Quasi-Elastic Neutron Scattering

- What is it ?
- Why do we care?
- How do we measure it?
- How do we analyse the data?

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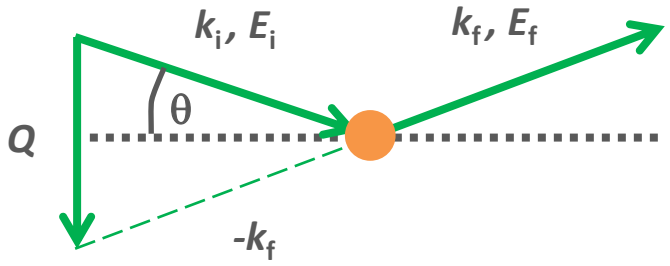
The Scattering Process

Interaction of neutron with nuclei – there can be an exchange of **momentum** and of **energy**



Elastic scattering:

$$|\boldsymbol{k}_i| = |\boldsymbol{k}_f| = \frac{2\pi}{\lambda}$$

$$\mathrm{Q} = 2|\boldsymbol{k}|\sin\boldsymbol{\theta} = \frac{4\pi}{\lambda}\sin\boldsymbol{\theta}$$

$$\Delta E = 0$$

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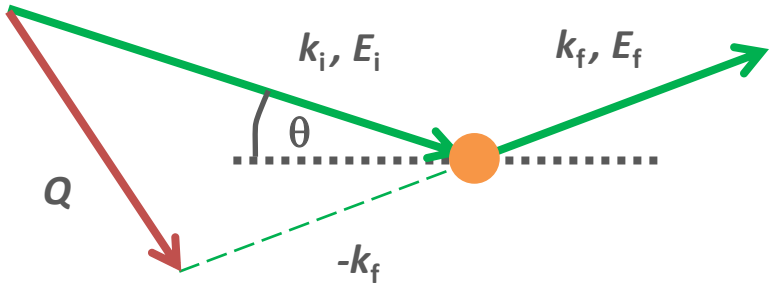


Scattering triangle
(cosine rule)

$$Q^2 = {k_i}^2 + {k_f}^2 - 2k_i k_f \cos 2\theta$$

Kinematic condition

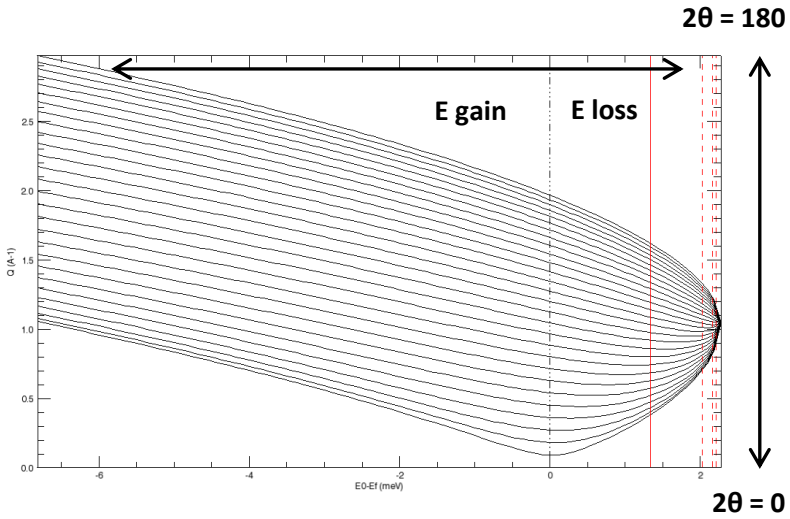
$$\frac{\hbar Q^2}{2m} = E_i + E_f - 2\sqrt{E_i E_f}\cos 2\theta$$

Inelastic scattering:

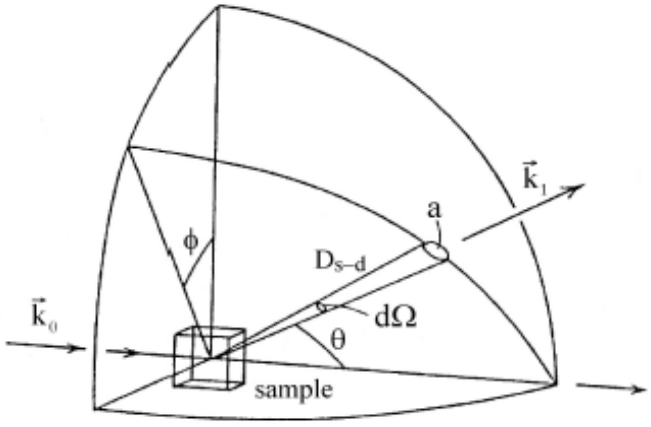
$$|\boldsymbol{k_i}| \neq |\boldsymbol{k_f}|$$

$$\hbar \boldsymbol{Q} = \hbar(\boldsymbol{k_i} - \boldsymbol{k_f})$$

$$\boldsymbol{\Delta E} = \hbar\boldsymbol{\omega} = E_i - E_f = \frac{\hbar}{2m}(k_i - k_f)$$



