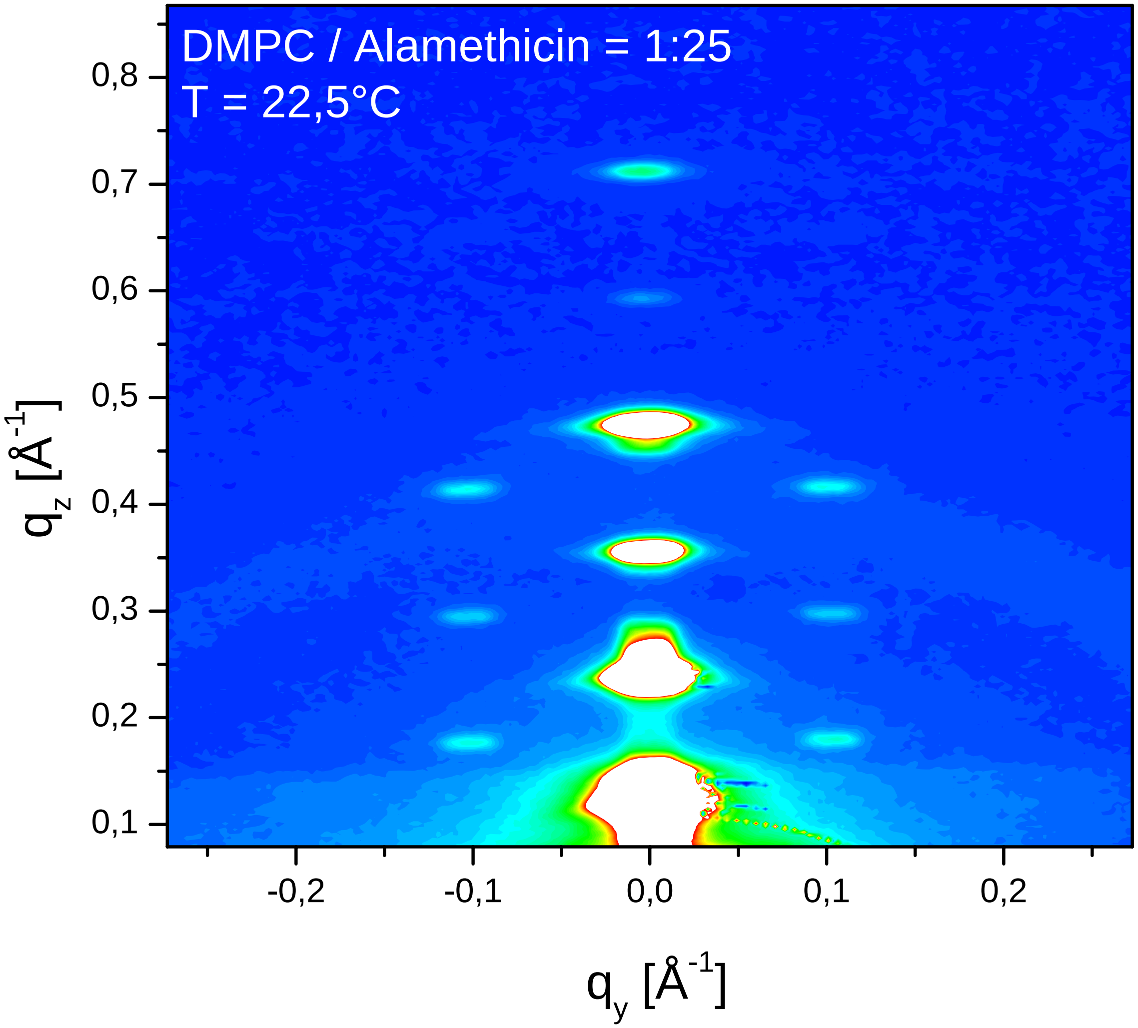
energy $\hbar\omega = \frac{1}{2} m \left(v_2^2 - v_1^2\right)$

