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Pontificia Universidad Catolica de Chile
Facultad de Fisica
Santiago de Chile, October 2009

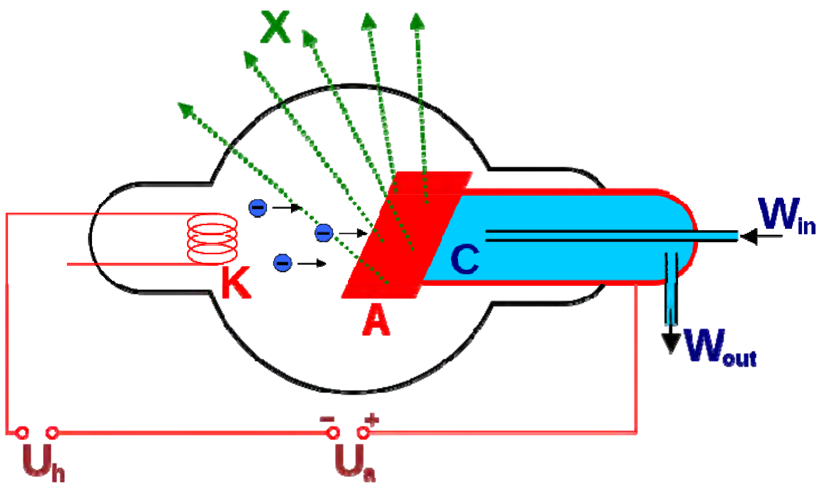
Collective Molecular Dynamics in Proteins and Membranes

Mini Curso III/III,
Red Nacional de Postgrado en Ciencias Físicas:
"Dynamics in Soft-Matter and Biology Studied by Coherent Scattering Probes"

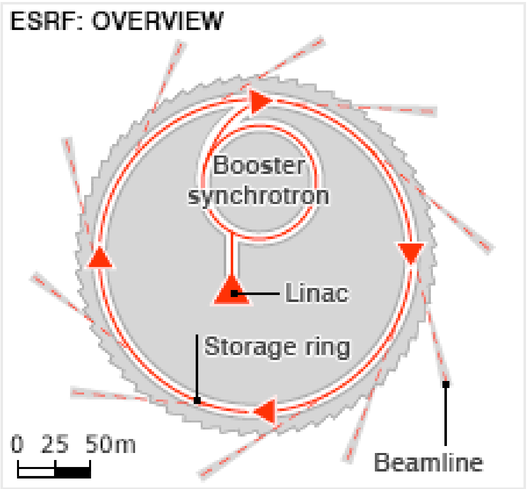
Production of X-rays

Laboratory for Membrane and Protein Dynamics

X-ray tube



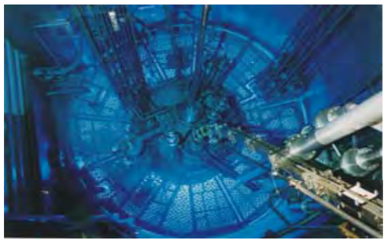
Synchrotron Sources



Production of Neutrons

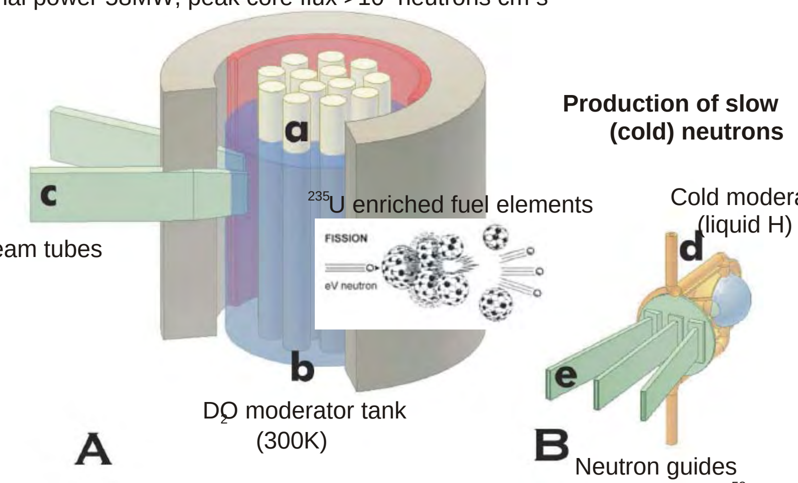
Production

Reactor Sources

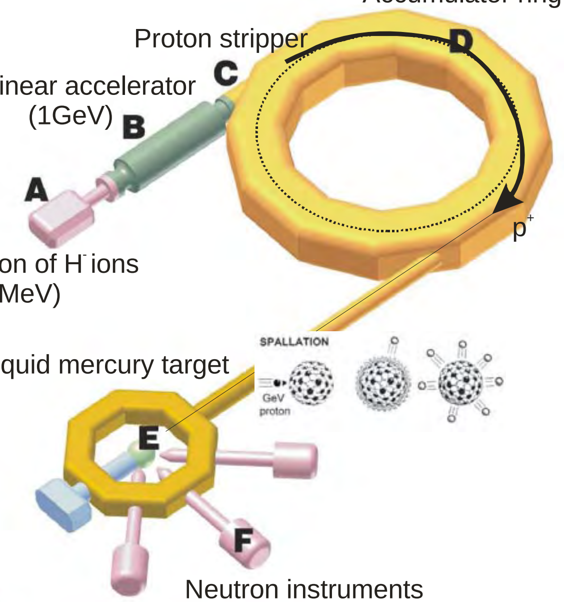


The Institut Laue-Langevin (ILL) in Grenoble, France, operates the world's most powerful neutron reactor

Thermal power 58MW, peak core flux $>10^{15}$ neutrons cm^{-2} s^{-1}



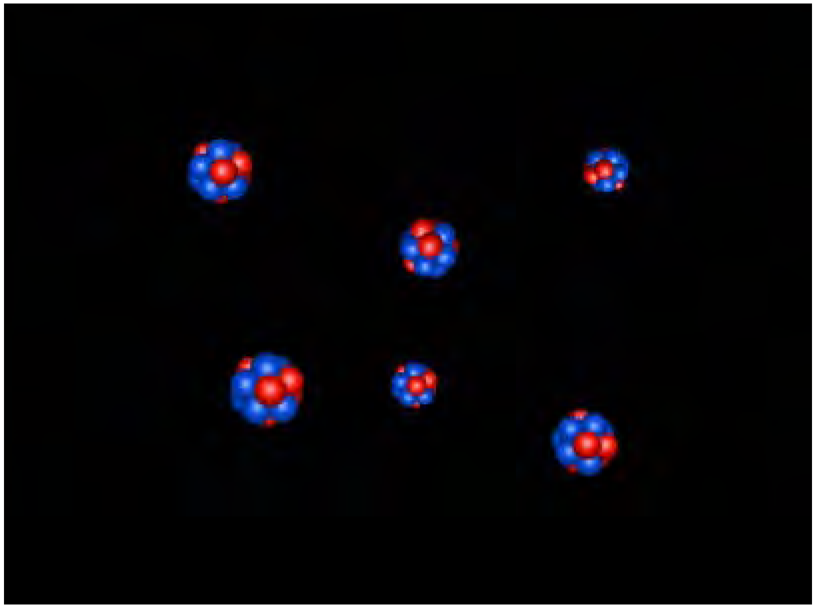
Spallation Sources

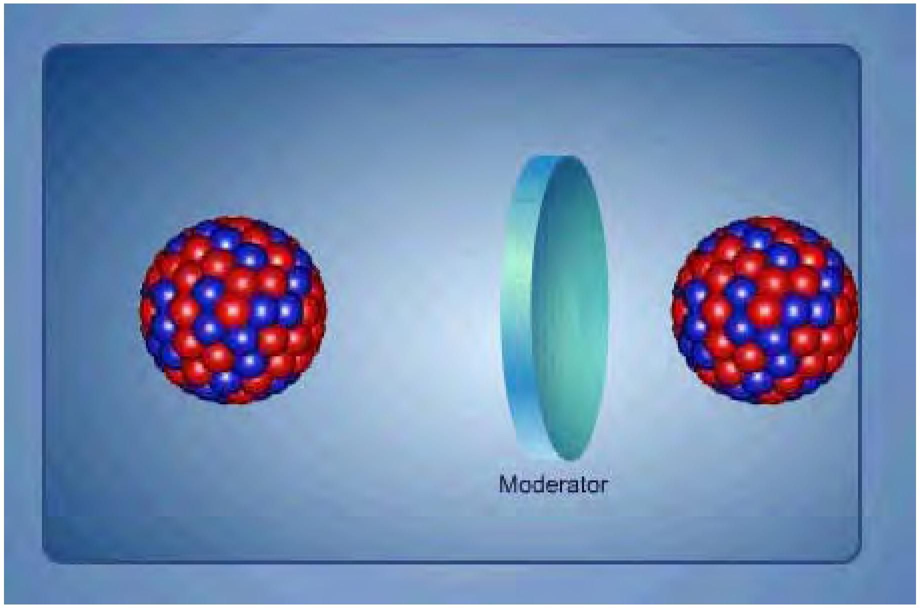


2 MW spallation neutron source

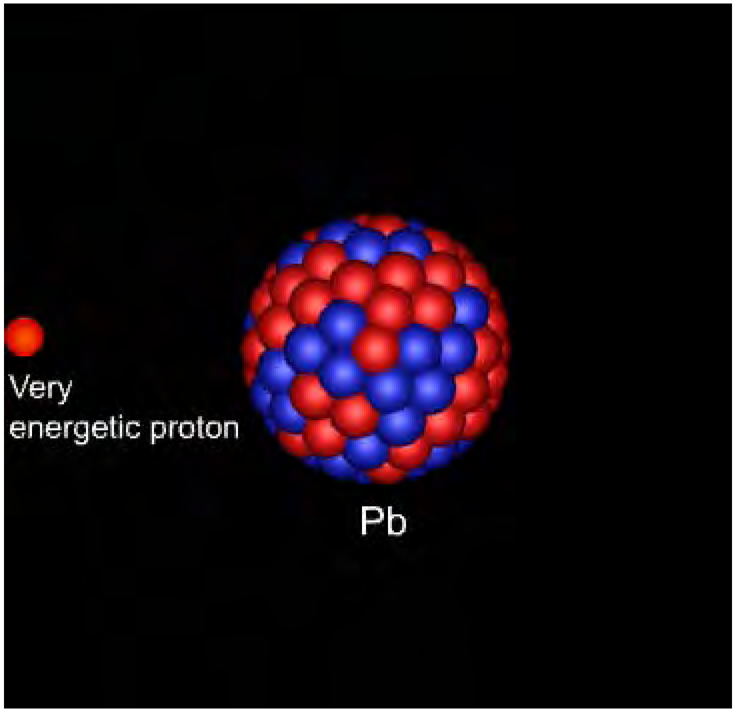
The Spallation Neutron Source (SNS) in Oakridge, USA, is the world's most powerful neutron spallation source

Production of Neutrons - Fission



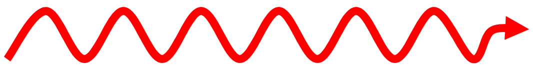


Production of Neutrons - Spallation

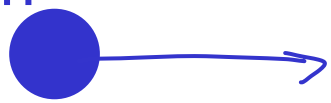


Properties of Neutrons and X-rays

x-rays electromagnetic



neutron particle



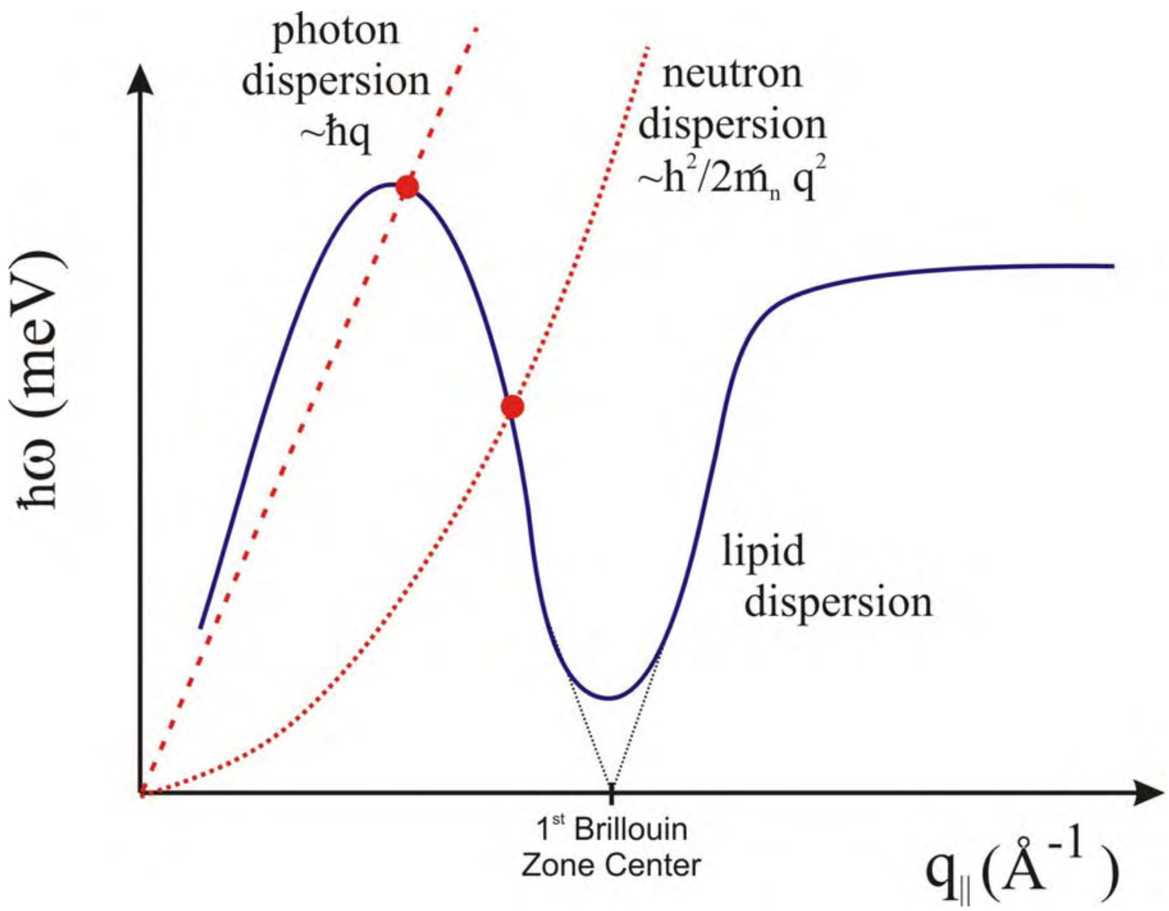
∅	mass	$1.675 \cdot 10^{-27}$ kg
c	velocity	$500\,m/s - 2{,}200\,m/s$
$p = \hbar q = \frac{h}{\lambda}$	Momentum	$p = m_n \cdot v$
$E = \hbar\omega = c \cdot p = c \cdot \hbar\, q$	energy	$E = \frac{1}{2} m v^2 = \frac{\hbar^2}{2m} \cdot q^2$
∅	charge	∅
∅	magnetic moment	Spin $\frac{1}{2}$