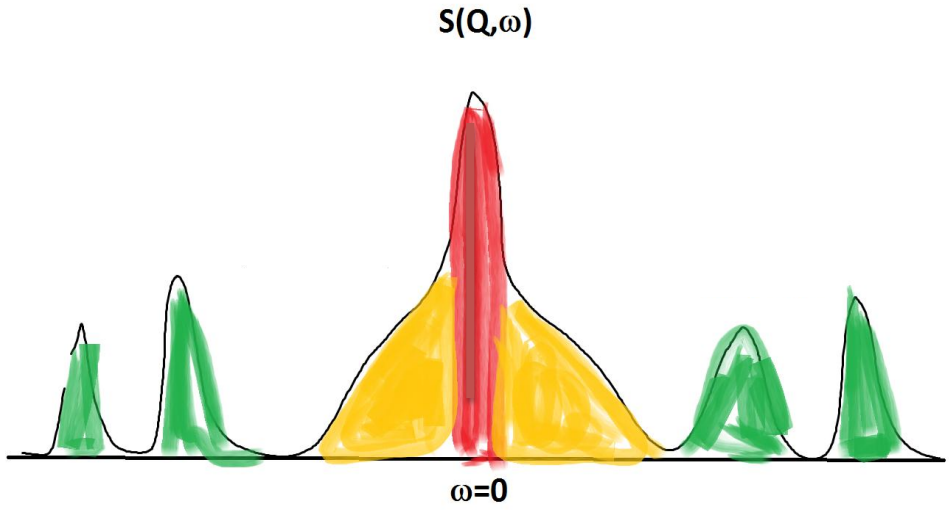
The Scattering Function, $S(Q,\omega)$



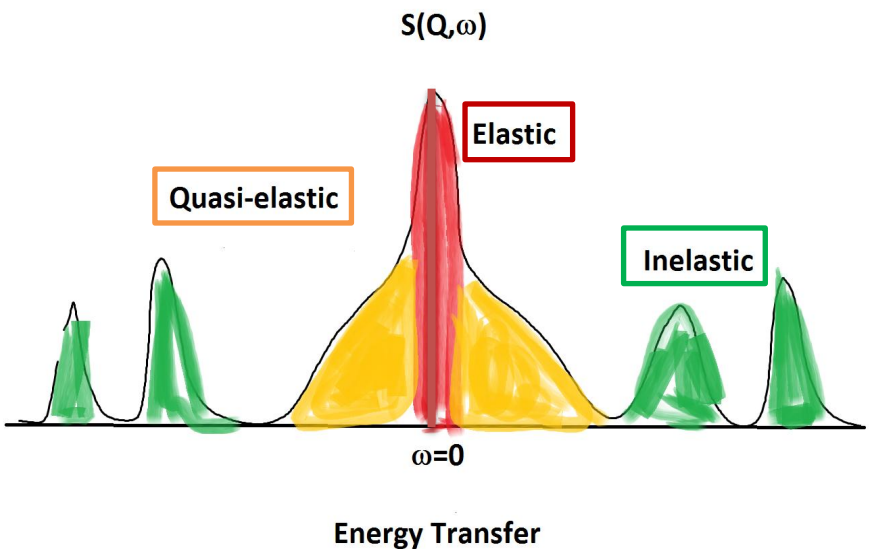
$$\frac{d^2\sigma}{d\Omega d\omega} \propto \frac{k_f}{k_i}\frac{\sigma}{4\pi}S(\boldsymbol{Q},\omega)$$

The **scattering function,** $S(\boldsymbol{Q},\omega)$ contains all the physics of the system (in space and time) and depends only on the system.

This is our measurable in the scattering experiment.



Quasi-Elastic Scattering



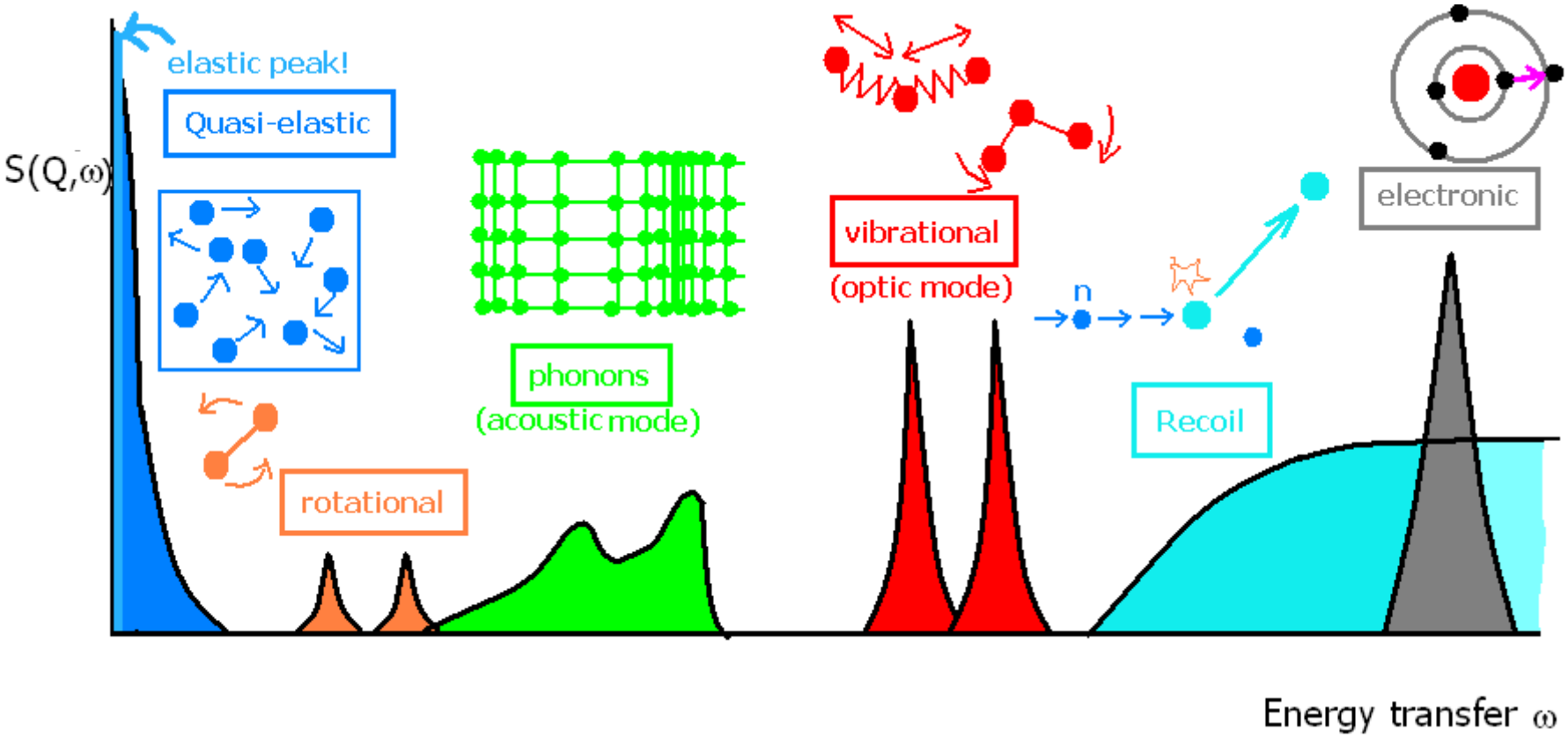
Elastic scattering – no energy exchange ħω=0. In an ideal world this should be a delta function. Of course, this is not the case giving rise to an instrumental resolution.

$$S(\boldsymbol{Q},\omega) = S^*(\boldsymbol{Q},\omega) \otimes R(\boldsymbol{Q},\omega)$$

Inelastic scattering – there is energy exchange ħω≠0. Due to processes occurring discrete energy steps such as vibrational modes, stretching modes…

Quasi-elastic scattering (QENS)– there is small energy exchange ħω≠0≈neV or μeV . **High energy resolution**. Due to processes occurring with a distribution of energies (rotations, translations…).