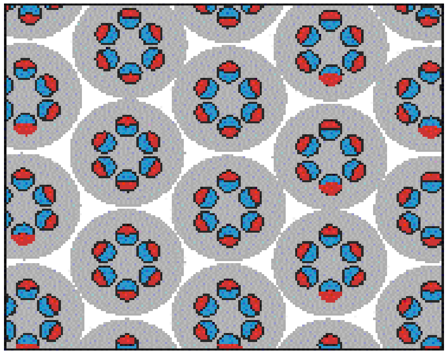
Reciprocal Space of a Membrane

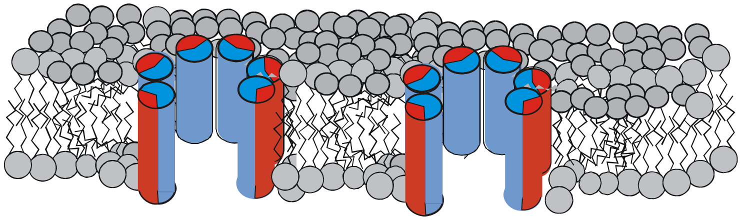




Complex Membrane

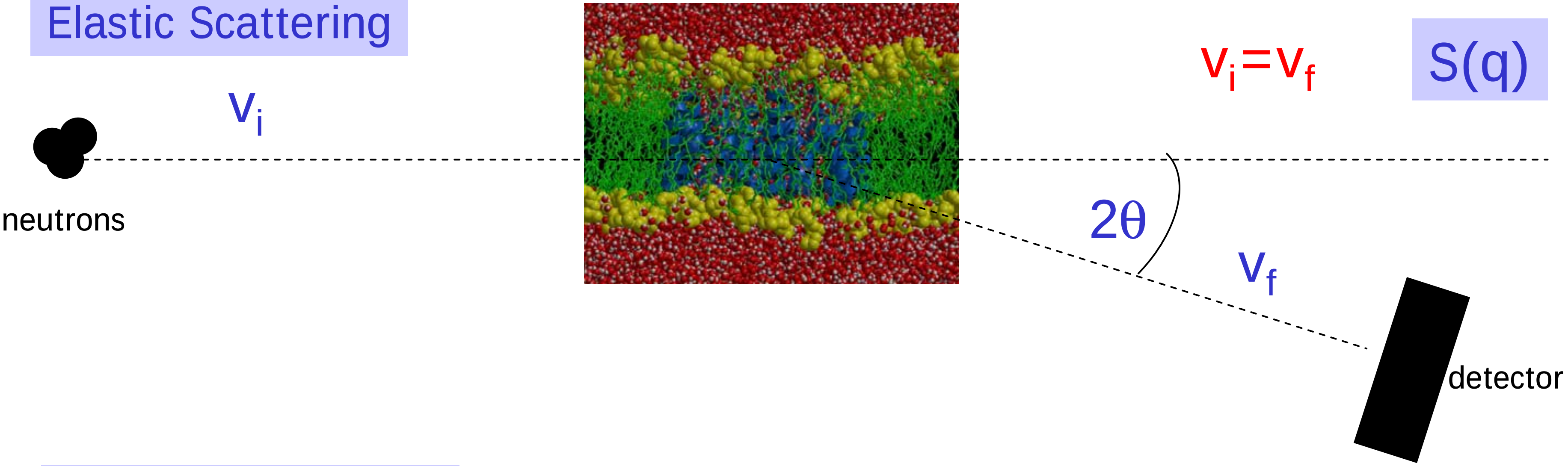






Elastic and Inelastic Neutron Scattering

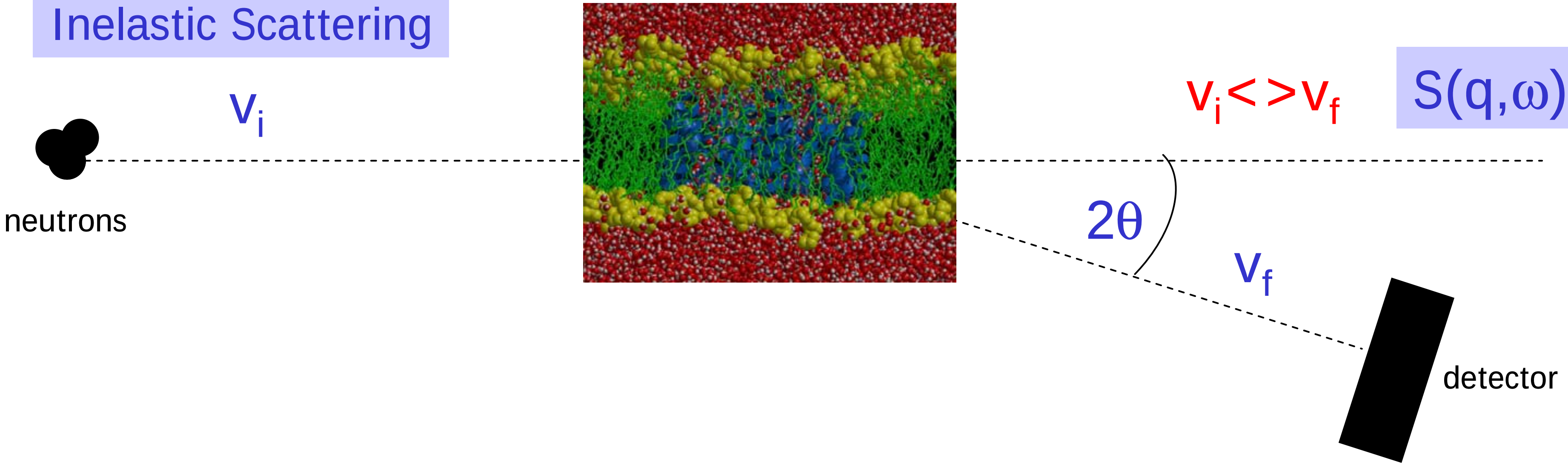
Elastic Scattering



$v_i = v_f$

$S(q)$

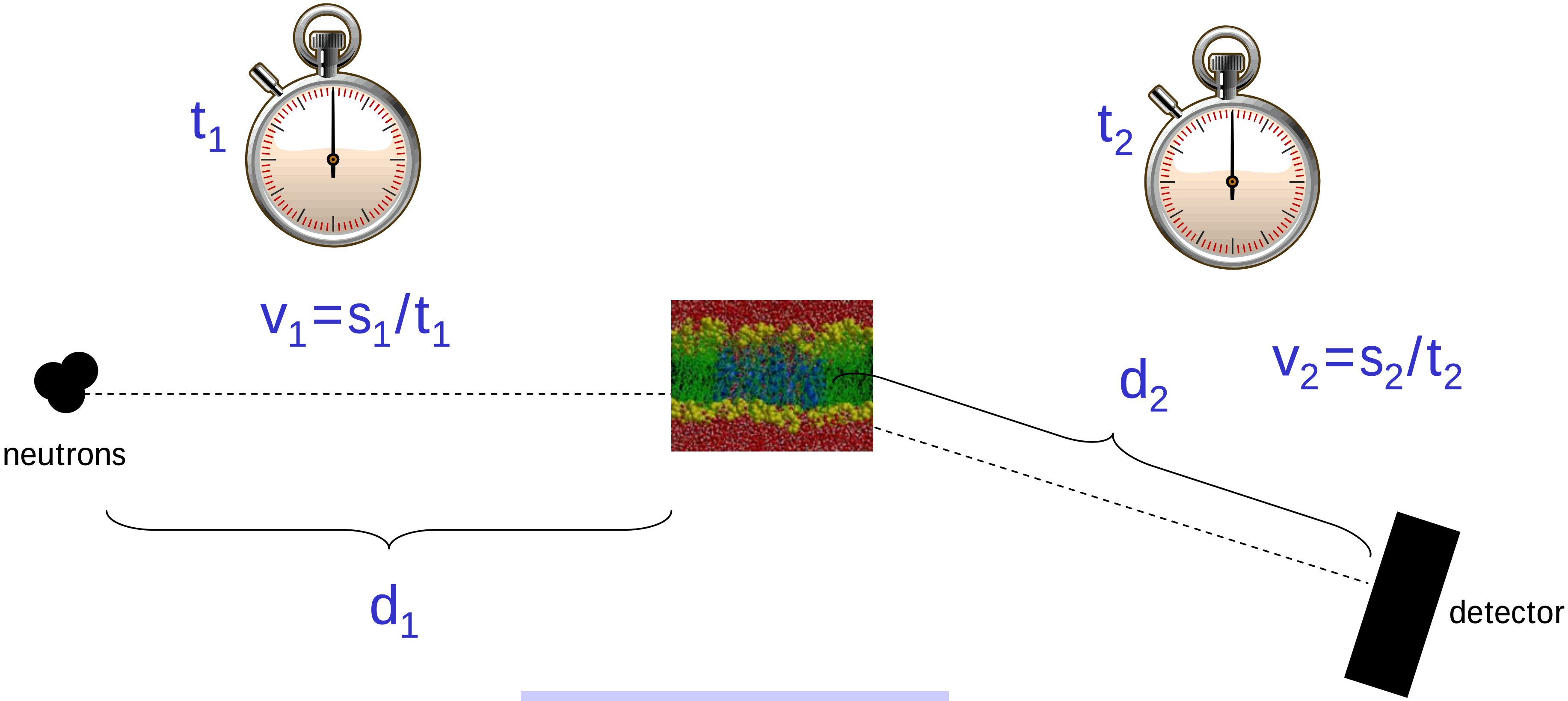
Inelastic Scattering



$v_i <> v_f$

$S(q,\omega)$

Neutron **T**ime **o**f **F**light Technique



t_1