Scattering Laws

Scattering laws

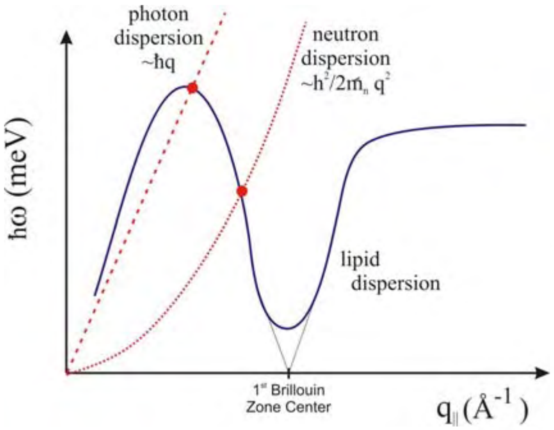
momentum $\vec{q} = \frac{m}{\hbar}(\vec{v}_1 - \vec{v}_2)$

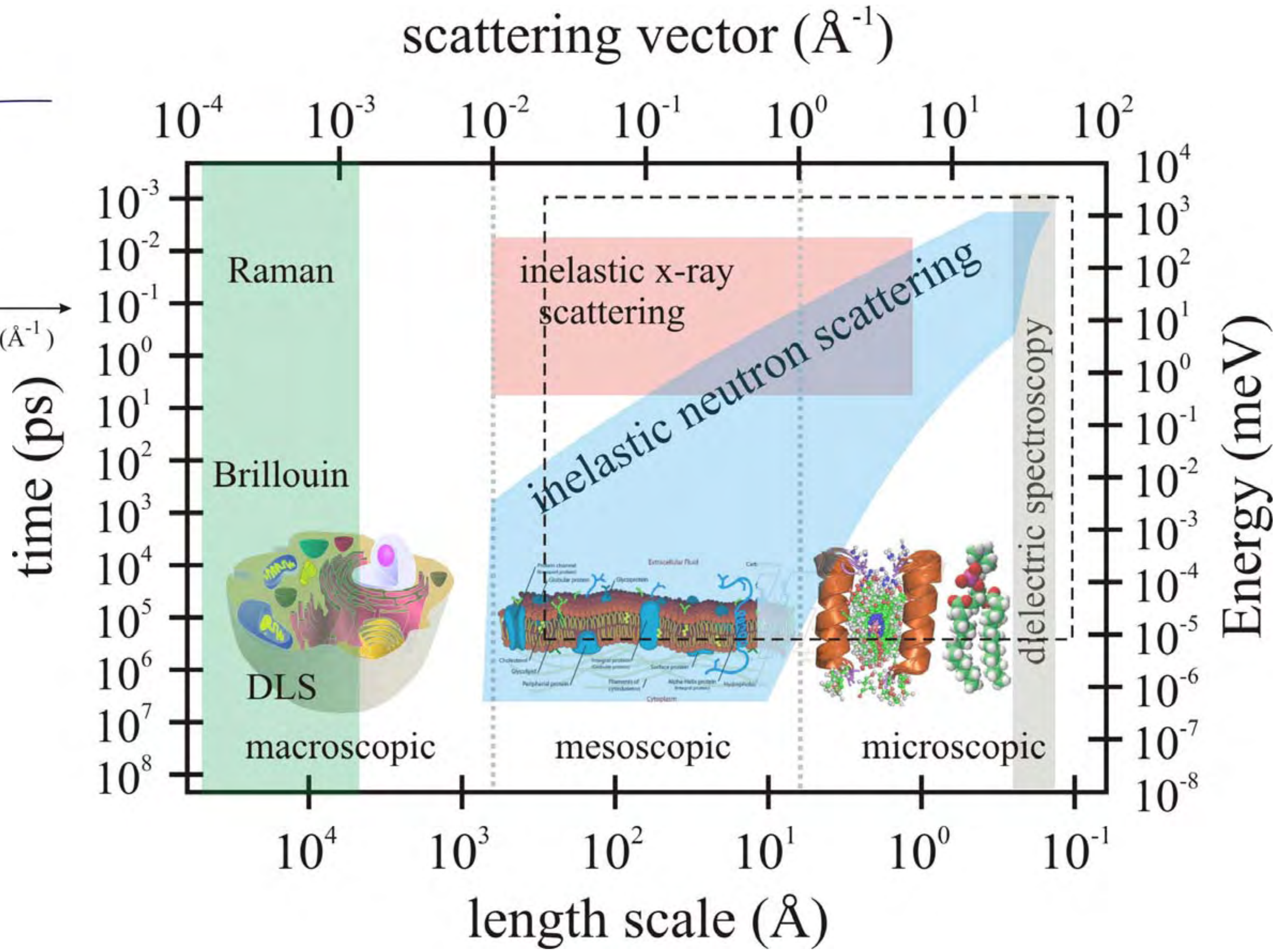
energy $\hbar\omega = \frac{1}{2}m\left(v_2^2 - v_1^2\right)$



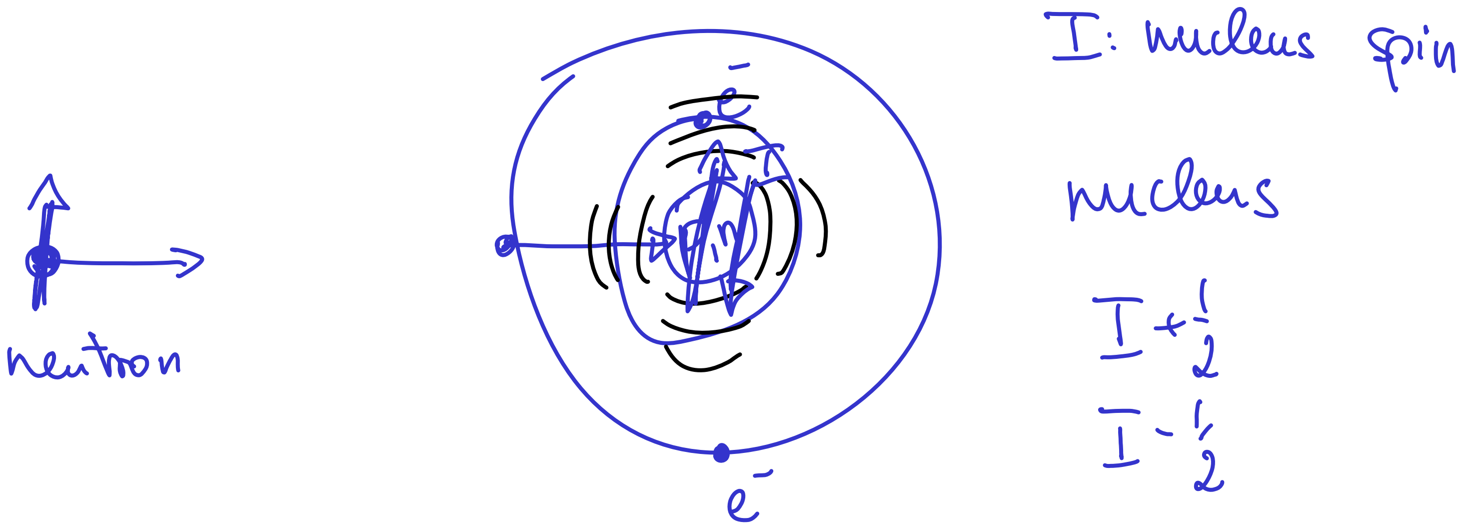
Limits of inelastic x-ray and neutron scattering?