Map of dynamical modes



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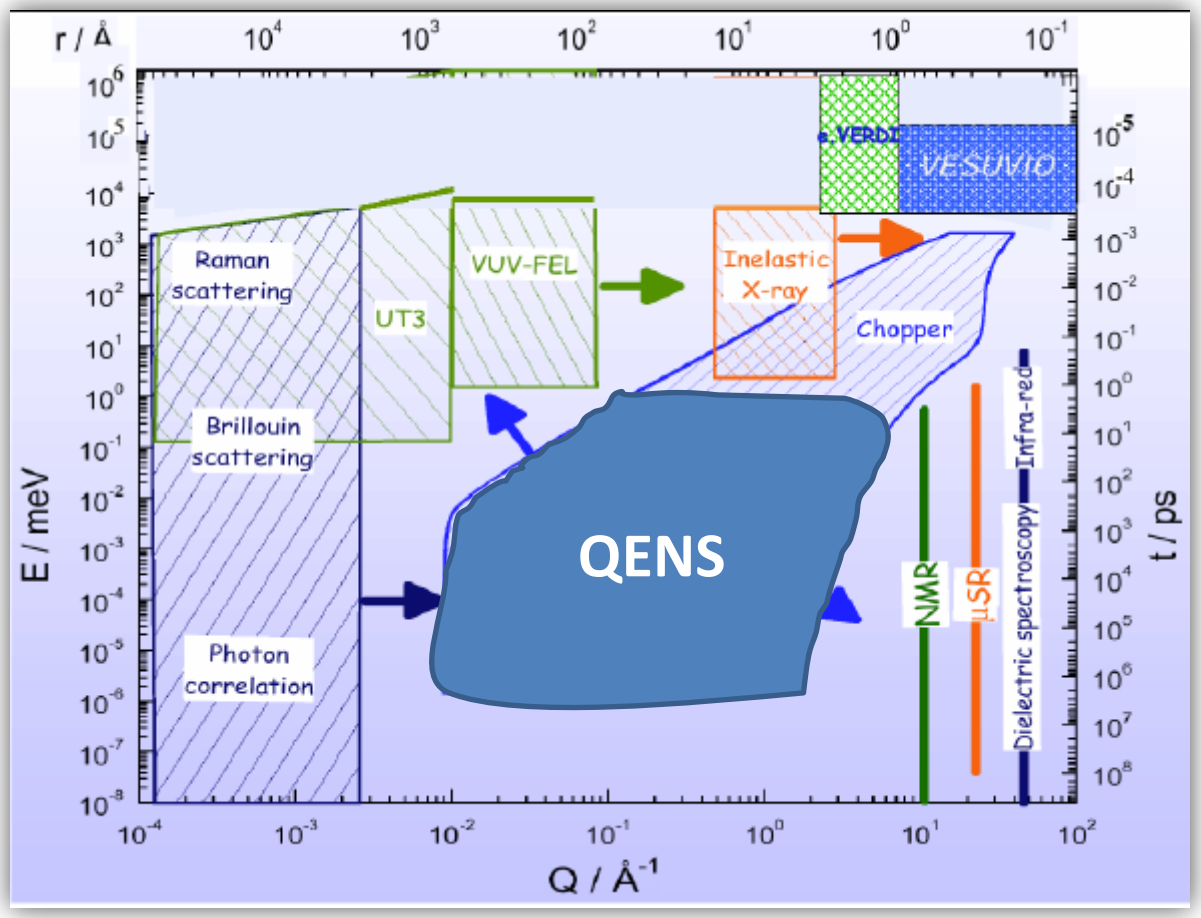

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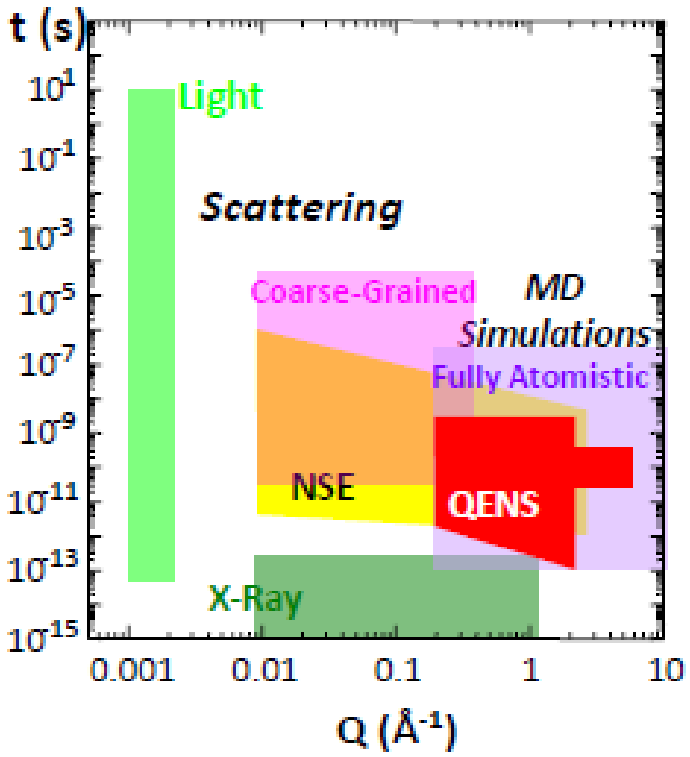
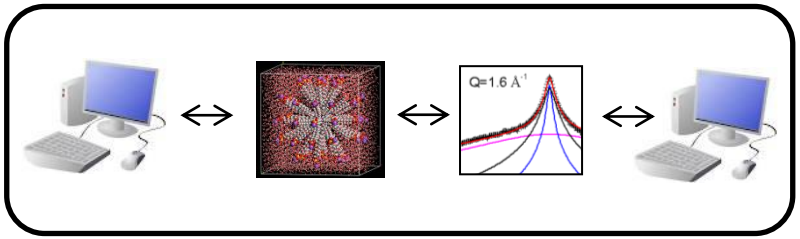


Molecular Dynamics Simulations



- Flexible parameter space
- Large parameter space
- Need to optimize and choose FF
- Directly comparable with neutron data

Quasi-Elastic Scattering – Why care?

- Probes dynamics in a wide **range of science** areas
  - *Materials science*: hydrogen storage, surface science, fuel cells
  - *Soft Matter*: polymer nanocomposites and blends, organic photovoltaics, polymer electrolytes
  - *Biology*: hydration water, protein structure-dynamics-function relationships, cell membrane-protein/small molecules interactions, drug delivery, protein binding
  - *Chemistry*: ionic liquids, clays, porous media, complex fluids

Quasi-Elastic Scattering – Why care?

- Probes diffusion at a molecular scale
- Is able to differentiate bulk from confined dynamics
- Analytical functions used to describe motions
- Can be used as a systematic tool for comparisons
- Time and spatial scale are directly comparable to results from Molecular Dynamics simulations
- Complementarities with other experimental techniques
- Unique view of motions (eg. contrast)

QENS scattering function

$$S(\boldsymbol{Q},\omega) = S_{\mathrm{inc}}(\boldsymbol{Q},\omega) + S_{\mathrm{coh}}(\boldsymbol{Q},\omega)$$

- **Incoherent** scattering
  - Contains no information about structure
  - Describes the **dynamics of individual particles**
- **Coherent** scattering
  - Contaminates elastic signal arising from **structure**
  - Describes **correlations between nuclei**
  - Describes the **collective dynamics** of nuclei