t_2

$v_1=s_1/t_1$

$v_2=s_2/t_2$

d_2

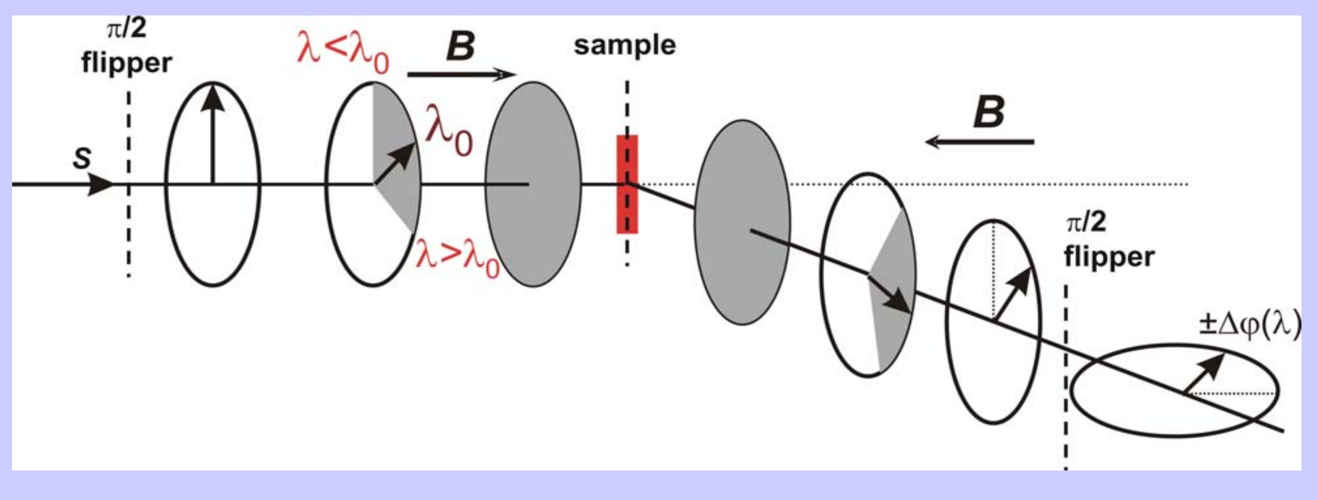
neutrons

d_1

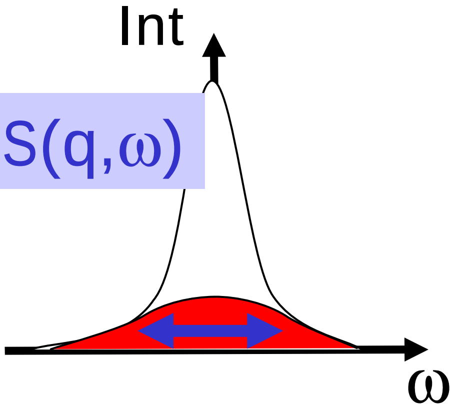
detector

$$\hbar\omega=\frac{1}{2}m\left(v_2^2-v_1^2\right)$$

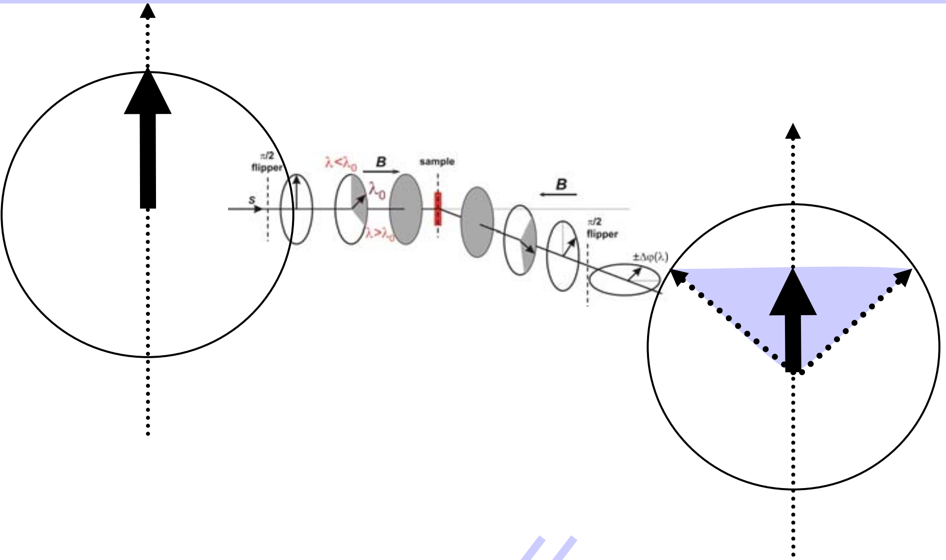
Neutron **S**pin-**E**cho



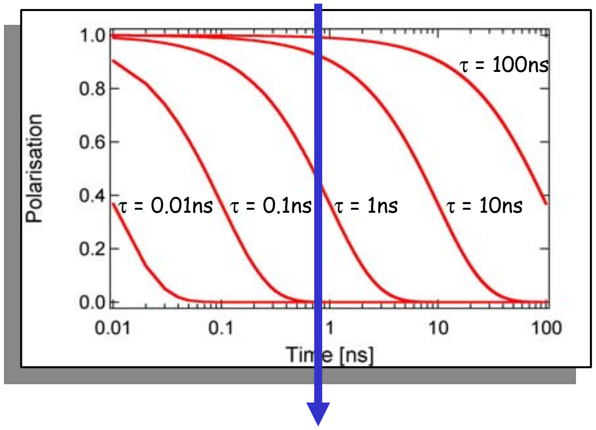
$\Delta\lambda/\lambda \cong 15\%$



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



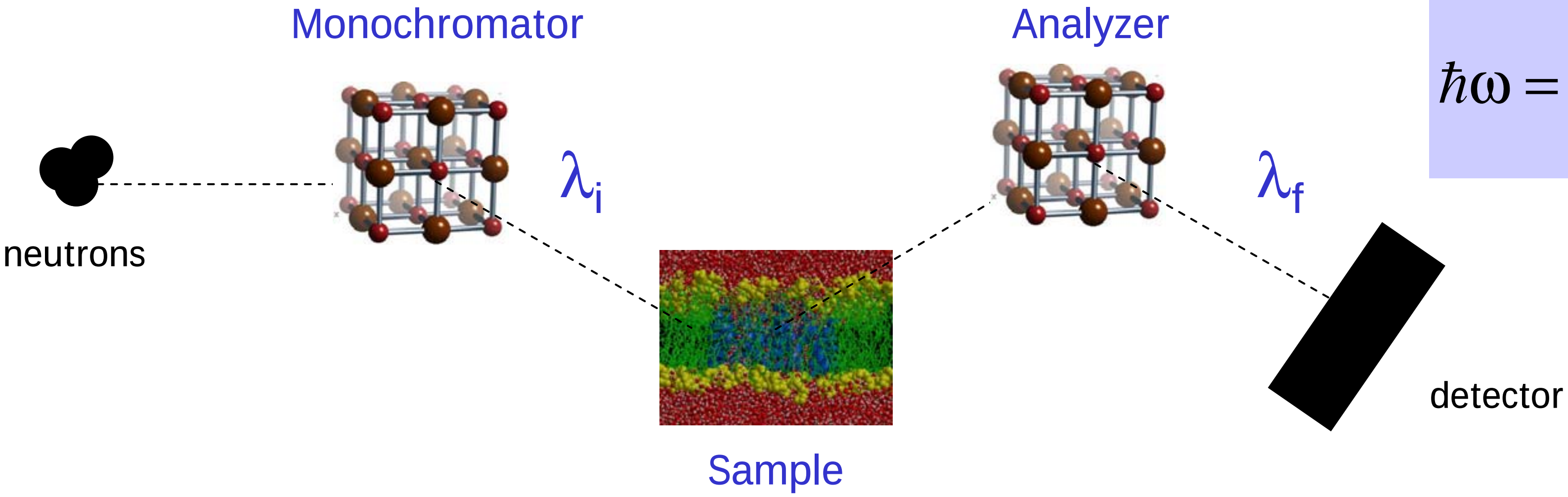
S(q,t)