Neutron and X-ray Spectroscopy

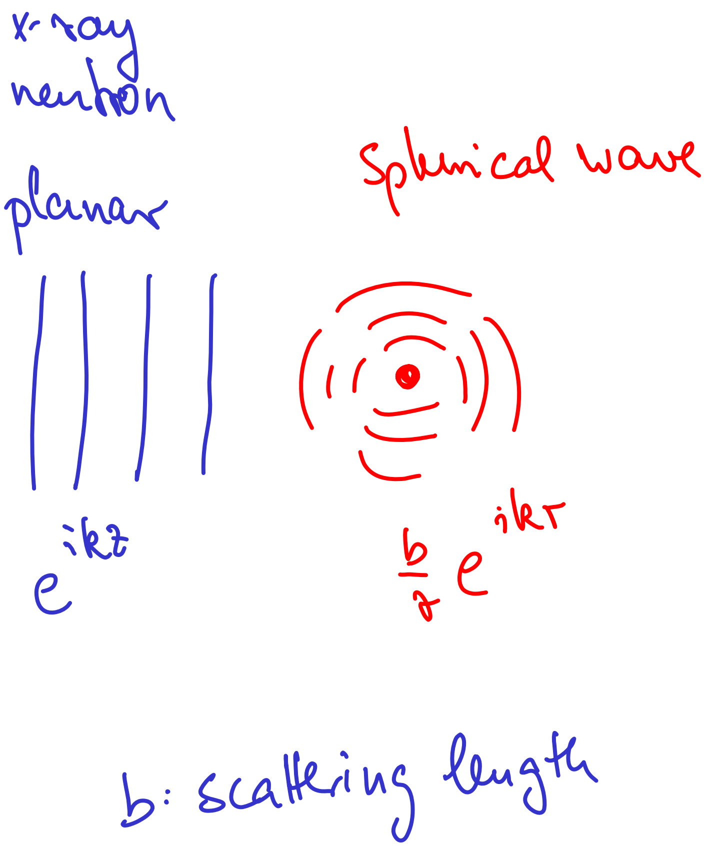


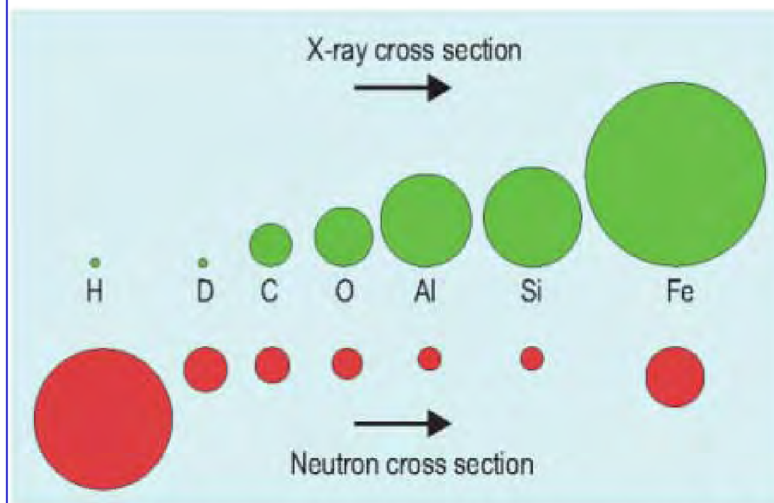


Interaction with Matter



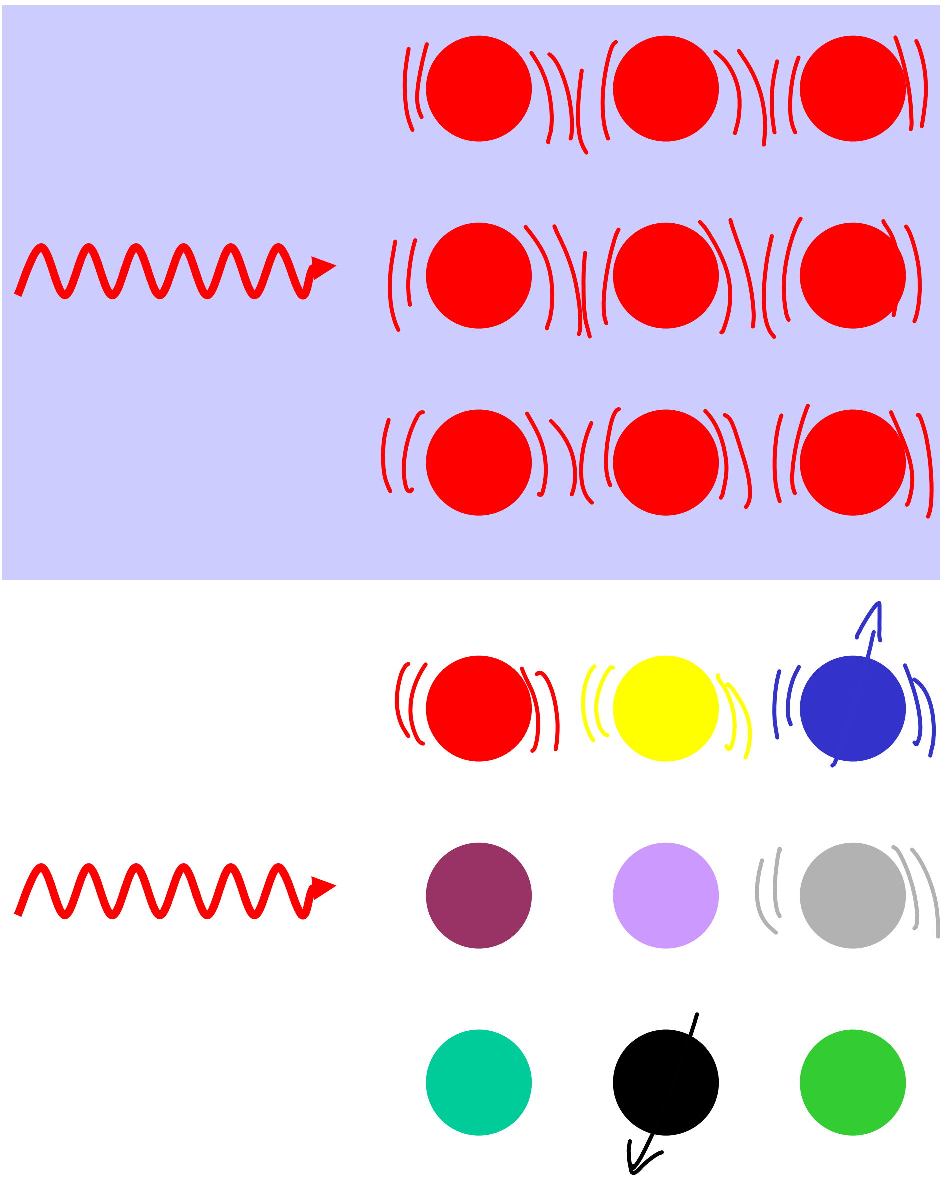
Scattering Cross Sections



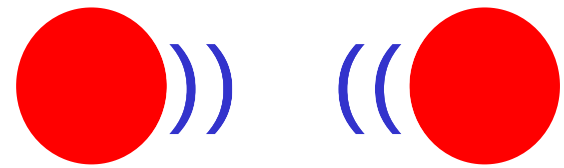


Scattering Cross Section:
Probability that a neutron will interact with a nucleus

Coherent and Incoherent Scattering



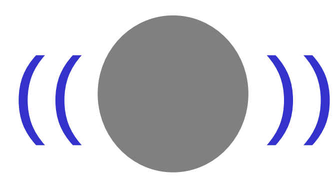
Interactions between molecules



coherent scattering

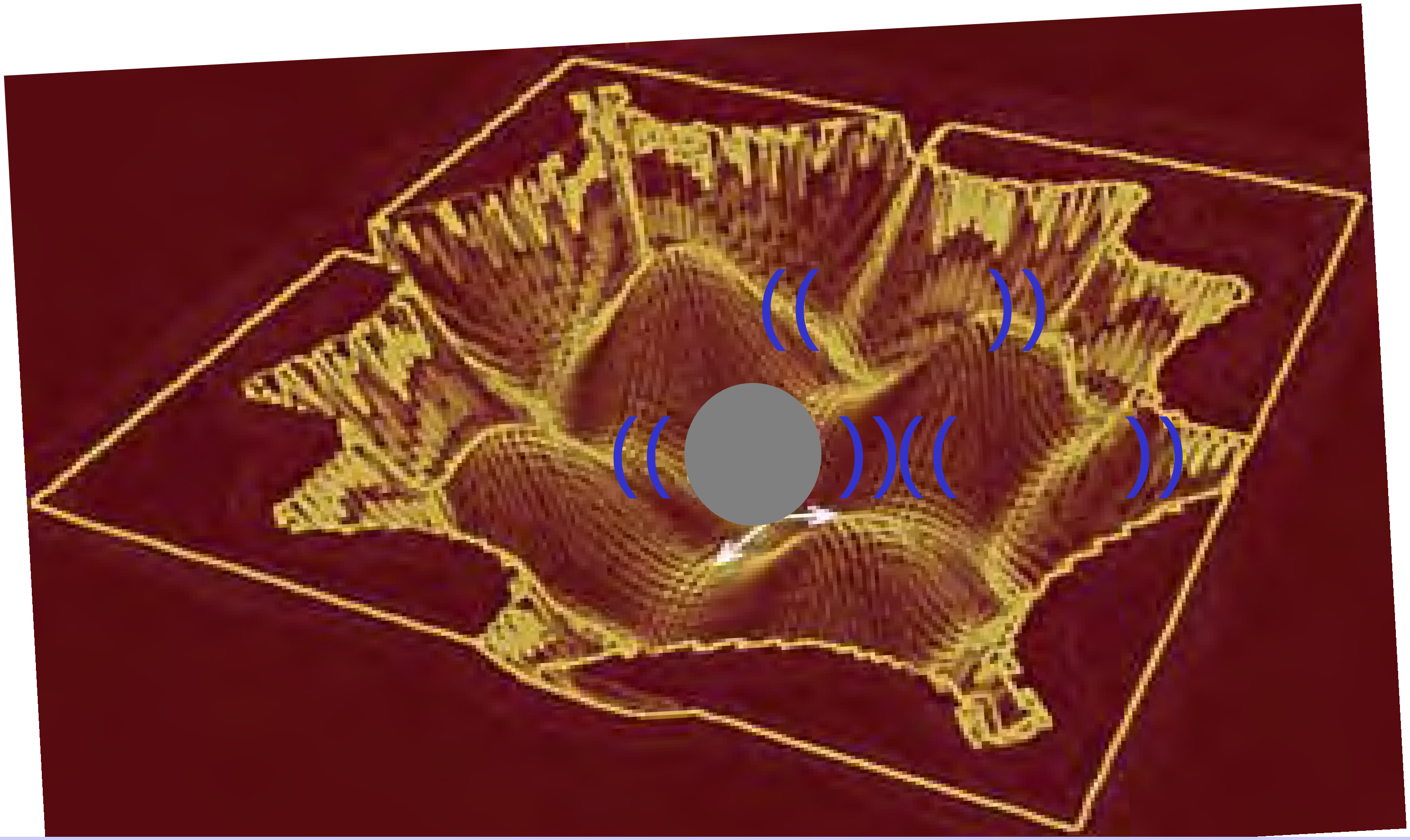
x-rays, neutrons?

incoherent scattering



Individual molecule

Incoherent Scattering



Structure of energy landscape: geometry and potential barriers

Coherent Scattering

Interactions between molecules

Coherent and Incoherent Scattering

X-rays

all atoms are the same

⇒ only coherent scattering

⇒ interactions, collective dynamics

Neutrons

different isotopes, different orientations of nuclear spin

⇒ coherent <u>and</u> incoherent scattering

⇒ interactions <u>and</u> local dynamics

Membrane Dynamics

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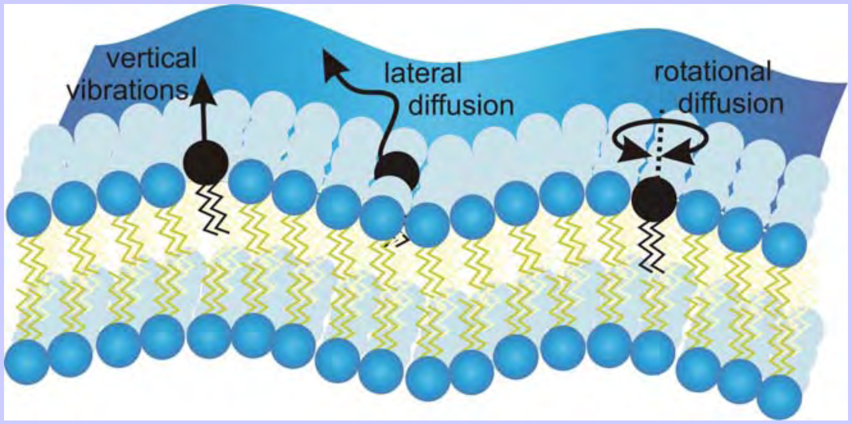
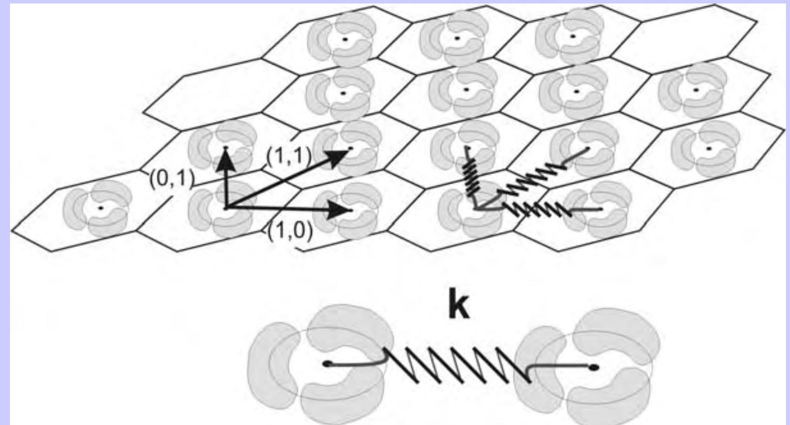
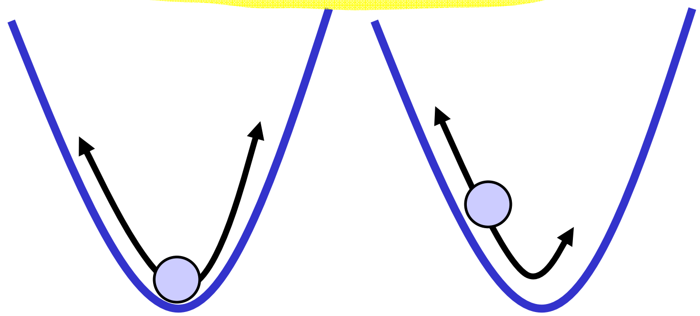
Local modes in bilayers



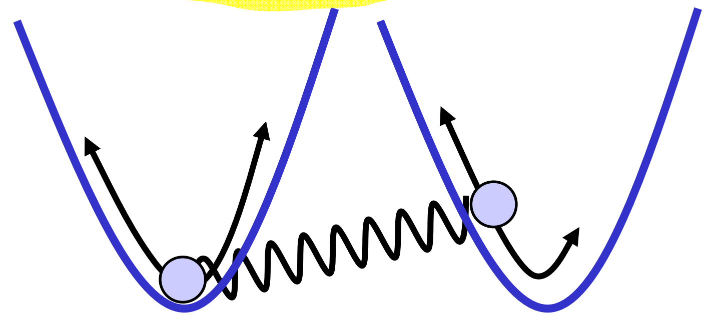


Collective excitations

Incoherent, single molecule

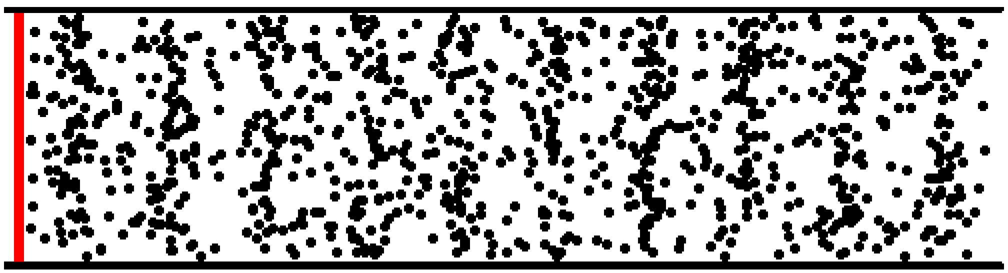


Coherent, interactions



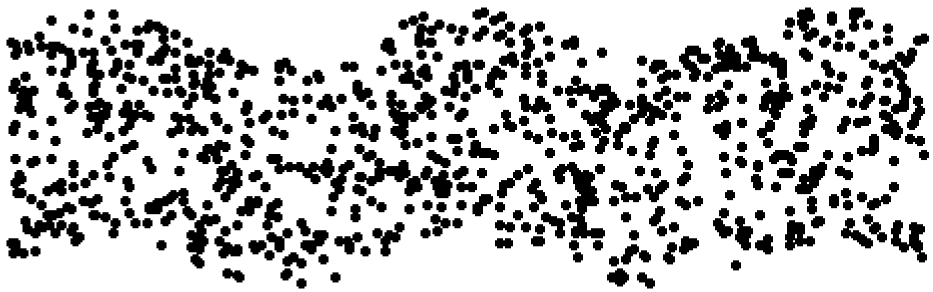
Correlated molecular motions drive “functionalities” of membranes and proteins and structural changes