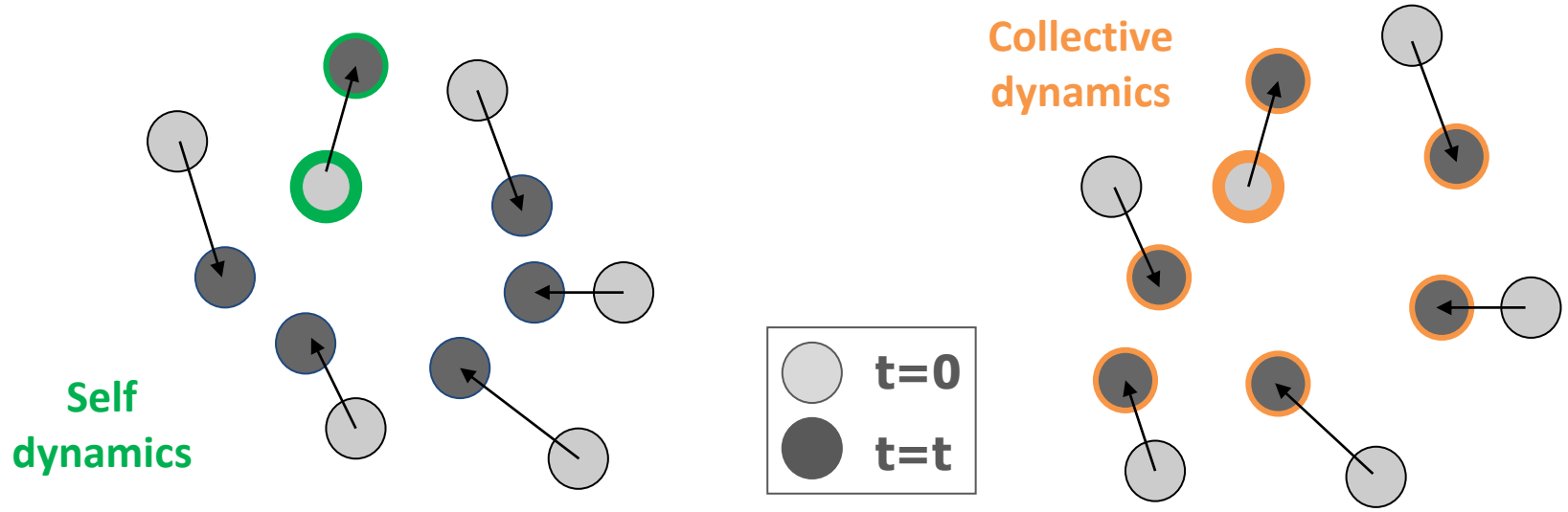
Scattering Functions- Correlations

Remember that in the experiment we measure the total $S(\boldsymbol{Q},\omega)$ and that each term, coherent and incoherent is weighted by its respective cross-section σ

$$S(\boldsymbol{Q},\omega) = S_{\mathrm{inc}}(\boldsymbol{Q},\omega) + S_{\mathrm{coh}}(\boldsymbol{Q},\omega)$$

$$S_{\mathrm{inc}}(\boldsymbol{Q},\omega) = \frac{1}{2\pi}\int_{-\infty}^{+\infty}\sum_{i}\langle \exp(-i\boldsymbol{Q}\cdot\boldsymbol{R}_i(0))\exp(-i\boldsymbol{Q}\cdot\boldsymbol{R}_i(t))\rangle \exp(-iwt)\,dt$$

$$S_{\mathrm{coh}}(\boldsymbol{Q},\omega) = \frac{1}{2\pi}\int_{-\infty}^{+\infty}\sum_{i,j}\langle \exp(-i\boldsymbol{Q}\cdot\boldsymbol{R}_i(0))\exp(-i\boldsymbol{Q}\cdot\boldsymbol{R}_j(t))\rangle \exp(-iwt)\,dt$$



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$$S_{\mathrm{coh}}(\boldsymbol{Q},\omega) = \frac{1}{2\pi}\int_{-\infty}^{+\infty}\sum_{i,j}\left\langle \exp(-i\boldsymbol{Q}\cdot\boldsymbol{R}_i(0))\exp(-i\boldsymbol{Q}\cdot\boldsymbol{R}_j(t))\right\rangle \exp(-iwt)\,dt$$

These expressions can also be re-written in terms of the self and collective **intermediate scattering functions, I(Q,t)**, such that**:**

$$S_{\mathrm{inc}}(\boldsymbol{Q},\omega) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} I_{\mathrm{self}}(\boldsymbol{Q},t)\exp(-iwt)\,dt$$

$$S_{\mathrm{coh}}(\boldsymbol{Q},\omega) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} I_{\mathrm{coll}}(\boldsymbol{Q},t)\exp(-iwt)\,dt$$

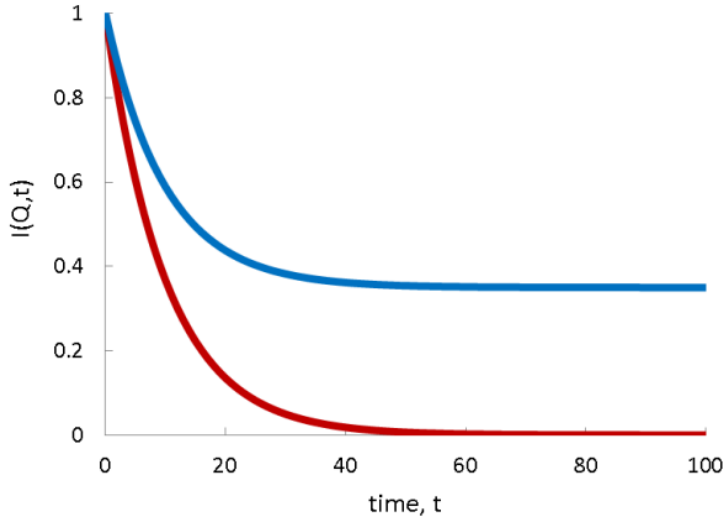
Intermediate Scattering Function

The intermediate scattering functions are **the time and space Fourier transform** of **the self autocorrelation function** and the **pair correlation function** (incoherent and coherent scattering functions respectively).

They describe the position of particle *i* in space as a function of time.

$$S_{\mathrm{inc}}(\boldsymbol{Q},\omega) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} I_{\mathrm{self}}(\boldsymbol{Q},t)\exp(-iwt)\,dt$$

$$S_{\mathrm{coh}}(\boldsymbol{Q},\omega) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} I_{\mathrm{coll}}(\boldsymbol{Q},t)\exp(-iwt)\,dt$$