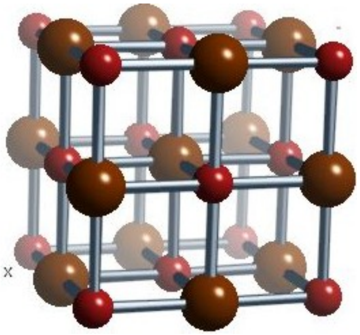
τ

good monochromatization $\not\Leftrightarrow$ good energy resolution

Neutron **T**riple **A**xis **S**pectrometer

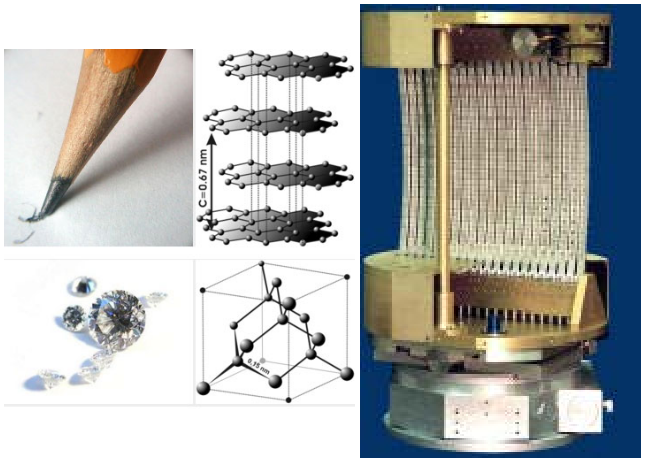


$$\hbar\omega = \frac{h^2}{2m}\frac{1}{\lambda_i^2 - \lambda_f^2}$$



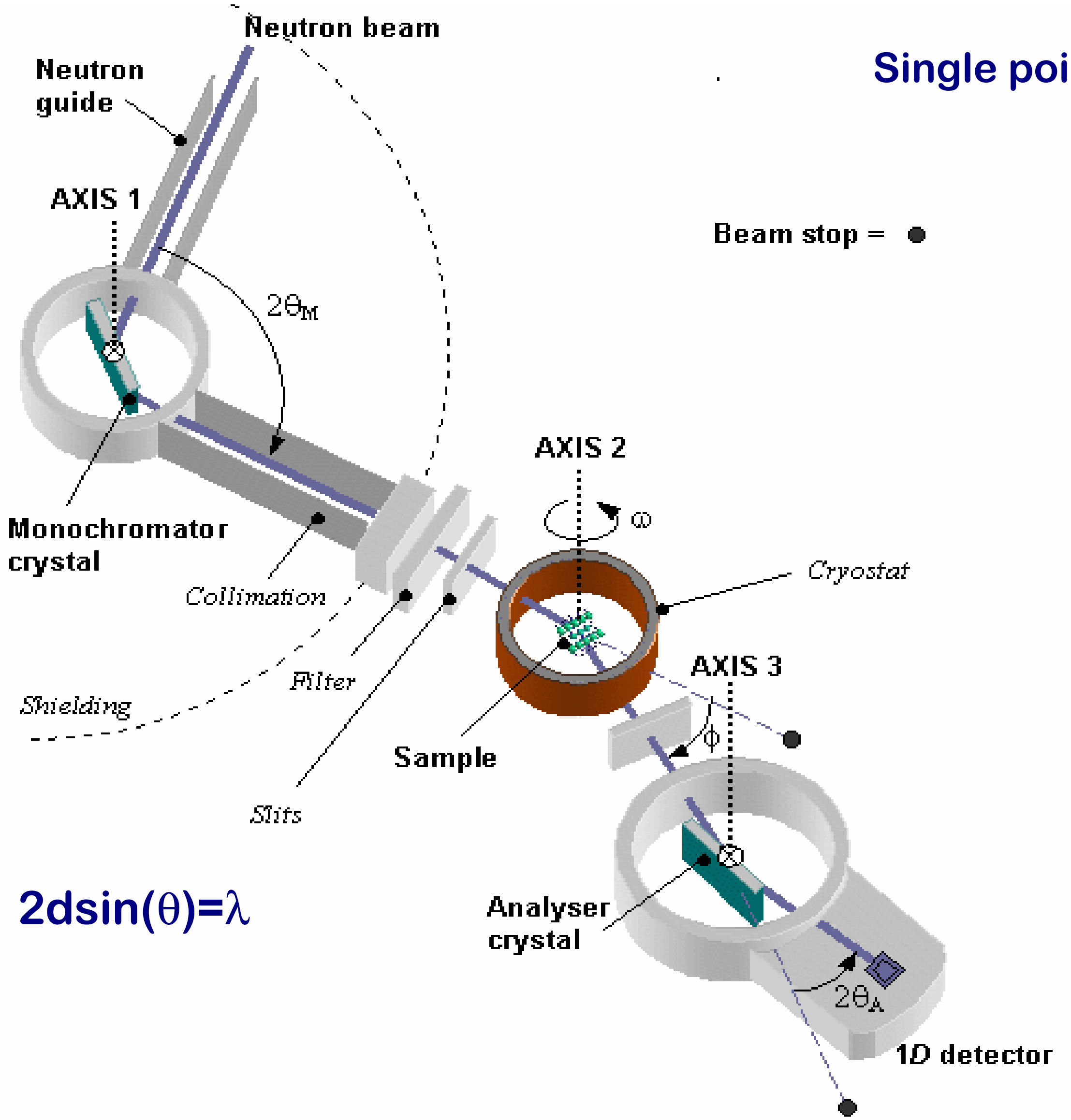
Bragg's Law

$$2d\sin\theta = \lambda$$

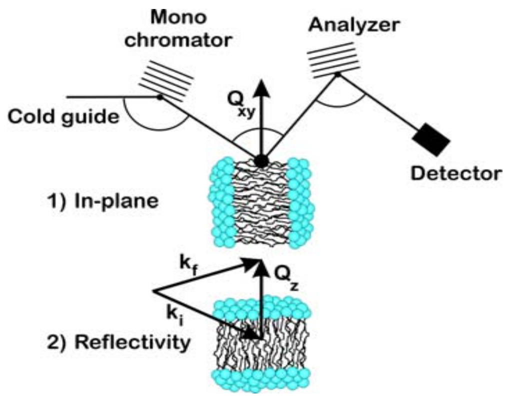


Triple-axis spectrometers

Single point in (Q,ω) space

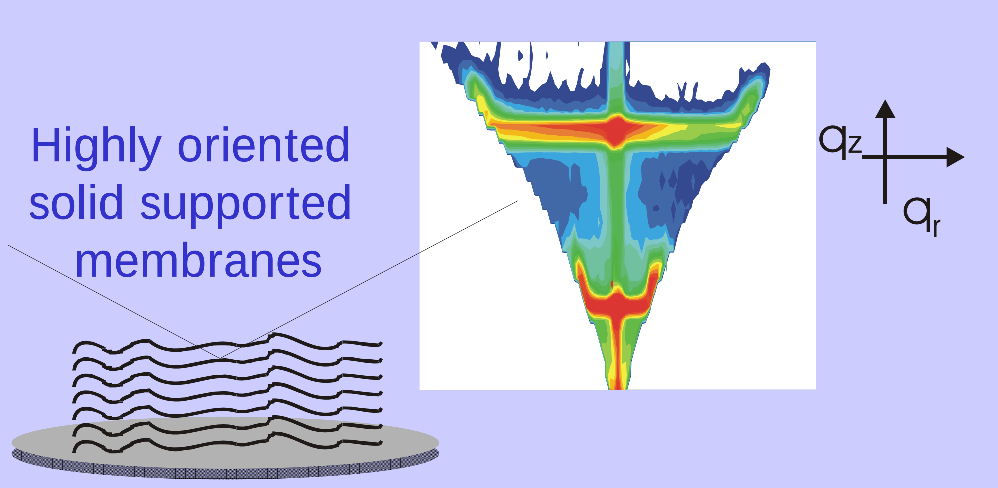


$2d\sin(\theta)=\lambda$



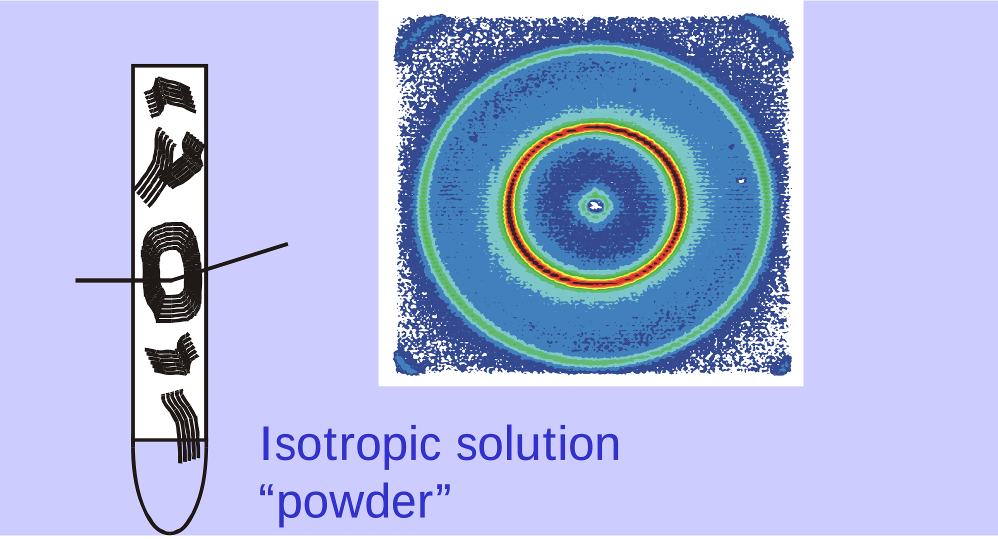
By rotating the sample, Q can be placed within the plane of the membranes or perpendicular to the bilayers

Scattering from aligned phases

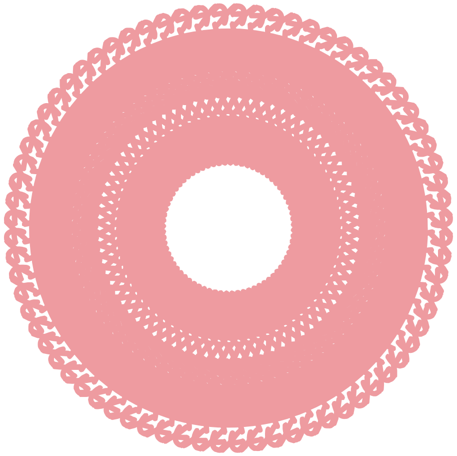


Highly oriented solid supported membranes

Si-wafer



Isotropic solution “powder”