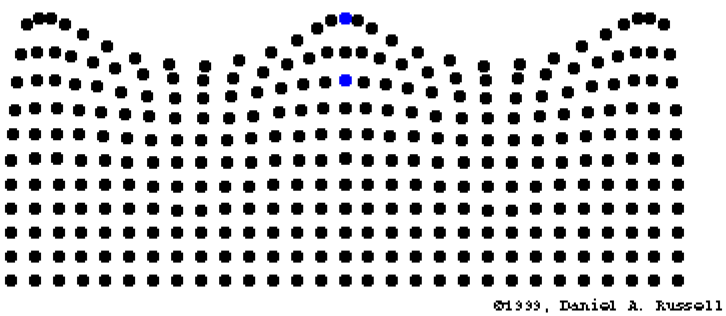
Cooperative Phenomena



Longitudinal Wave

Transverse Wave





Surface Wave

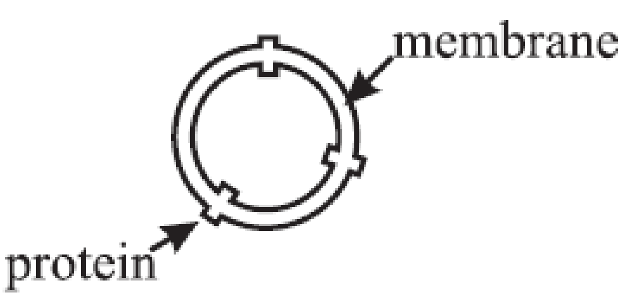
Selective Deuteration

Coherent and Incoherent Scattering Cross Sections

Nuclide	σ_{coh} (b)	σ_{inc} (b)	Nuclide	σ_{coh} (b)	σ_{inc} (b)
^{1}H	1.7583	80.27	^{12}C	5.559	0
^{2}H	5.592	2.05	^{13}C	4.81	0.034
^{3}H	2.89	0.14	^{16}O	4.232	0
^{14}N	11.03	0.5	^{17}O	4.2	0.004
^{15}N	5.21	0.00005	^{18}O	4.29	0

Protonated ←→ Incoherent

Deuterated ←→ Coherent



Part V and VI

- Inelastic Scattering and excitations
- Quasi- and inelastic scattering
- Neutron Instruments
- Coherence Length

Excitation Spectrum

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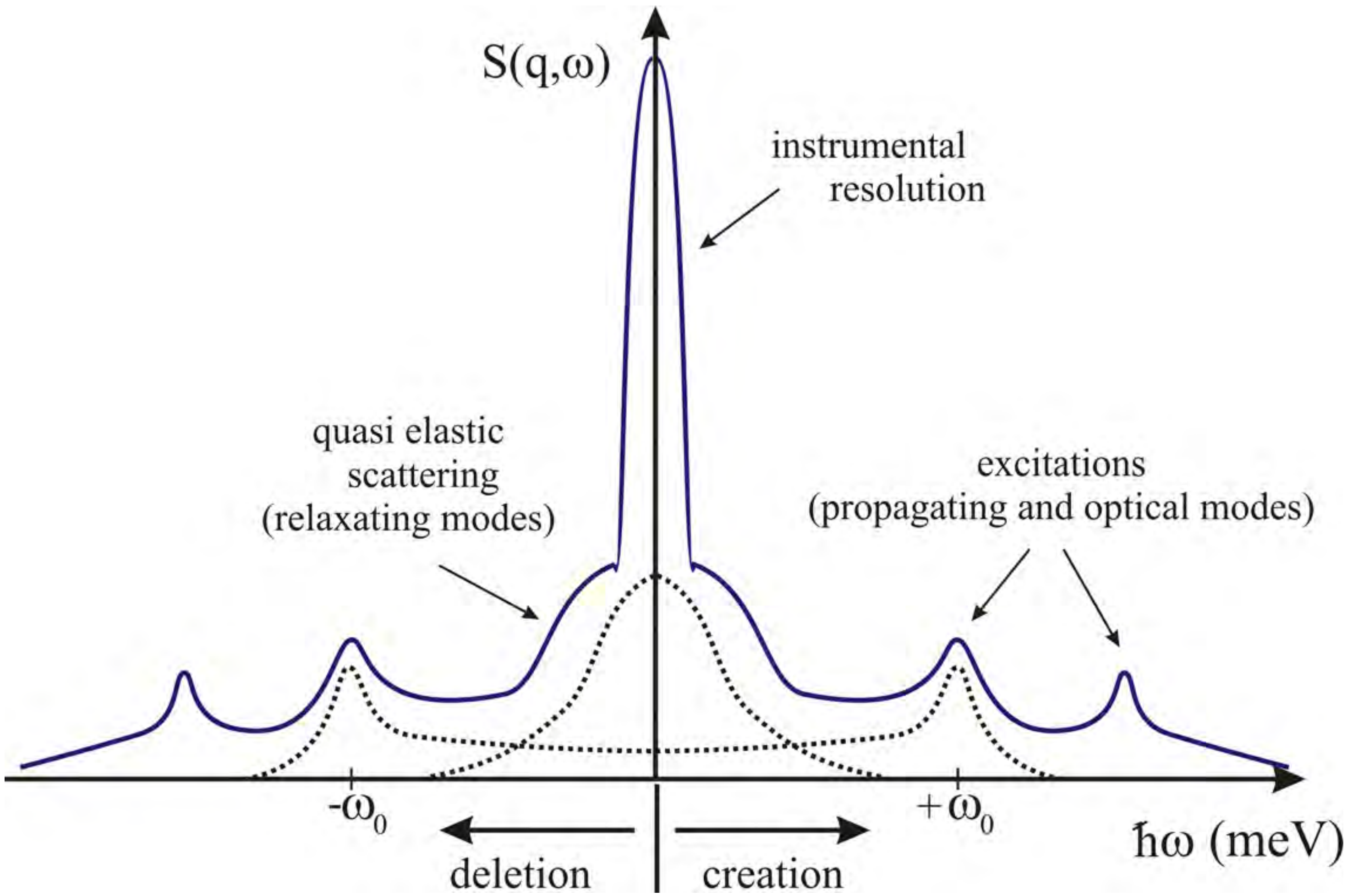
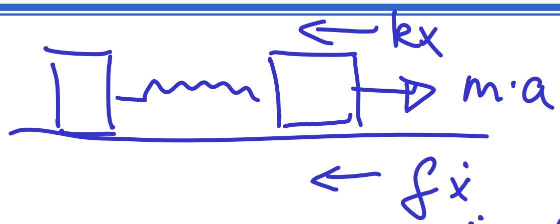


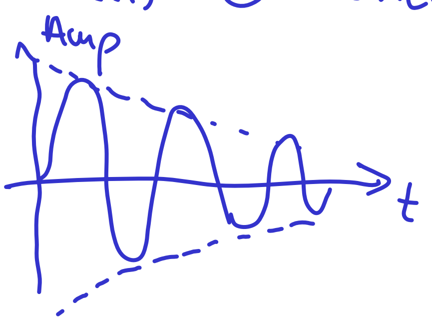
Coherent, incoherent?

Quasi- and Inelastic Neutron Scattering

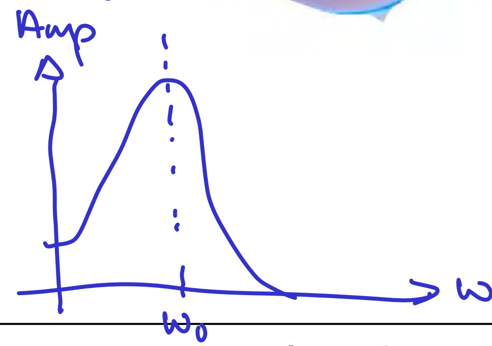


$m\cdot a = -kx - f\dot{x} \Rightarrow \ddot{x} + \underbrace{\frac{f}{m}}_{\lambda}\dot{x} + \underbrace{\frac{k}{m}}_{\omega_0^2}x = 0$

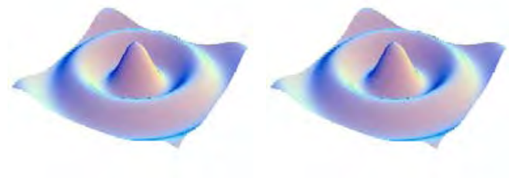
$\Rightarrow x(t) = e^{-\lambda\cdot t}\cdot\sin(\omega t)$

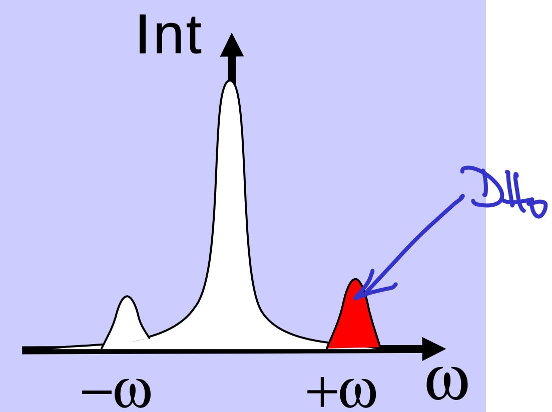


$\Longleftrightarrow$

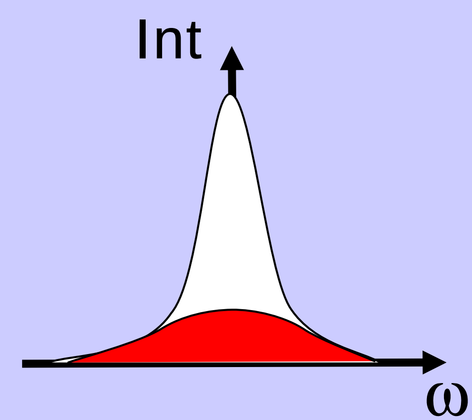


Propagating,
Oscillating Mode





Energy

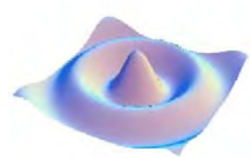


Relaxator

$m\ddot{x} + f\dot{x} = 0$

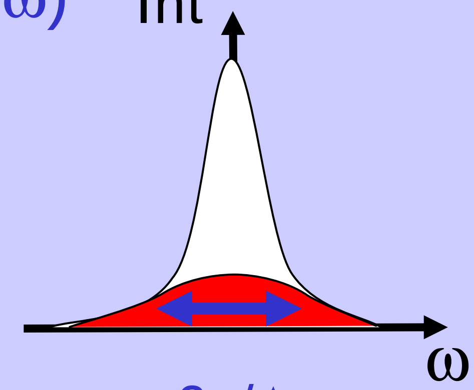
$\Rightarrow x(t) = e^{-\lambda\cdot t}$

Relaxating
(overdamped) Mode



Energy-Time domains

S(q,ω)



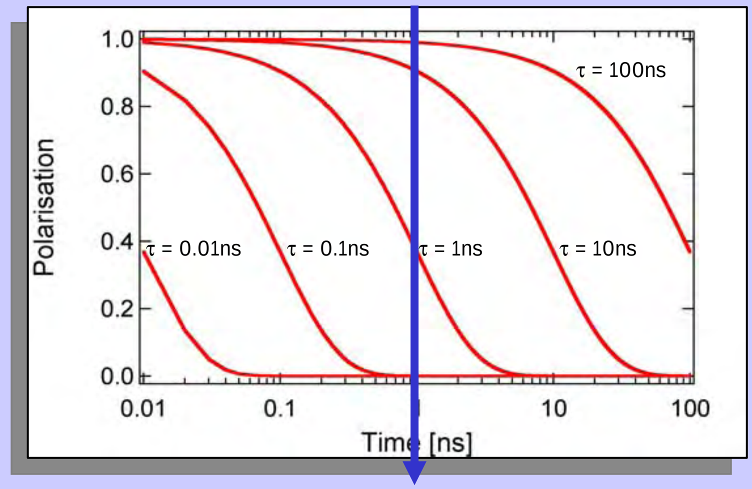
$\tau = 2\pi/\Delta\omega$

Lorentzian

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

Line shape

S(q,t)