… for QENS …

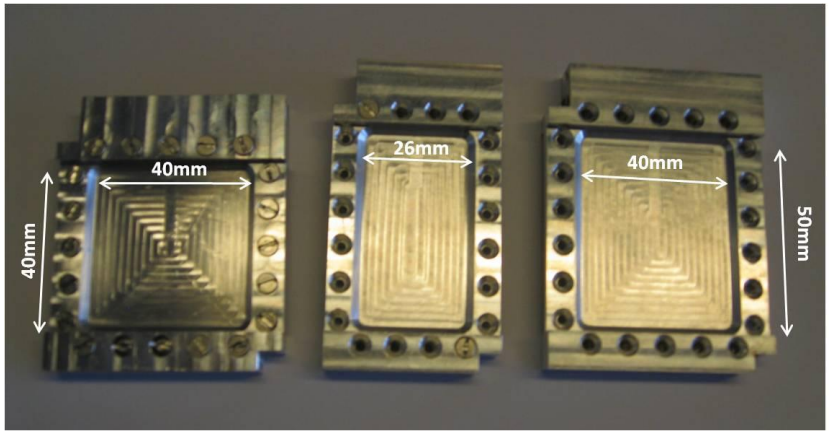
	σ_{coh} (b)	σ_{incoh} (b)	σ_{abs} (b)
Hydrogen	1.76	**80.2**	0.33
Deuterium	5.59	2.05	0.00
Carbon	5.56	0.00	0.00
Nitrogen	11.0	0.50	1.90
Oxygen	4.23	0.00	0.00
Phosphorus	3.31	0.01	0.17
Aluminium	1.50	0.01	0.23
Silicon	2.17	0.00	0.17

The QENS experiment

- Minimise possibility of multiple scattering

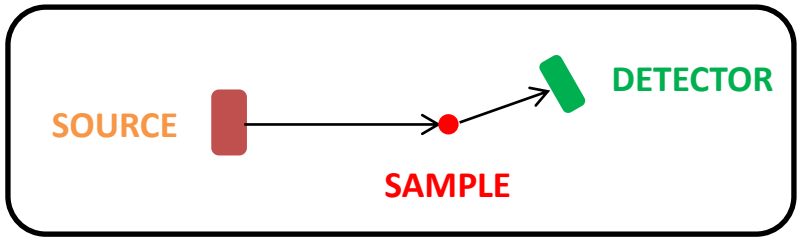
  => Keep transmission at 90 %

- Use annular or flat aluminium cans



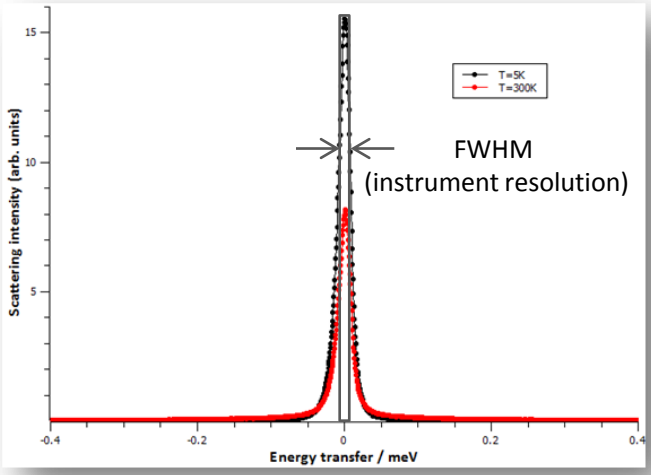
QENS Spectrometers - Direct

Direct geometry



LET on ISIS-TS2

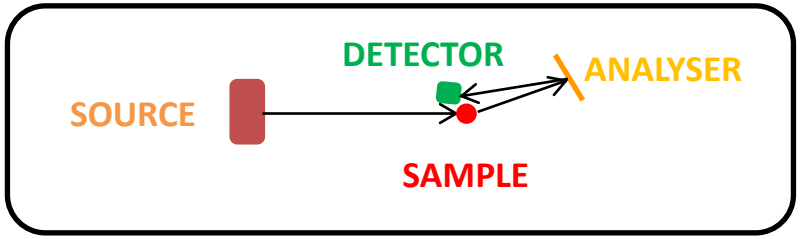
- Send neutrons of known **fixed E_i (v_i)** – neutron can loose as much energy as it has but can gain any (defines energy window)
- Source-sample and sample-detector distances known
- Time at which neutron is sent, known
- Time at which neutron is detected tells us E_f, thus we know ΔE

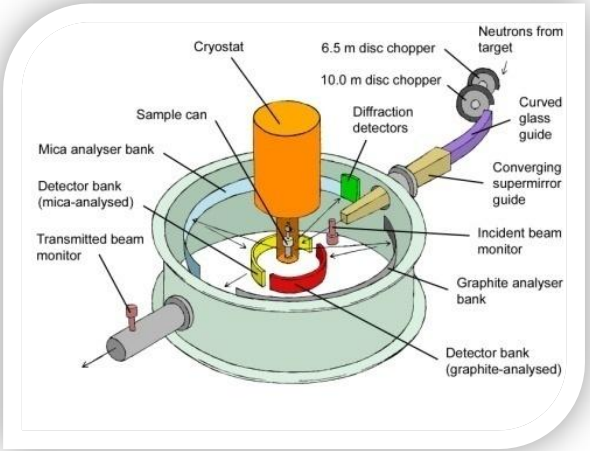


Elastic intensity is the integral of the line around $\Delta E=0$ as given by the instrumental resolution.