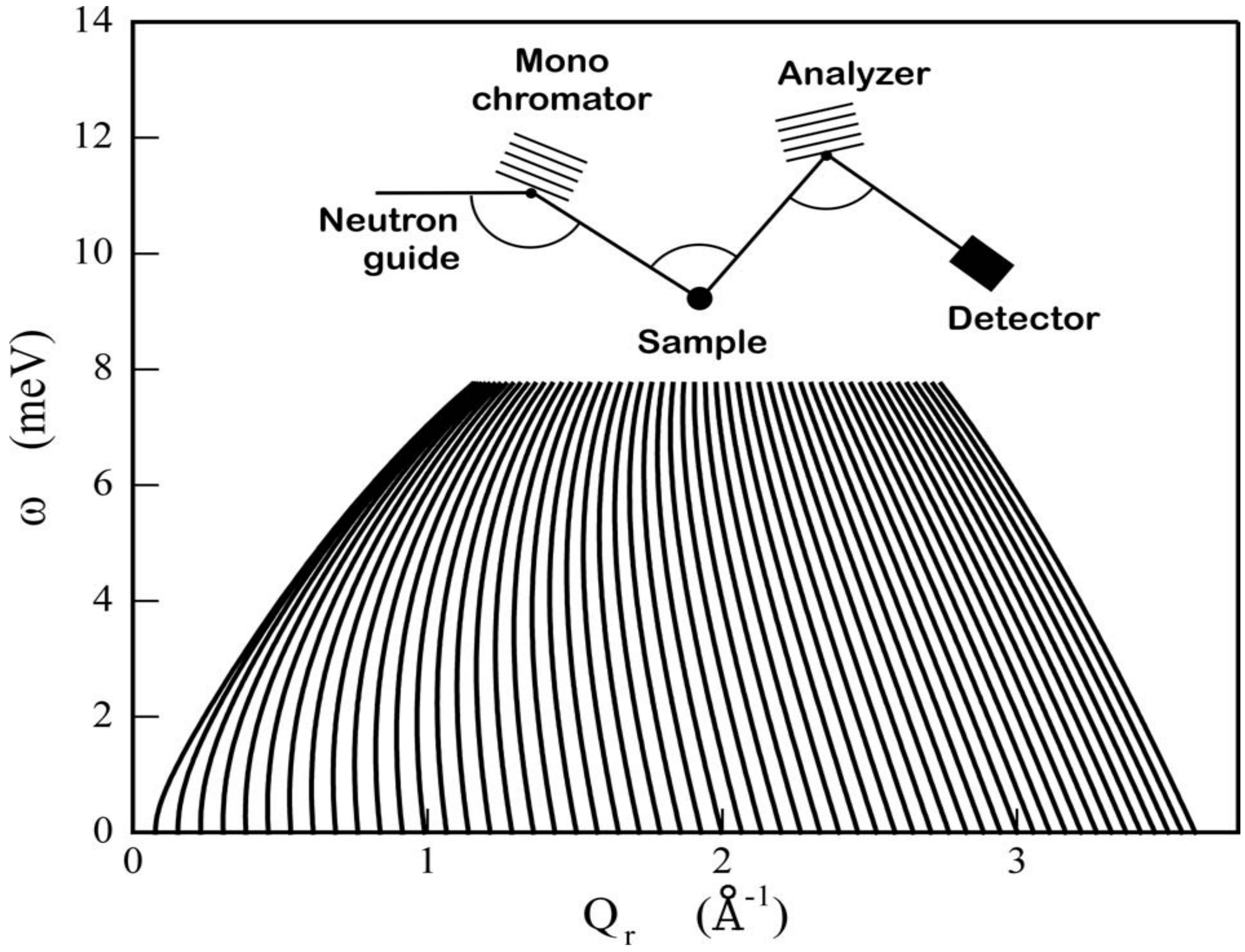
Triple-axis spectrometers

IN14 animation

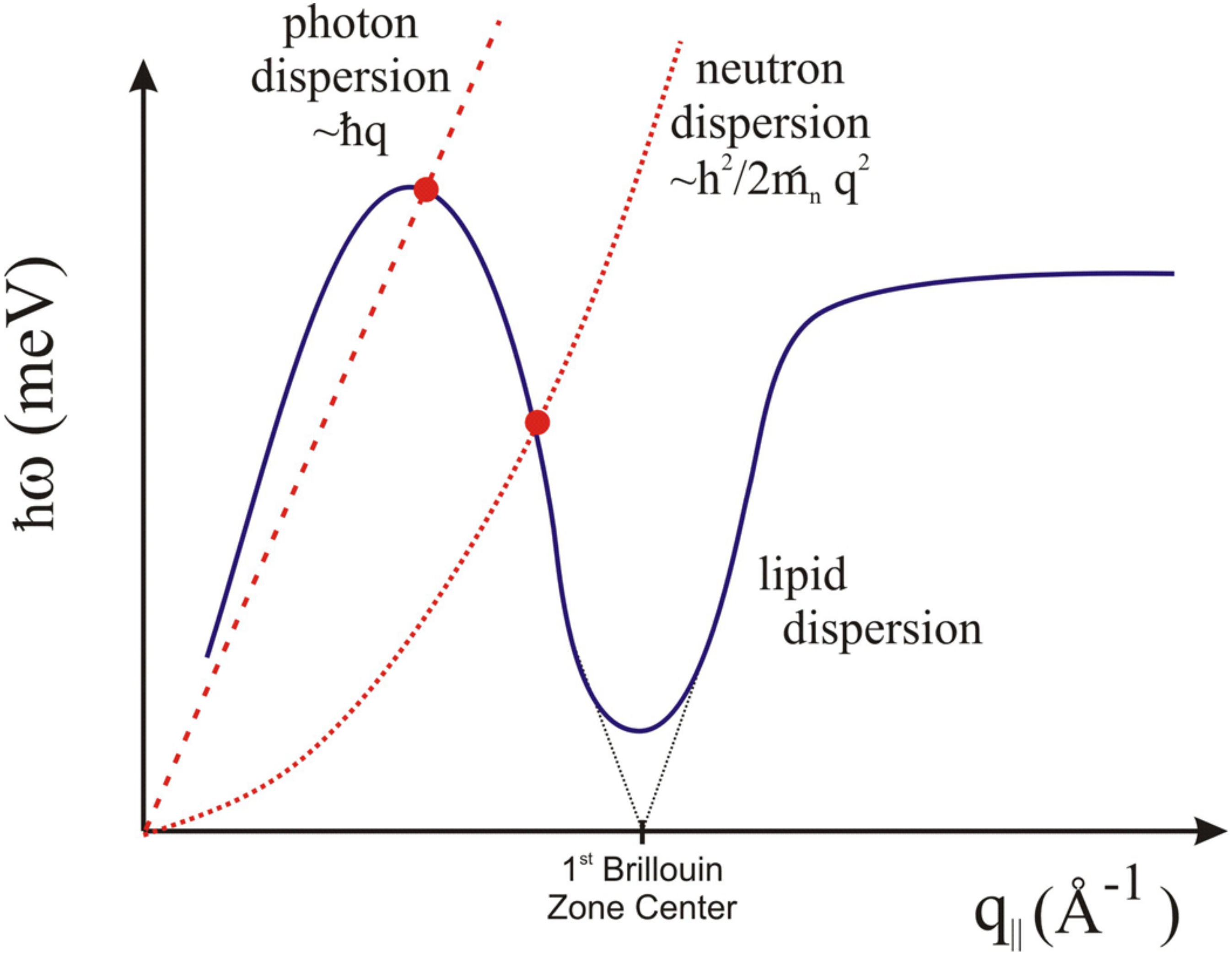
Matlab TAS Simulation

Triple-axis Resolution

accessible (Q,ω) range for a cold TAS