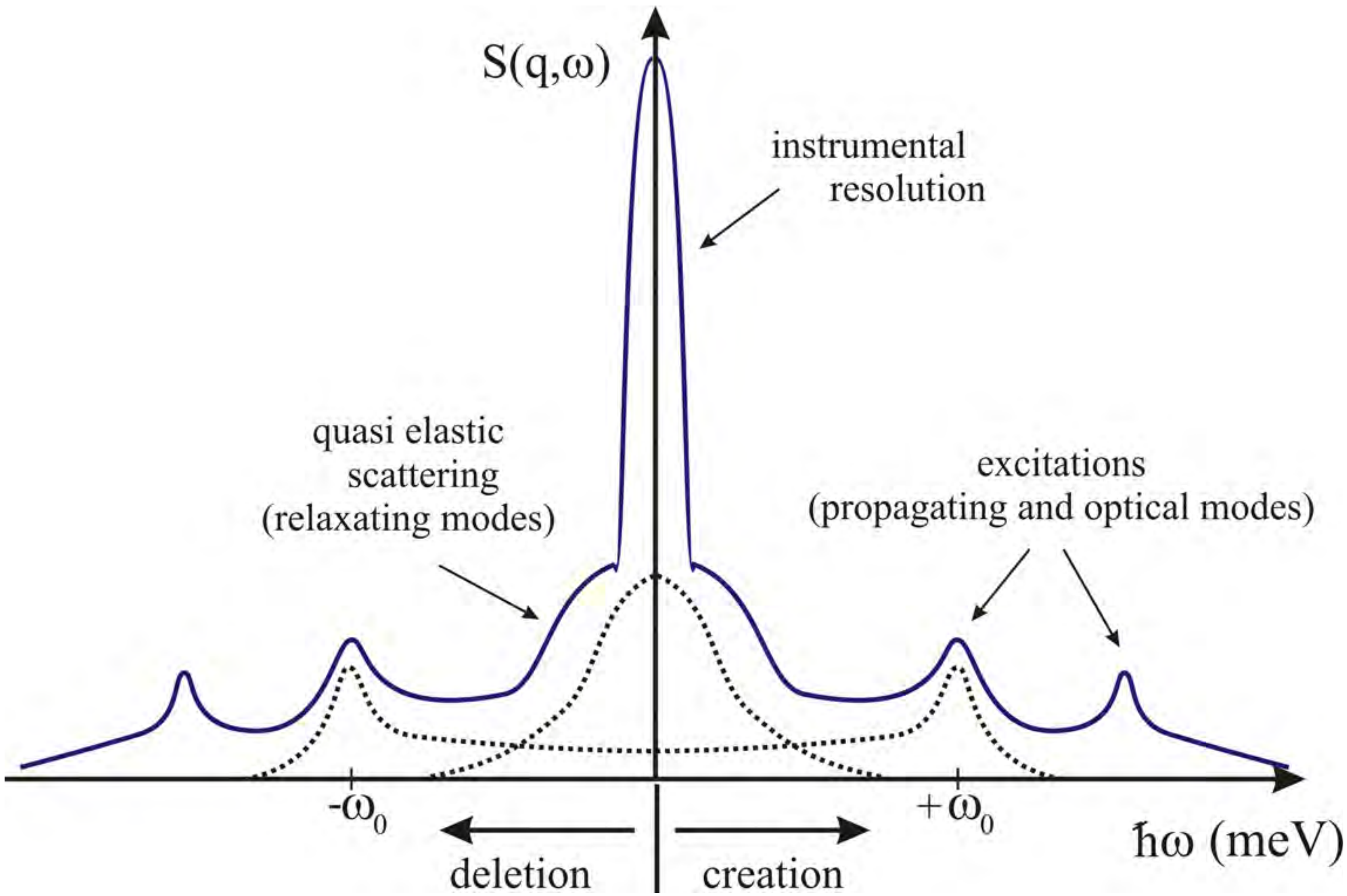


τ

Exponential decay
Debye relaxation

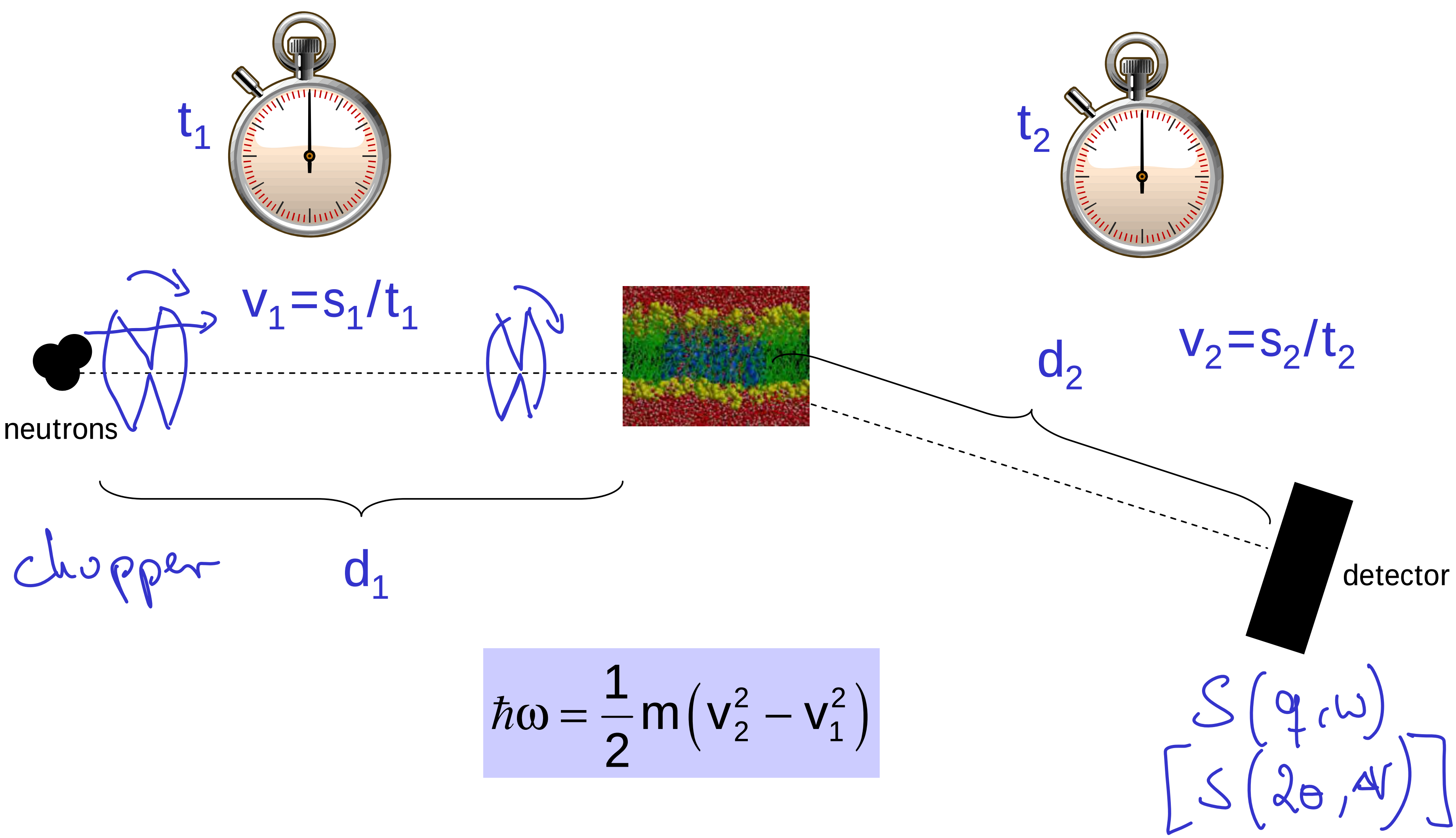
$$1ps = \frac{4.14}{1meV} \qquad 1ns = \frac{4.14}{1\mu eV} \qquad 1\mu s = \frac{4.14}{1neV}$$

Excitation Spectrum



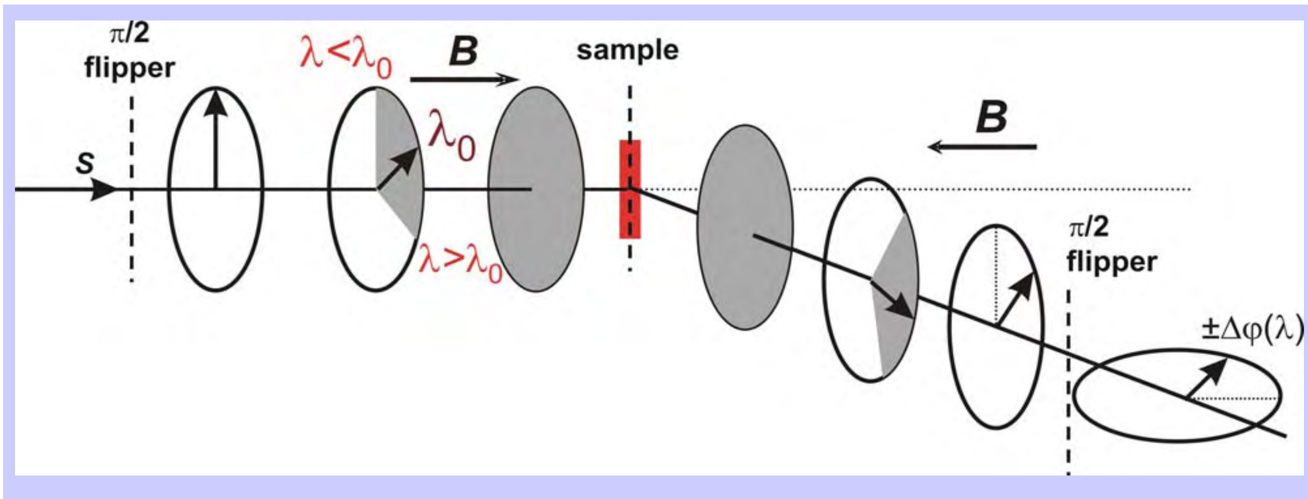
Coherent, incoherent?

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

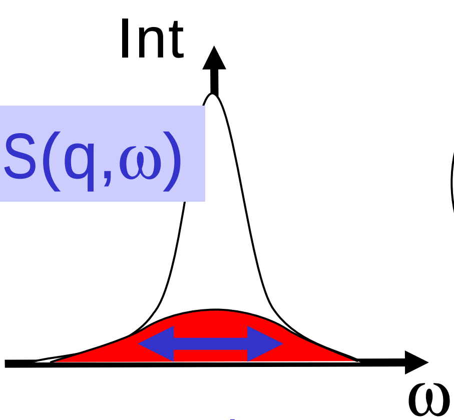


$$\hbar\omega = \frac{1}{2} m \left(v_2^2 - v_1^2 \right)$$

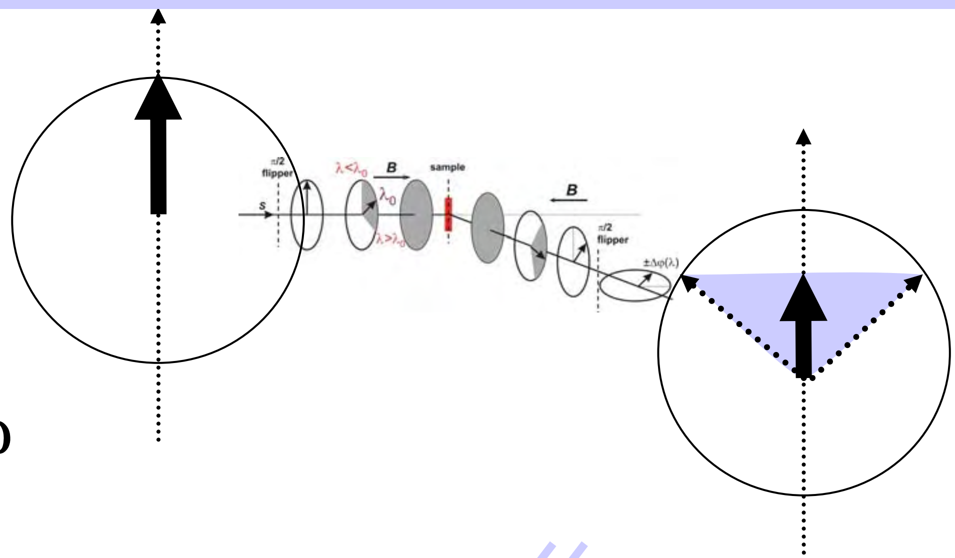
Neutron **S**pin-**E**cho



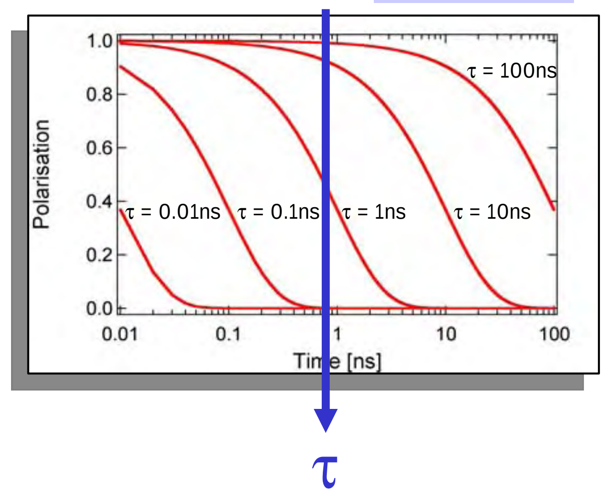
$\Delta\lambda/\lambda \cong 15\%$



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

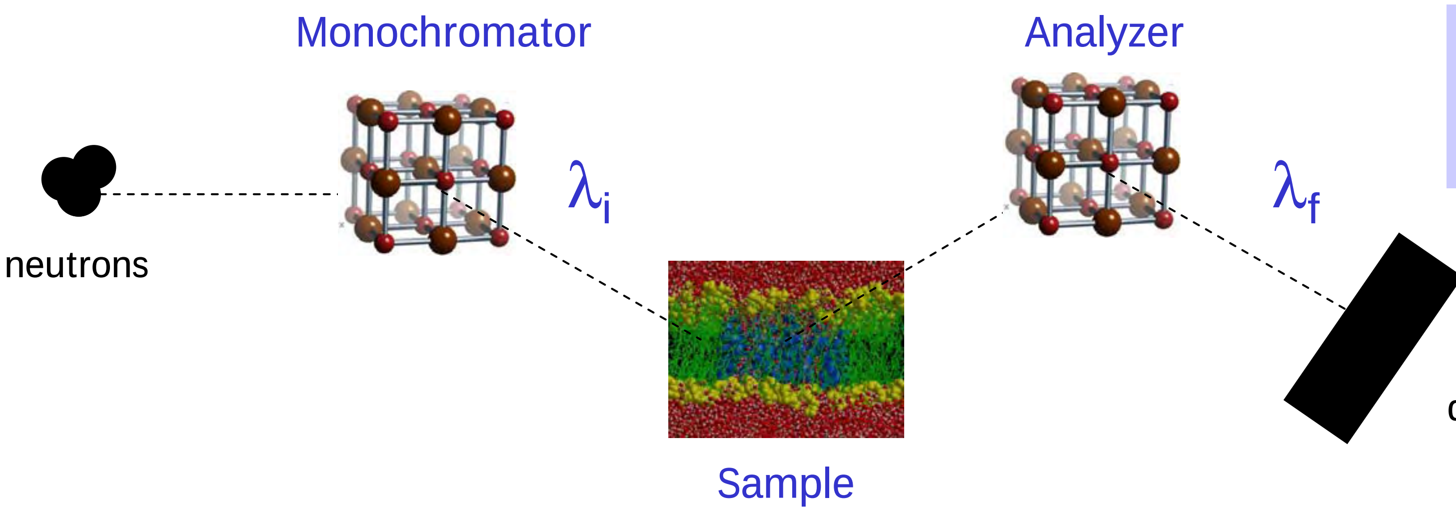


S(q,t)