QENS Spectrometers - Indirect

Indirect geometry or Backscattering

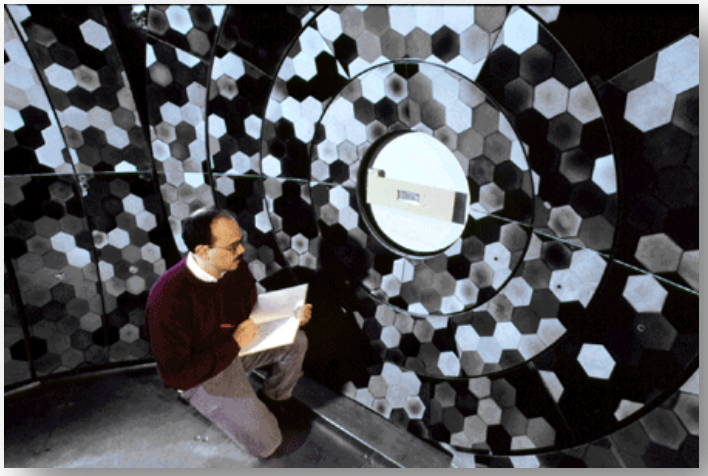




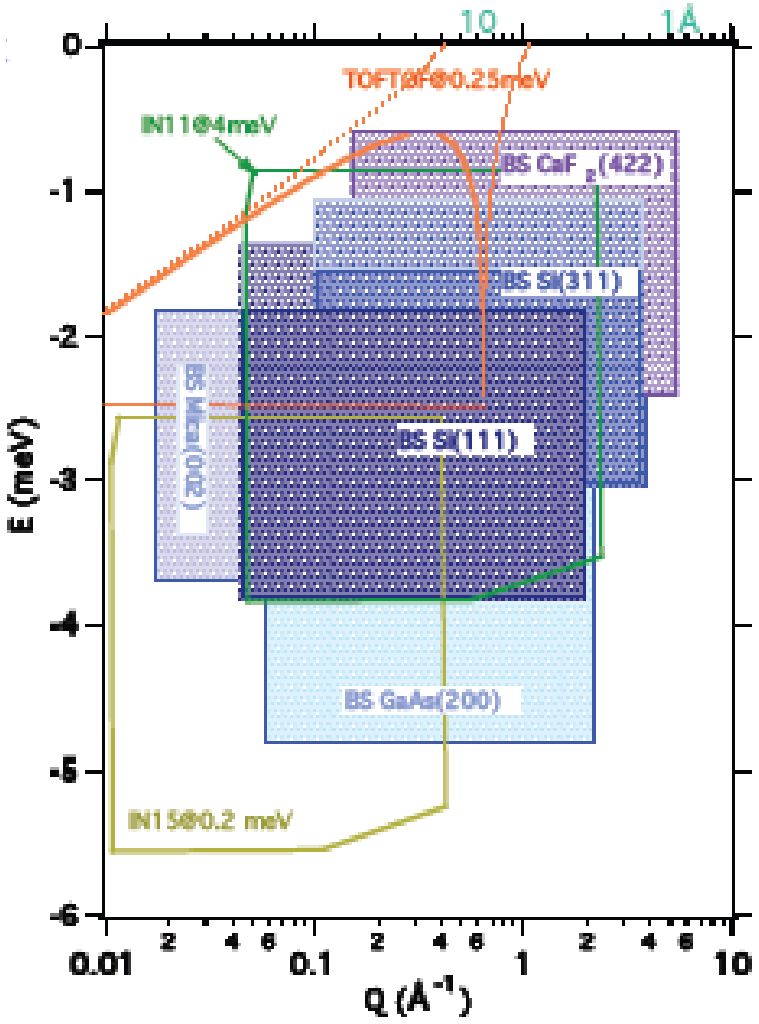
IRIS on ISIS-TS1

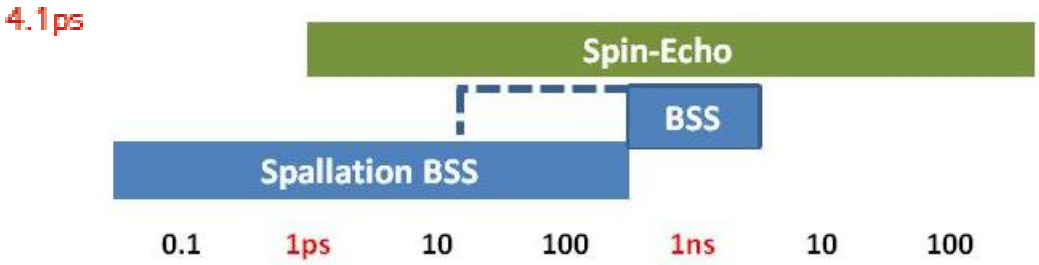
- Send neutrons of a known band of wavelengths or E_i (v_i)s (defines your energy window)
- In reactor source, use a Doppler drive; in a spallation source, use choppers
- Analyser crystals reflect back only a **fixed** $\boldsymbol{E_f}$ (Bragg's Law)
- Times & distances known, so detected neutron gives us ΔE

HFBS at the NCNR, USA



QENS Spectrometers – Which one?



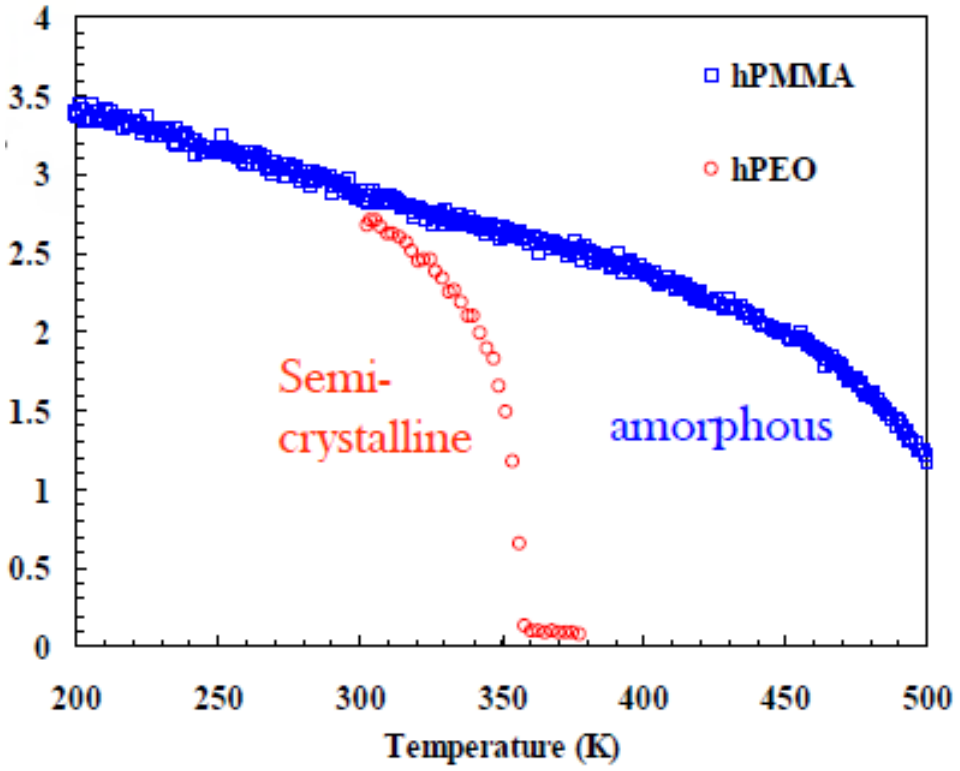


- Direct geometry:
  - Poorer resolution, higher energies, wider E transfer window, small Q range.
- Indirect geometry:
  - @ reactor, highest resolution with good intensity but limited E transfer range
  - @ spallation, medium resolution, high flux, wider E transfer range

Elastic Window Scan

Measurement of the elastic **intensity as a function of temperature** is a typical technique in QENS spectrometers. It resembles a DSC scan and is very good for locating **transitions** – at what temperatures do the dynamics enter the time window of the neutron spectrometer?

A lot of **biology and soft matter** experiments start with this type of measurement.