Scattering Probes



“Broadband” Neutron Spectroscopy

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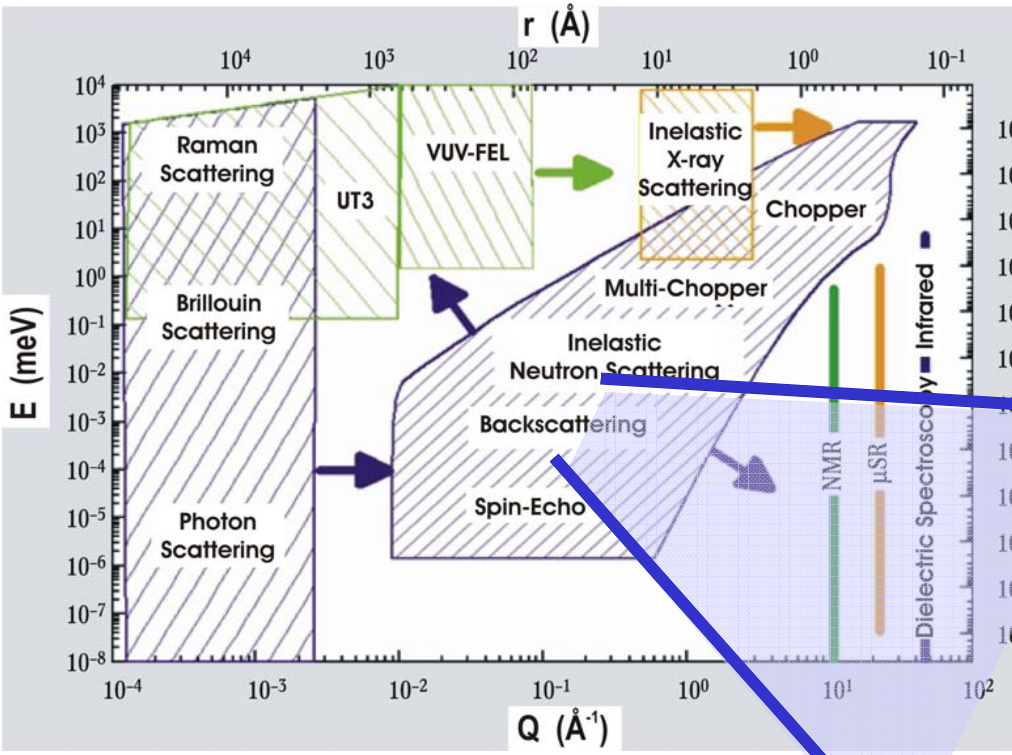
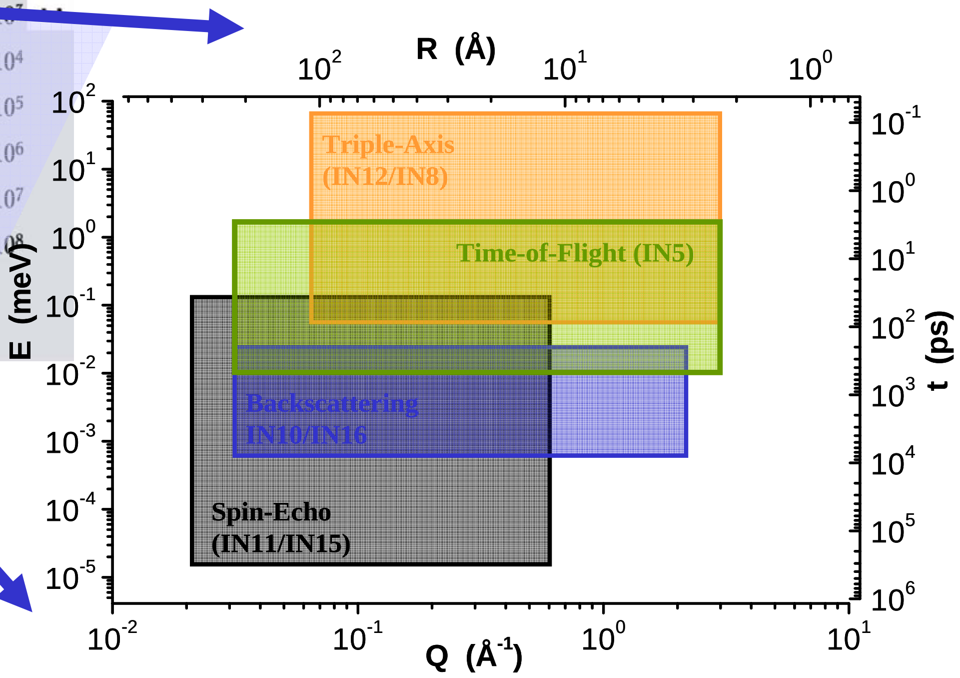
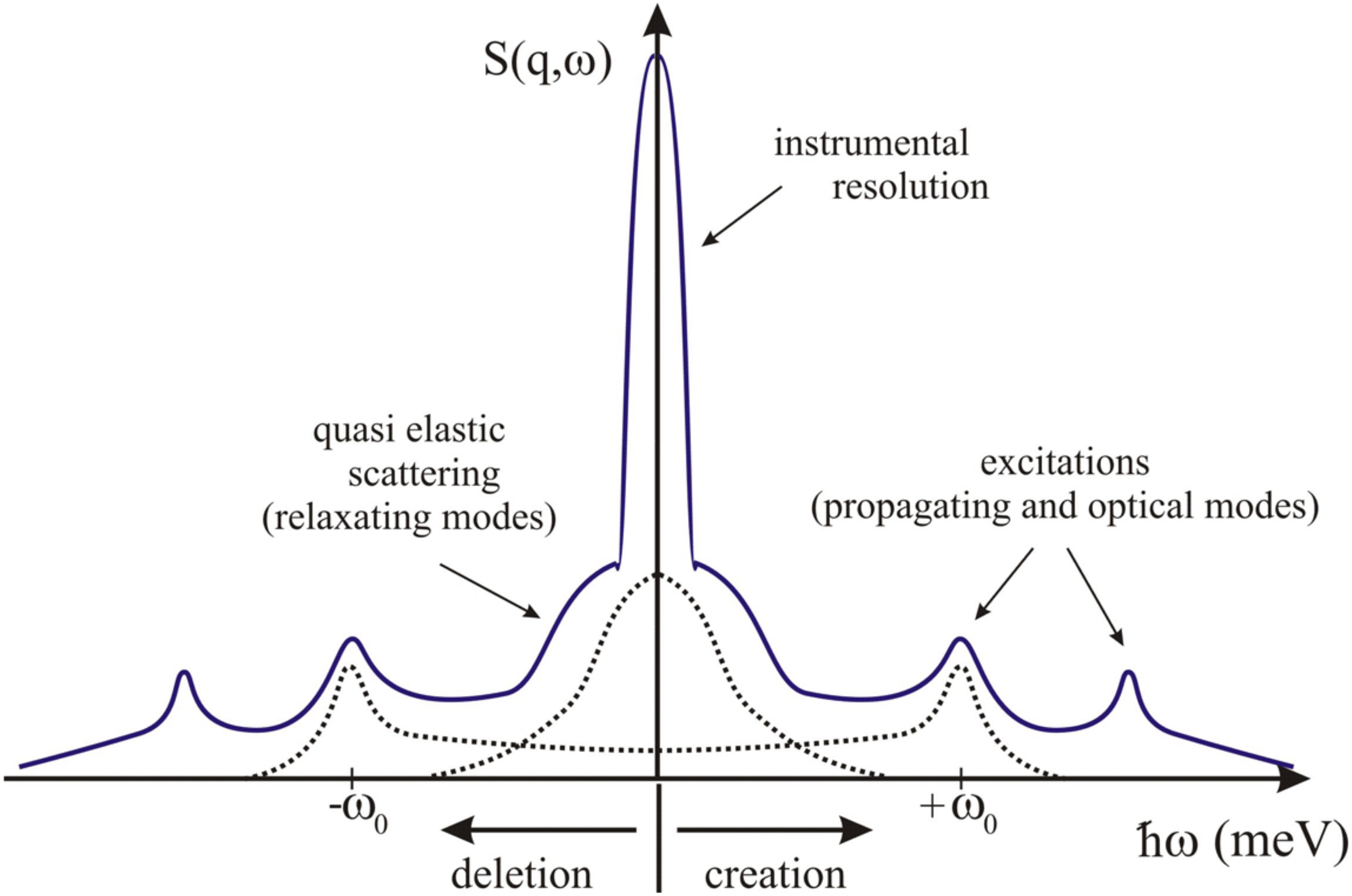