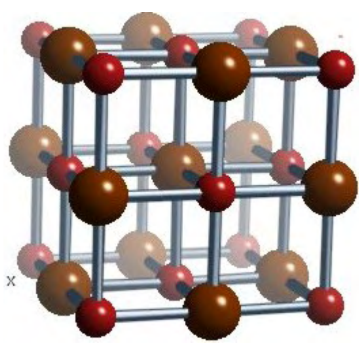


good monochromatization ⟺̸ good energy resolution

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

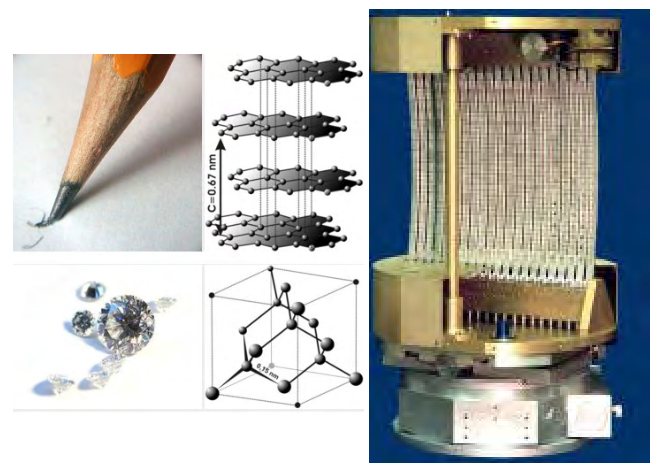


$$\hbar\omega = \frac{h^2}{2m}\frac{1}{\lambda_i^2 - \lambda_f^2}$$



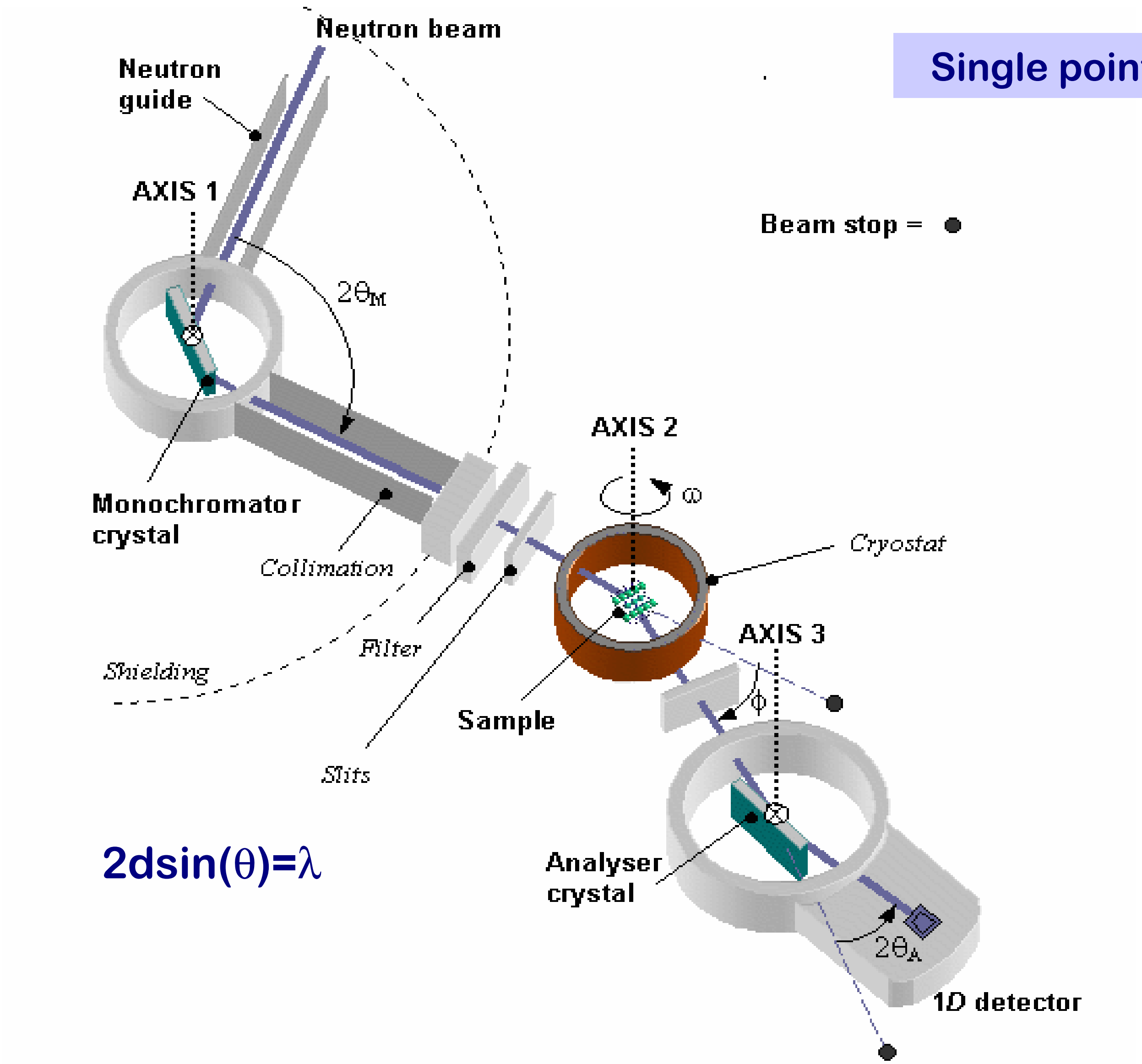
Bragg's Law

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

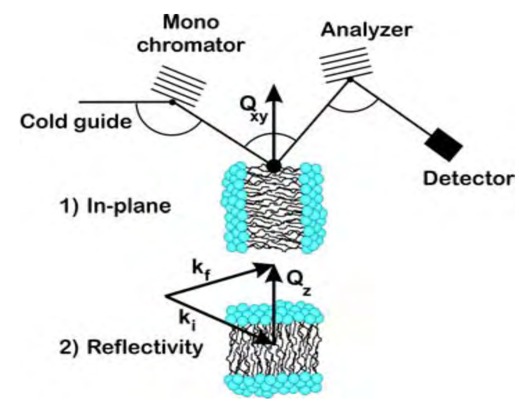


Triple-axis spectrometers

Single point in (Q,ω) space

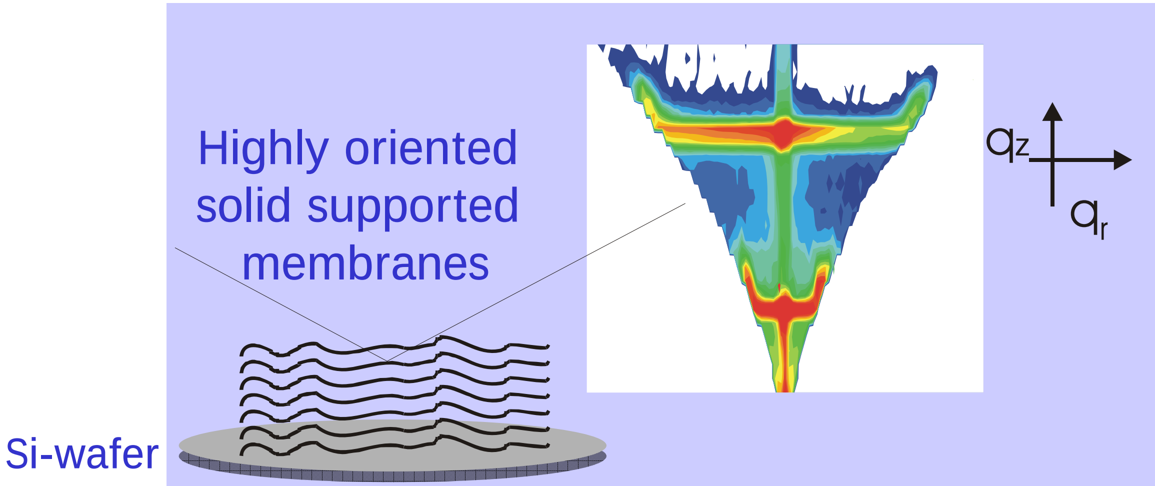


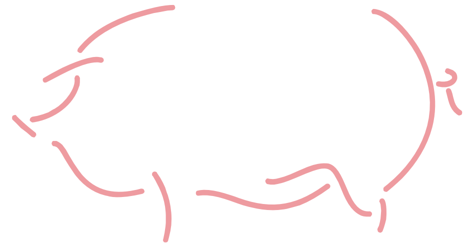
$2d\sin(\theta)=\lambda$

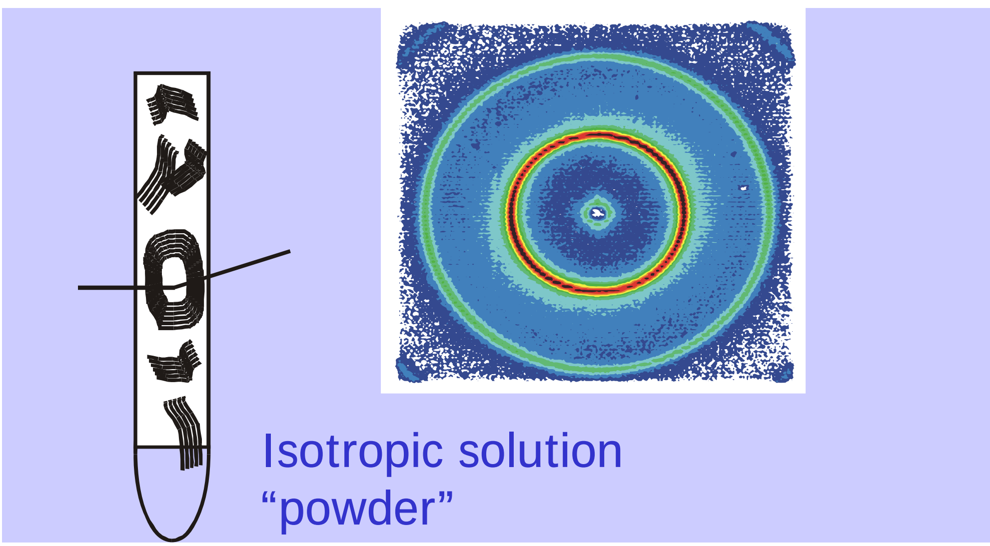


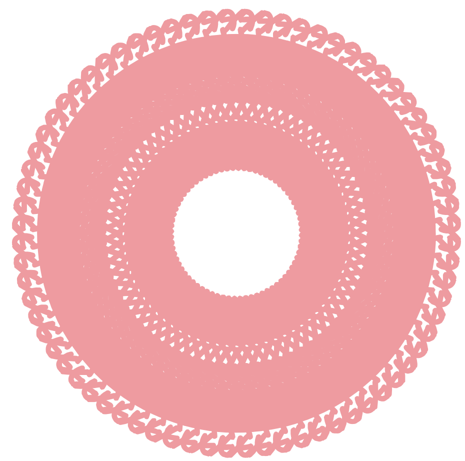
By rotating the sample, Q can be placed within the plane of the membranes or perpendicular to the bilayers