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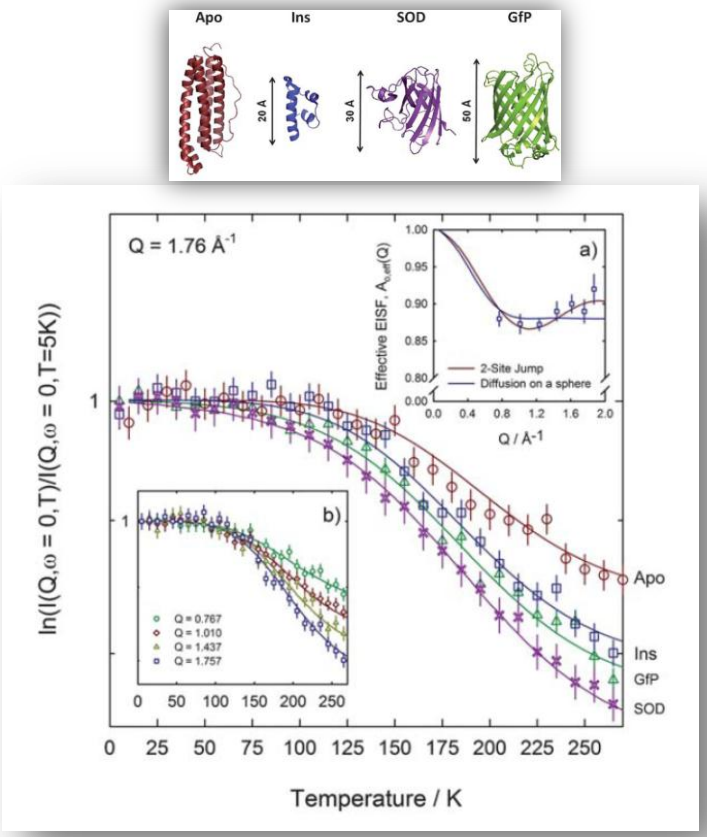
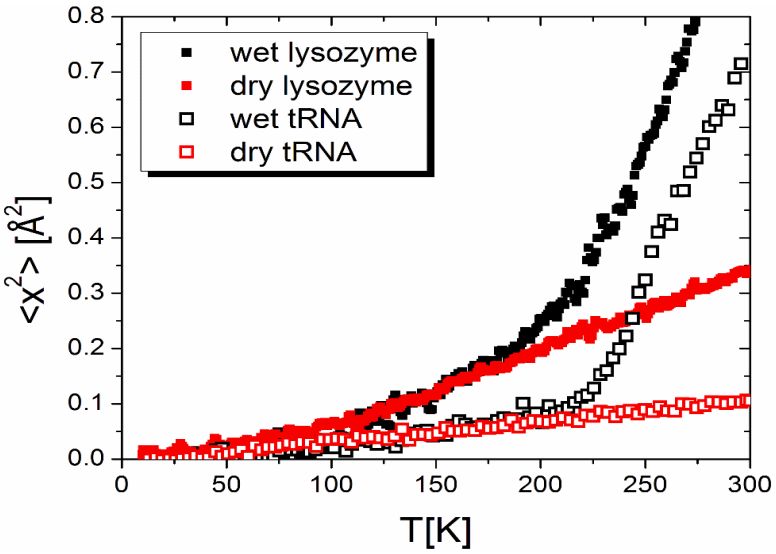
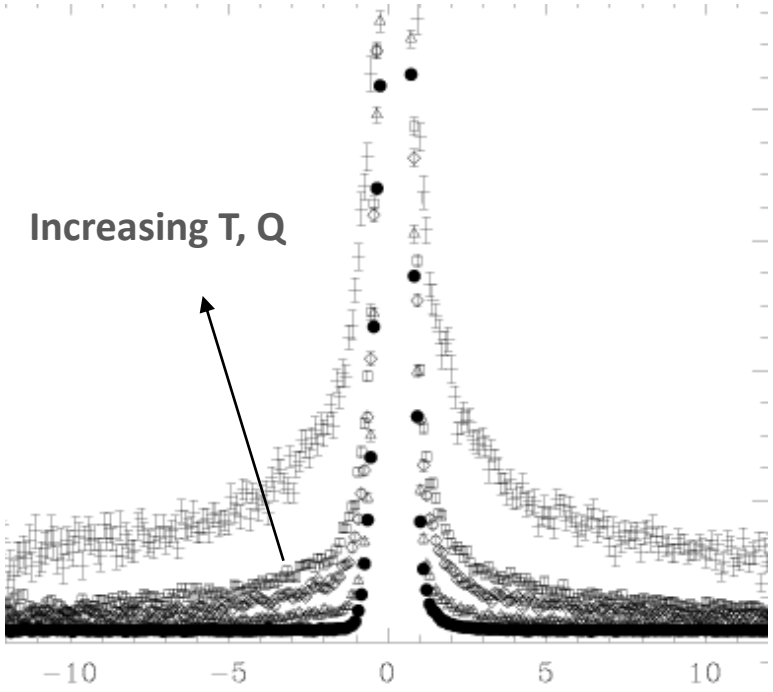


Fingerprinting as a *f*(*c*,*P*,..)



QENS Measurement

In elastic mode we only look at no change in energy, but QENS is all about measuring changes in energy which tells us about the **timescale of motion of the atoms as a function of T, P, c**… The initial scan allows us to pick temperatures where the dynamics will fall in our instrumental time window. Each spectrometer is different.



1. Elastic line - If motions are too slow for the spectrometer
2. Flat background – if motions are too fast for the spectrometer & all atoms are moving
3. Combo of 1 & 2 if not all atoms are moving or some are moving in a confined geometry
4. **Elastic line plus QENS broadening if motions are in the spectrometer's time window**

Self (incoherent) scattering function

Let's consider **the self correlation function**, ie. how particles move as a function of time. This corresponds as we have seen before to the incoherent signal. In general terms, the incoherent scattering function is written as:

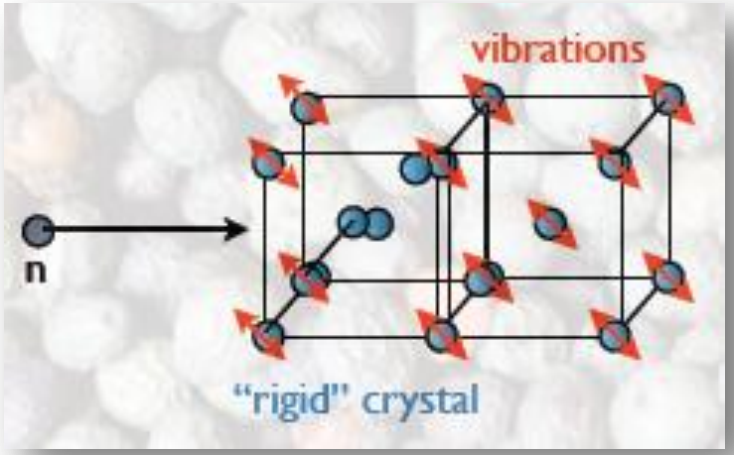
$$S_{\mathrm{inc}}(\boldsymbol{Q},\omega) = S_{\mathrm{vib}}(\boldsymbol{Q},\omega) \otimes S_{\mathrm{rot}}(\boldsymbol{Q},\omega) \otimes S_{\mathrm{trans}}(\boldsymbol{Q},\omega)$$

$$I_{\mathrm{self}}(\boldsymbol{Q},t) = I_{\mathrm{vib}}(\boldsymbol{Q},t) \times I_{\mathrm{rot}}(\boldsymbol{Q},t) \times I_{\mathrm{trans}}(\boldsymbol{Q},t)$$

the **convolution of components**, in its simplest case we can consider vibrations, rotations and translations. Note that for simplicity we assume that they are **independent** motions. Note that in the time domain we multiply the terms (easier!)