Inelastic neutron scattering gives wave vector resolved access to dynamics



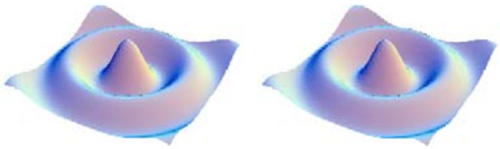
excitations
relaxations ⟷ specific motions

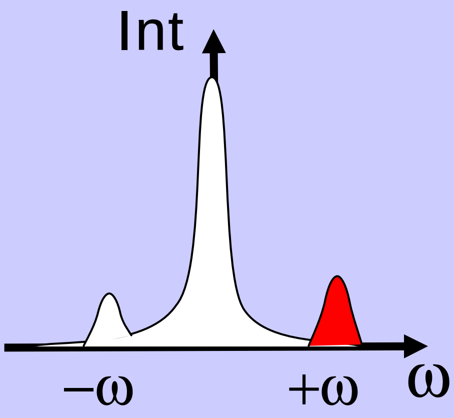
Excitation Spectrum



Quasi- and Inelastic Neutron Scattering

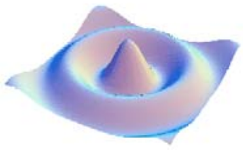
Propagating,
Oscillating Mode

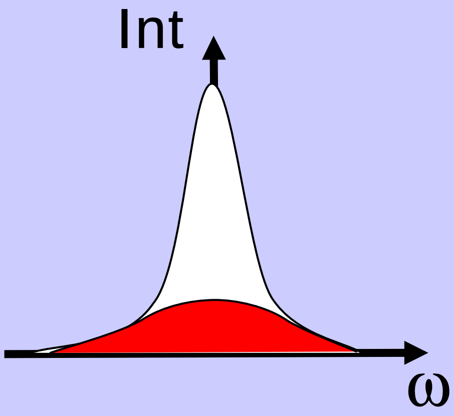




Energy

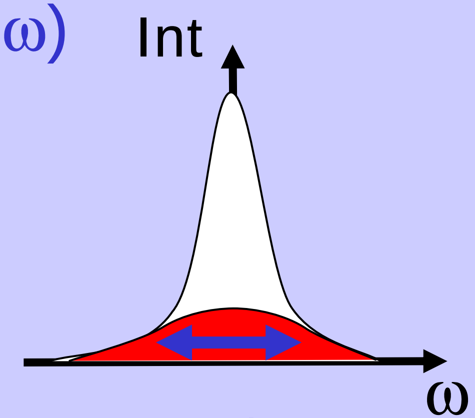
Relaxating
(overdamped) Mode





Energy-Time domains

S(q,ω)



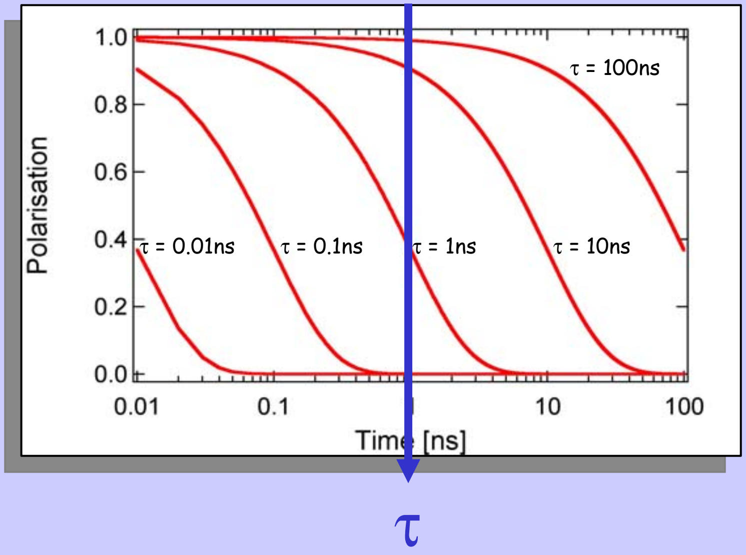
$\tau = 2\pi/\Delta\omega$

Lorentzian

$$E = \frac{h}{et}$$

Line shape

S(q,t)

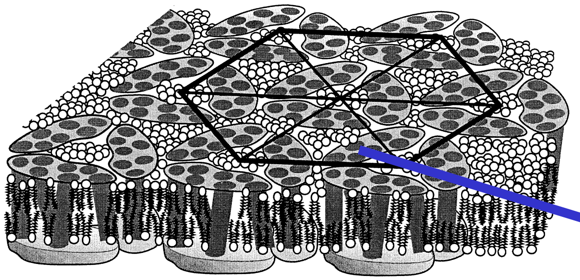


Exponential decay
Debye relaxation

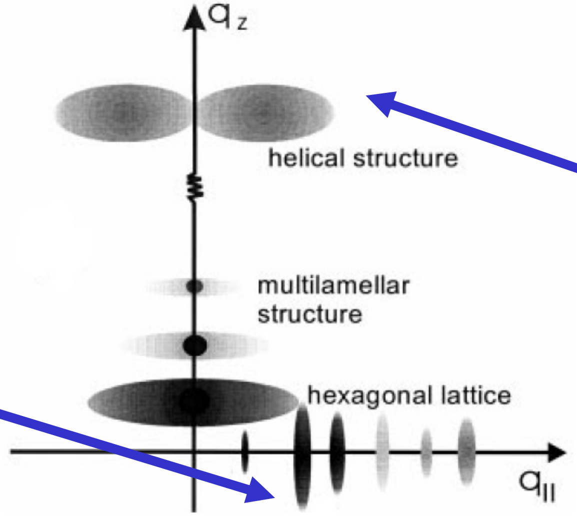
$$1ps = \frac{4.14}{1meV} \qquad 1ns = \frac{4.14}{1\mu eV} \qquad 1\mu s = \frac{4.14}{1neV}$$