Scattering from aligned phases









Triple-axis spectrometers

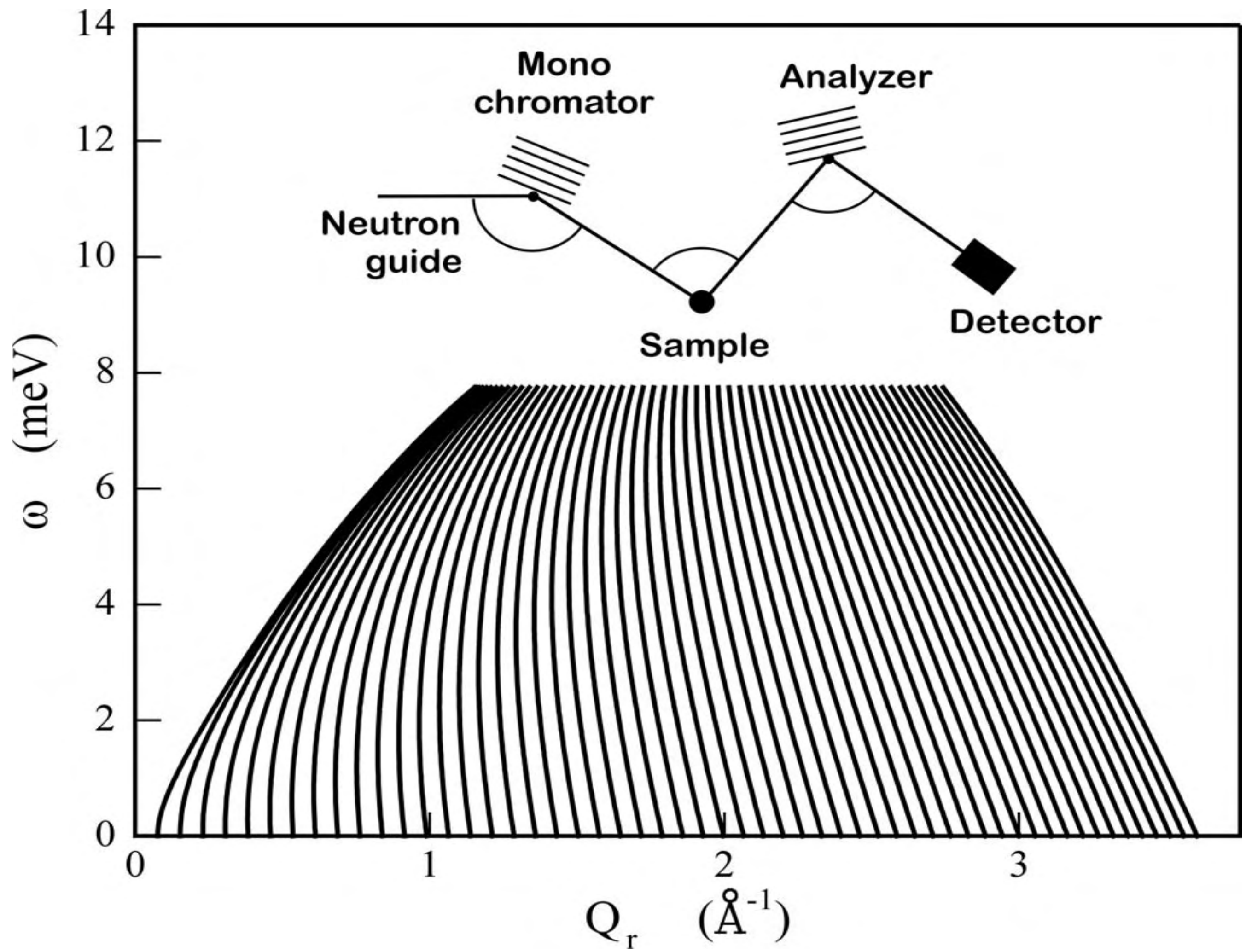
Triple-axis spectrometers

IN14 animation

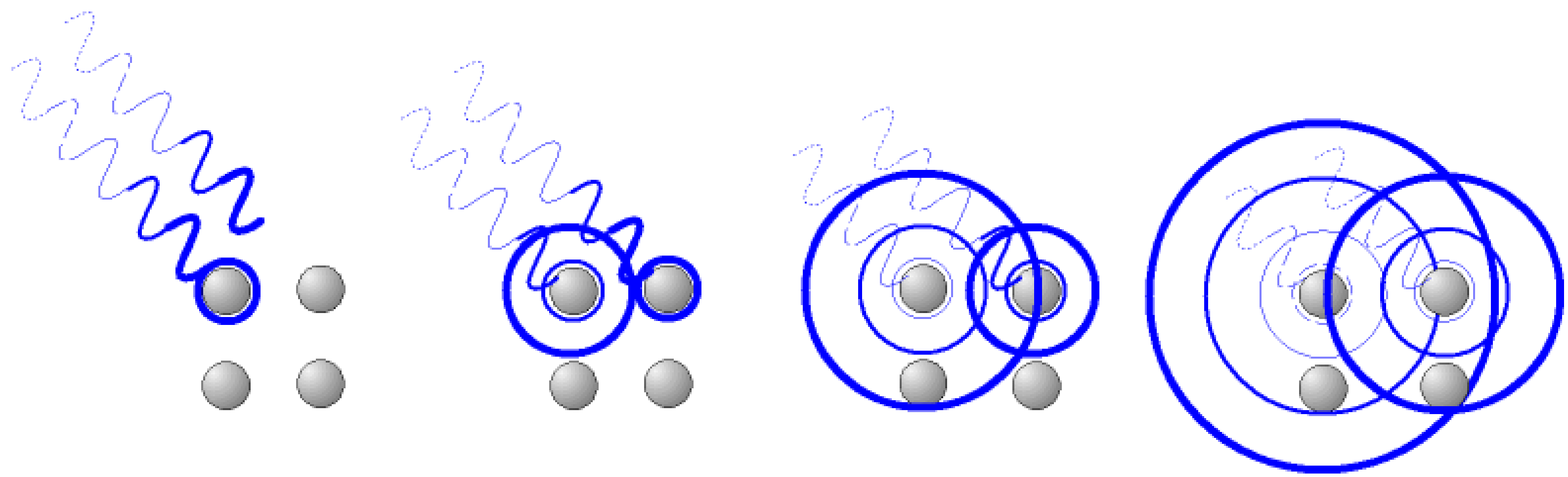
Matlab TAS Simulation

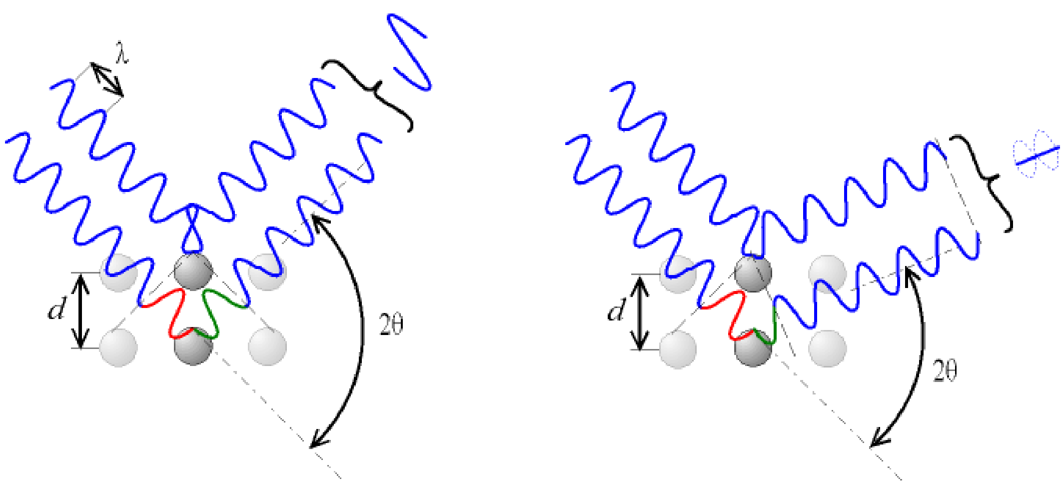
Triple-Axis Accessible Range

accessible (Q,ω) range for a cold TAS



Coherence of X-rays and Neutrons



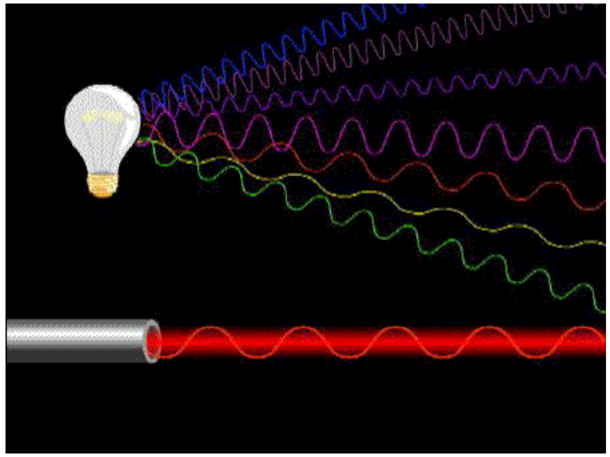


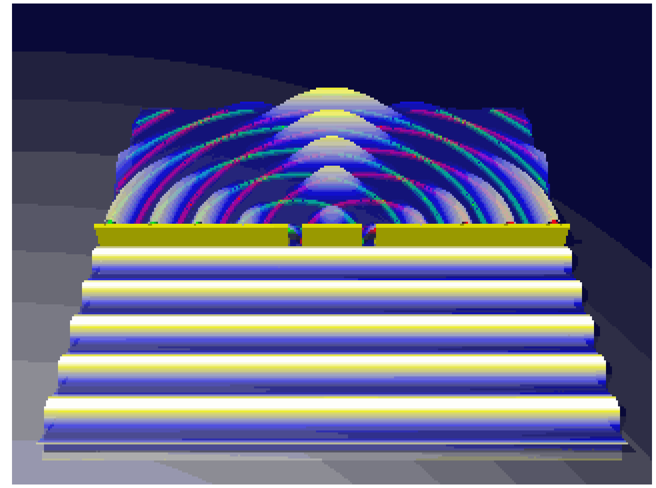
Constructive and destructive interference

Coherence?

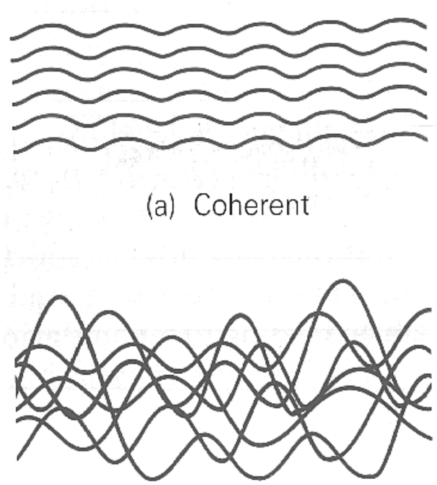
Coherence of Waves

Laser produce coherent light of one wave length





http://hsb.uni-frankfurt.de/web/research/atomic/photonmolecule/H2_double/3_double_slit/



(a) Coherent

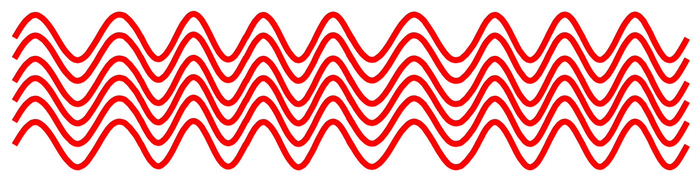
(b) Incoherent

In a Young type double slit experiment two phase coherent spherical waves are created by passing a plane wave

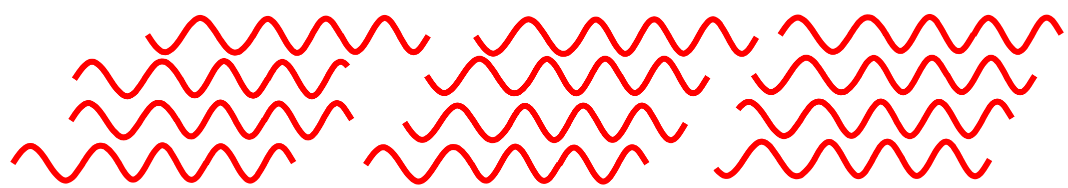
Coherence of Waves

Coherence:
highly monochromatic, emitted in long wave trains and so maintains a constant phase relationship over large distances

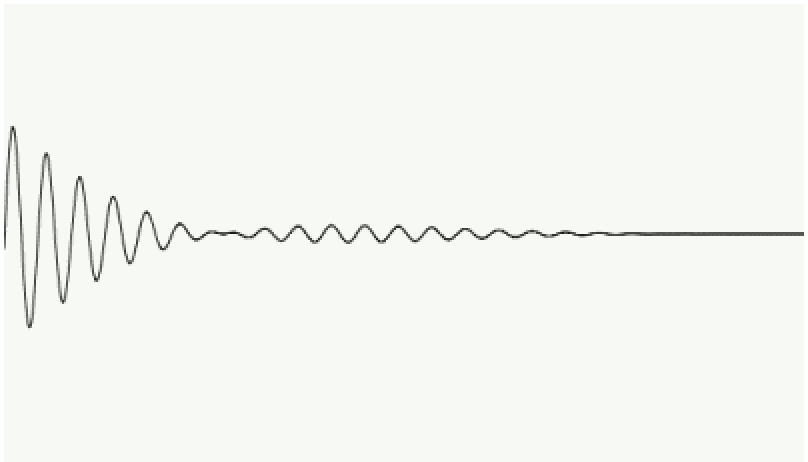
coherent

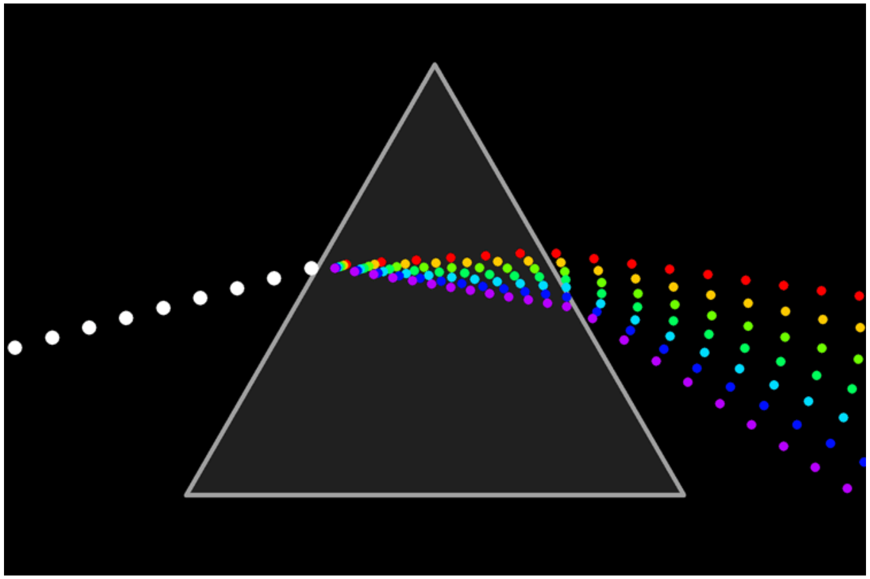


incoherent



Coherence





Longitudinal Coherence Length of a Wave

$$\lambda_C = \lambda^2 / \Delta\lambda$$

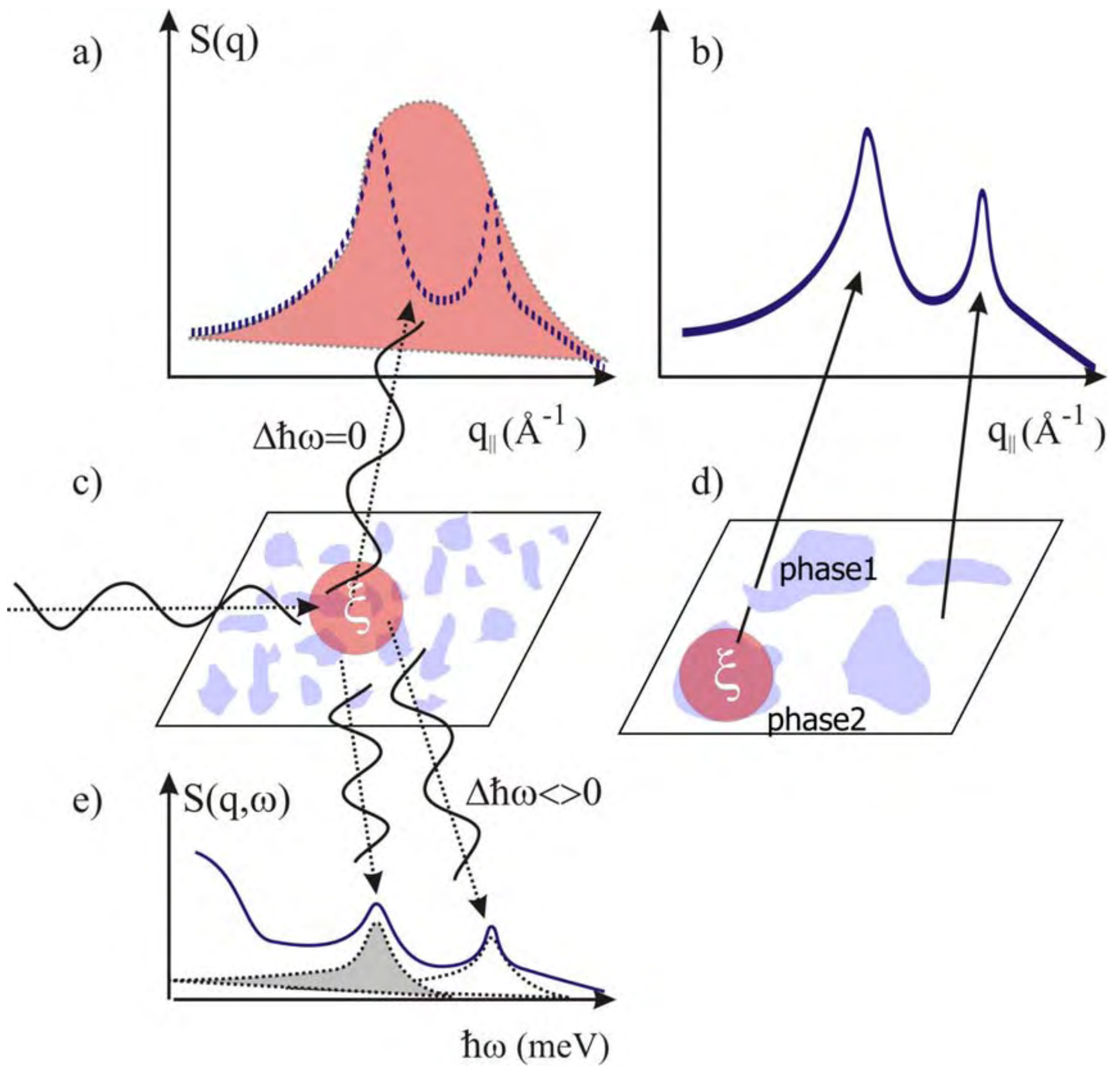
Coherence of X-rays and Neutrons

Laboratory for Membrane and Protein Dynamics

X-Rays		Neutrons
~ 1 Å	wavelength	1.8 Å $- 5$ Å
$\frac{\Delta\lambda}{\lambda} \sim 10^{-4}$	monochromaticity	$\frac{\Delta\lambda}{\lambda} \sim 0.05$
$10{,}000$ Å	coherence length	$100-500$ Å

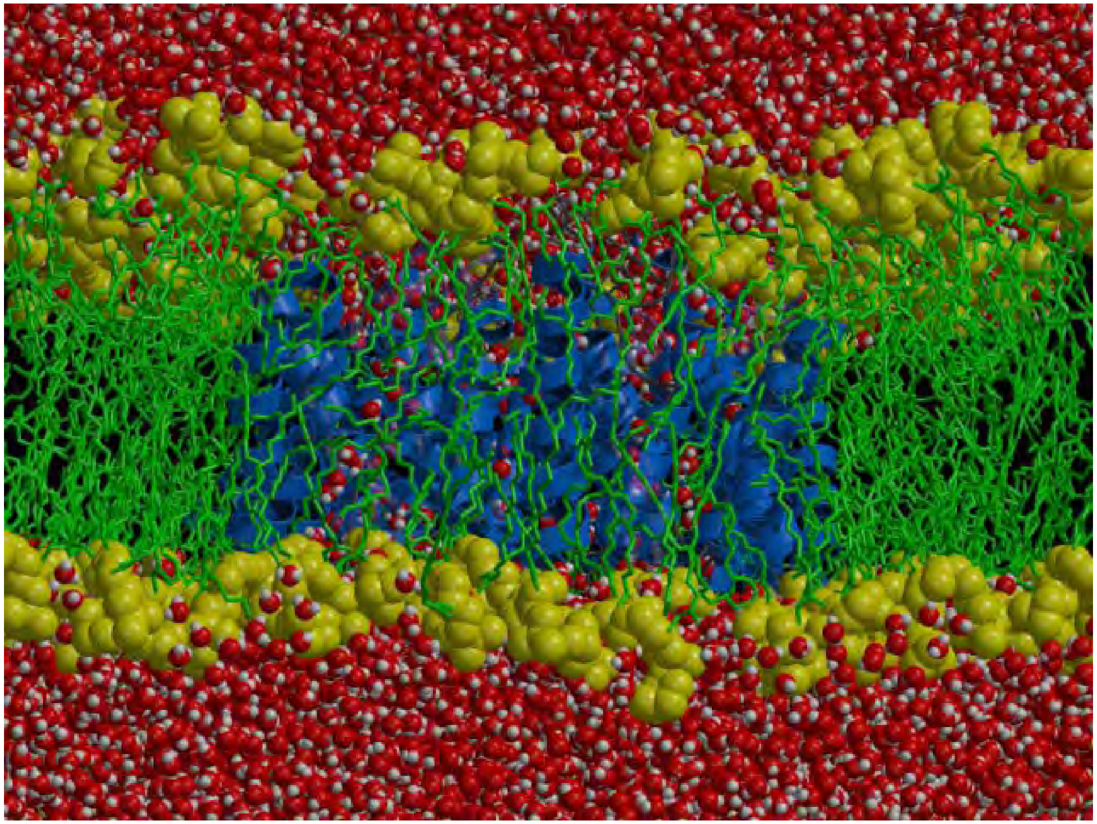
Matching of Coherent Properties

Investigation of
nano domains



Summary

Membrane Dynamics



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

Membrane is the primary site of (inter)action

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

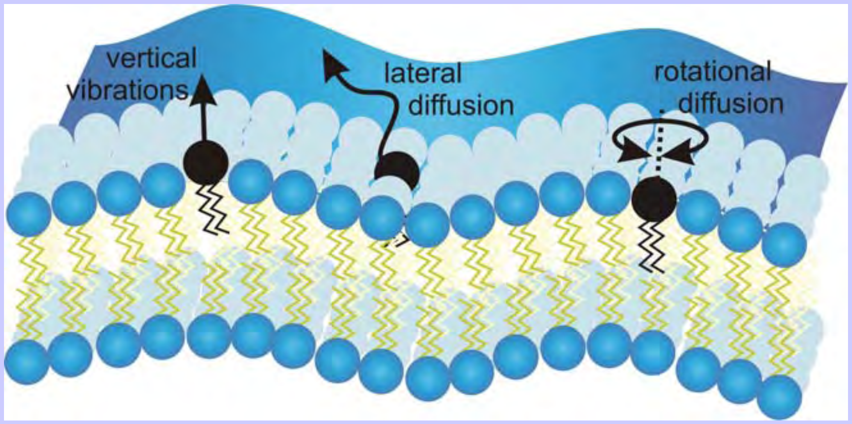
missing or not well developed periodic **structure** (BZ concept)

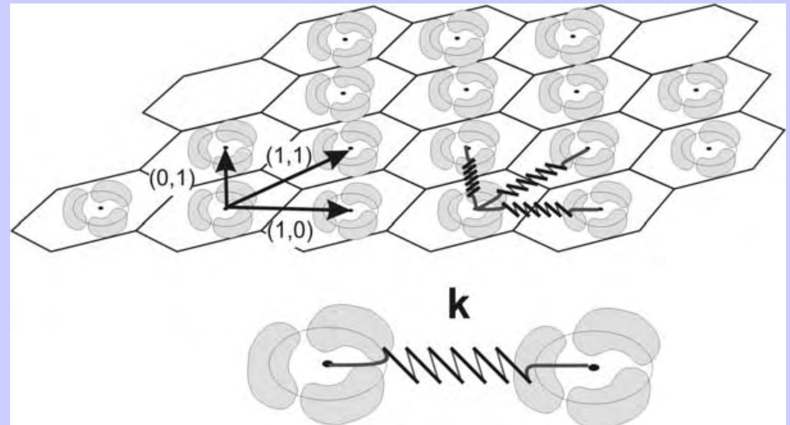
high ‘intrinsic’ background

- different molecular components
- single and collective molecular motions

Membrane Dynamics

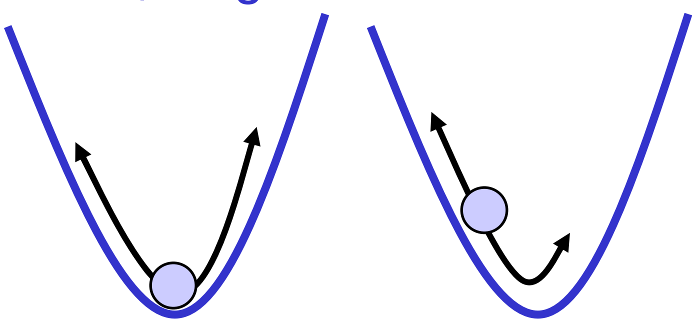
Local modes in bilayers



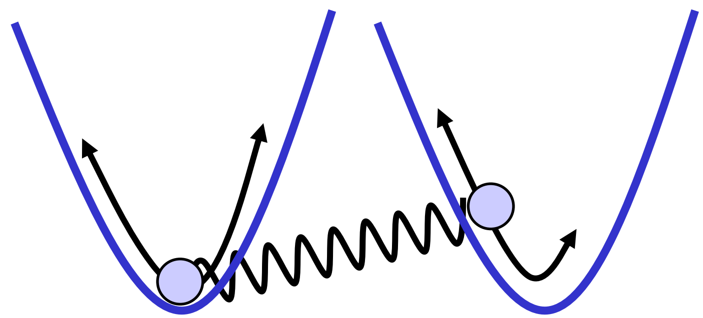


Collective excitations

Incoherent, single molecule



Coherent, interactions



Correlated molecular motions drive “functionalities” of membranes and proteins and structural changes