Cooperative Protein Dynamics

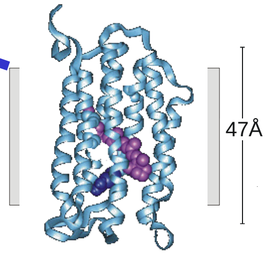
Bacteriorhodopsin in Purple Membrane



Sample: Dieter Oesterhelt, MPI Munich

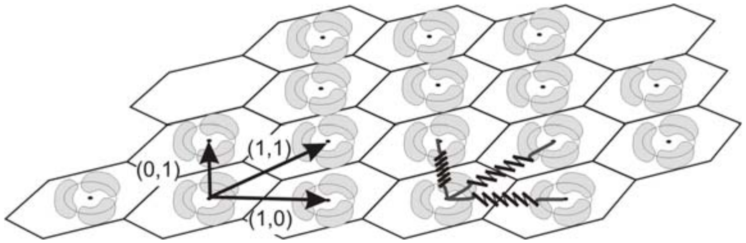


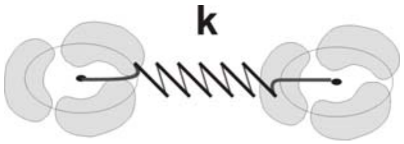
intra protein dynamics



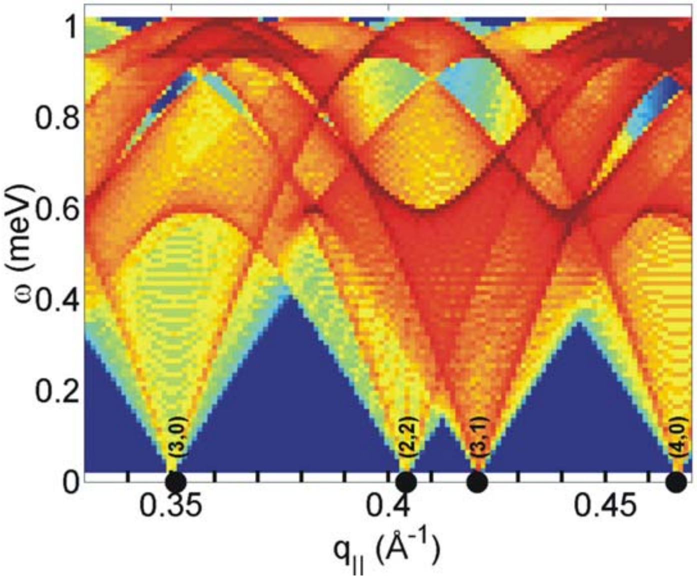
inter protein dynamics

a=62 Å

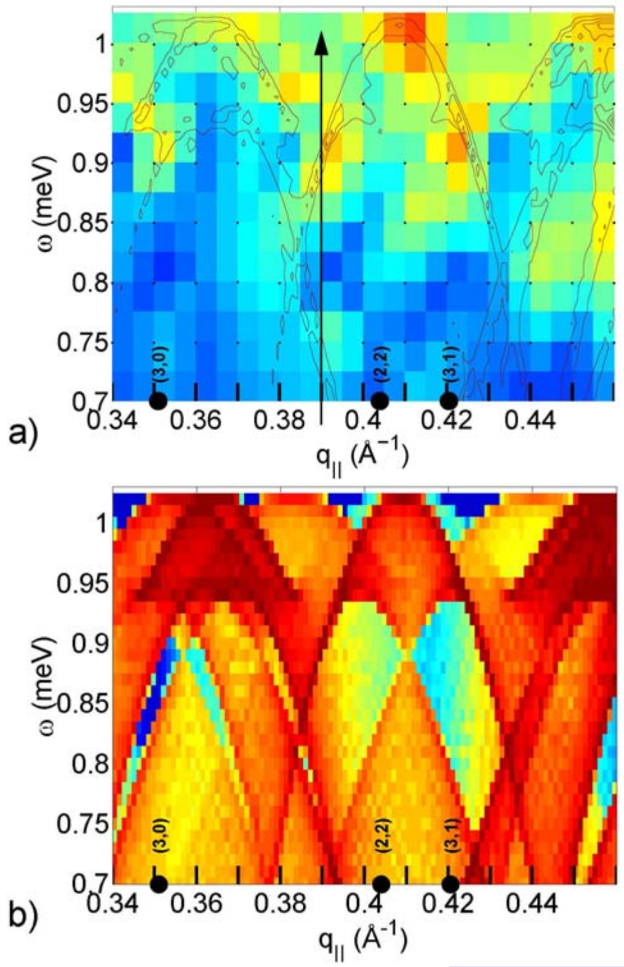


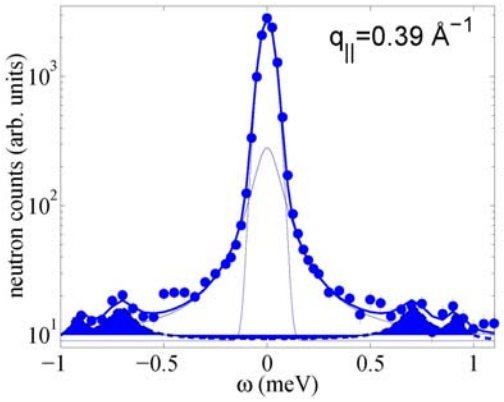


Karin Schmalzl, Dieter Strauch, ILL+U Regensburg



Cooperative Protein Dynamics



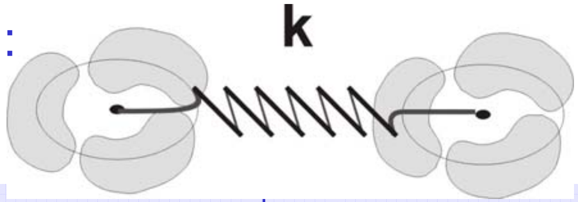


$$k = (l + t) \approx l \text{ (longitudinal)}$$

$$M_{BR}\omega^2 = 2(3l + t) \approx 6l$$

Equipartition theorem:

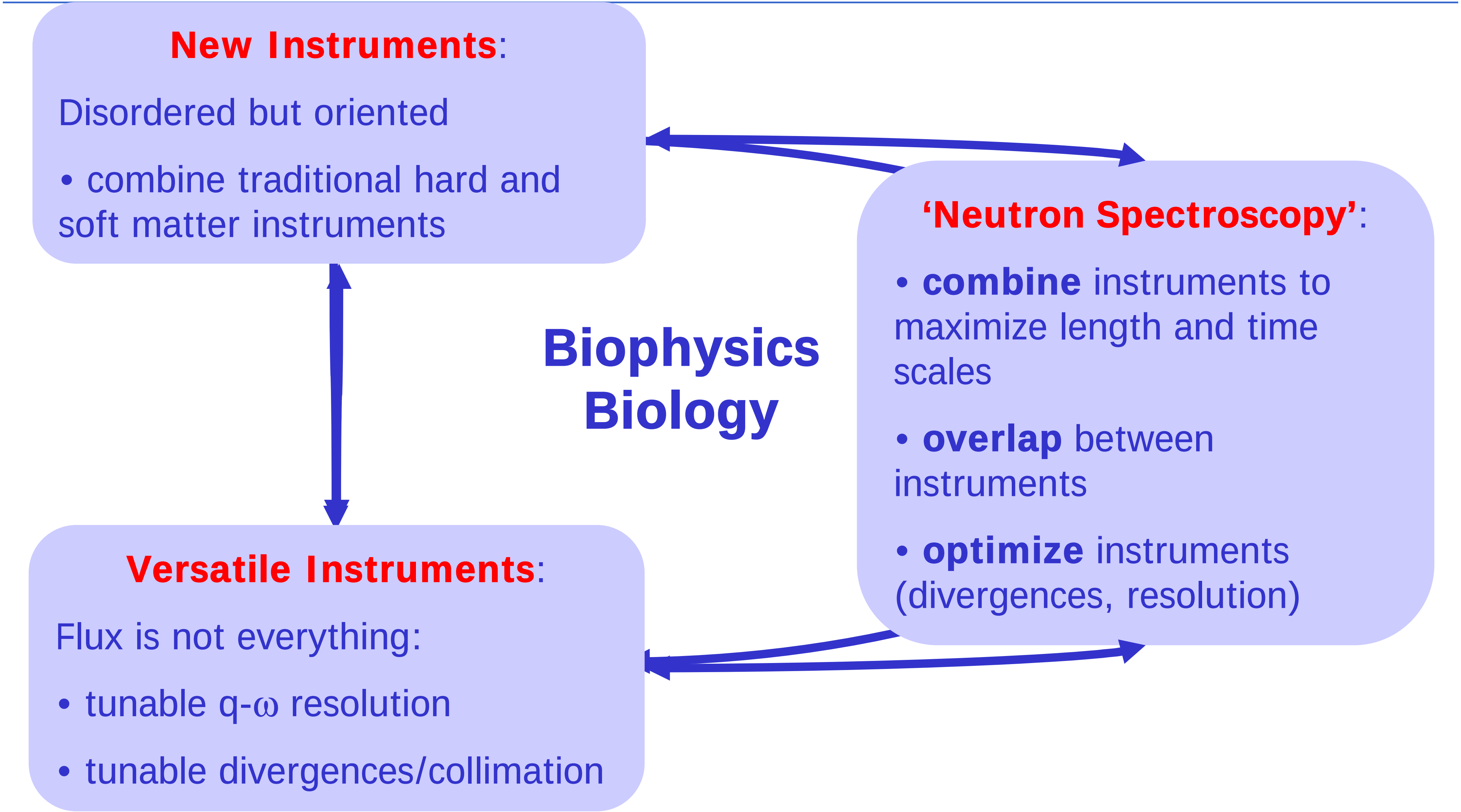
$\frac{1}{2}k\langle r^2\rangle = \frac{1}{2}k_BT$



k	52.4 N/m
Amplitude	0.2 Å
Interaction Force	~1 nN

“Protein Communication” in biological membranes

Hard and Soft Matter



New Instruments:

Disordered but oriented

- combine traditional hard and soft matter instruments

Biophysics
Biology

'Neutron Spectroscopy':

- **combine** instruments to maximize length and time scales
- **overlap** between instruments
- **optimize** instruments (divergences, resolution)

Versatile Instruments:

Flux is not everything:

- tunable q-ω resolution
- tunable divergences/collimation