Vibrations: Debye-Waller factor

In reality, nuclei (even in a rigid crystal) are **not stationary**, causing a decrease in the intensity of a diffracted beam (remember Bragg's law) because waves are not so well in phase. In addition, this smearing is a function of temperature. Assuming that **vibrations** are **harmonic** and **isotropic:**



$$DWF = \langle \exp(i\boldsymbol{Q}\cdot\boldsymbol{u})\rangle = \exp(-\langle(\boldsymbol{Q}\cdot\boldsymbol{u})^2\rangle) = \frac{1}{3}\exp(Q^2\langle u^2(T)\rangle)$$

Mean-square displacement of atoms, **$\langle u^2 \rangle$**, is measured as a function of temperature. Assuming particles are harmonic, we can think of them as springs and we can obtain an **effective force constant** – measurement of **flexibility** (used for proteins).

$$\langle k' \rangle = 2k_{\mathrm{B}}\left(\frac{d\langle u^2\rangle}{dT}\right)^{-1}$$

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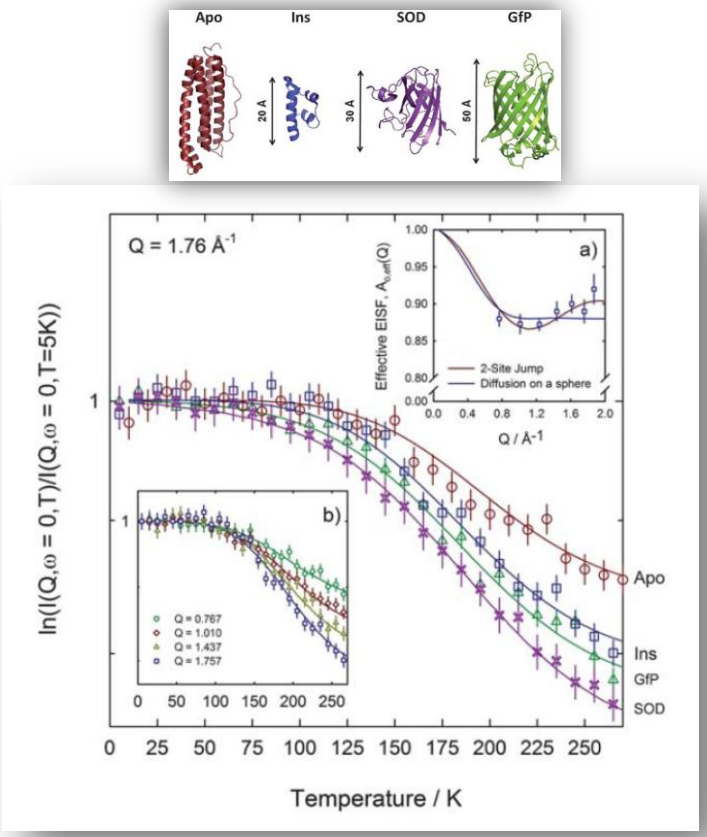

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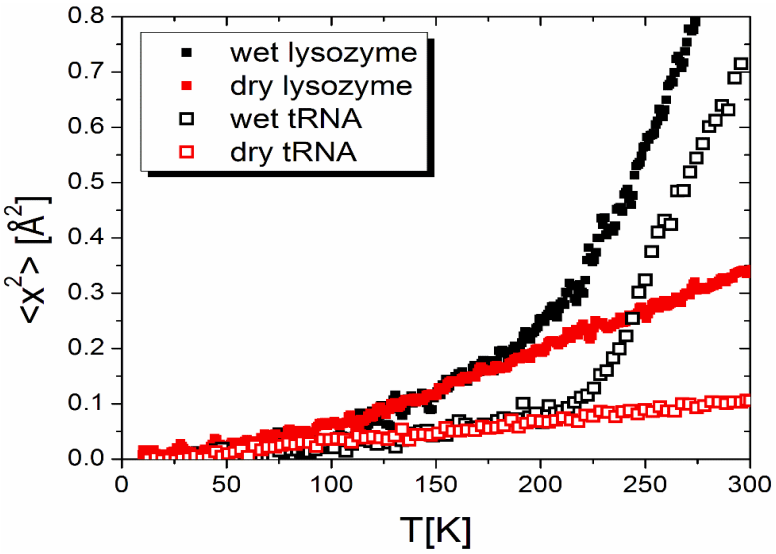
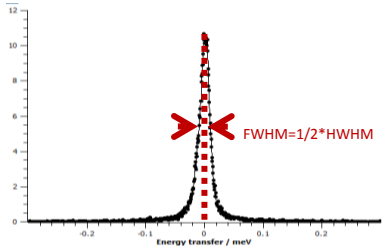


Simple Translational Diffusion

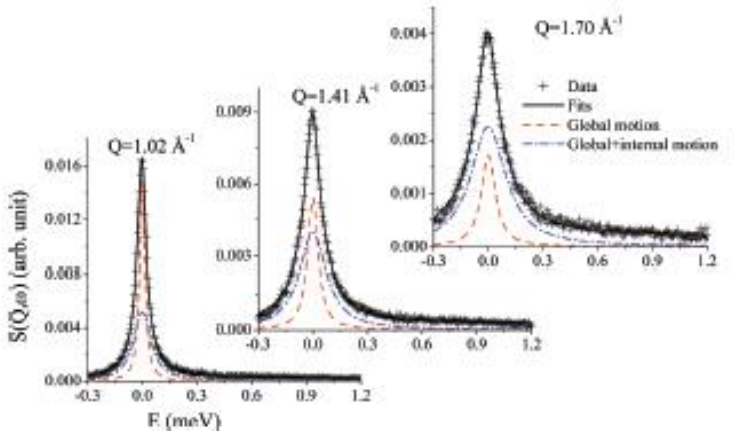
Let's go back to the incoherent scattering law and how to fit the data – in the energy space we typically fit with Lorentzians. Let's look at **continuous long-range isotropic translational diffusion**. In this case particles follow Fick's Law .

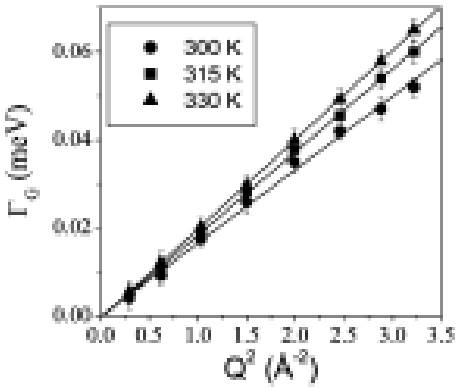
$$I(Q,t) = \exp(-Q^2 Dt) \qquad relaxation\,rate\ |\tau| = 1/(DQ^2)$$

$$S_{\mathrm{trans}}(\boldsymbol{Q},\omega) = \frac{1}{\pi}\frac{\Gamma}{\Gamma^2+\omega^2} \qquad \text{ie. a Lorentzian}$$



D (m^2/s) is the diffusion coefficient and Γ is the **half width at half maximum** (HWHM) which is this case = DQ^2. Leads to a broadening of the elastic line following a given Q-dependence. Diffusion coefficient follows Arrhenius Law





$$D \approx \exp(-E_a/kT)$$

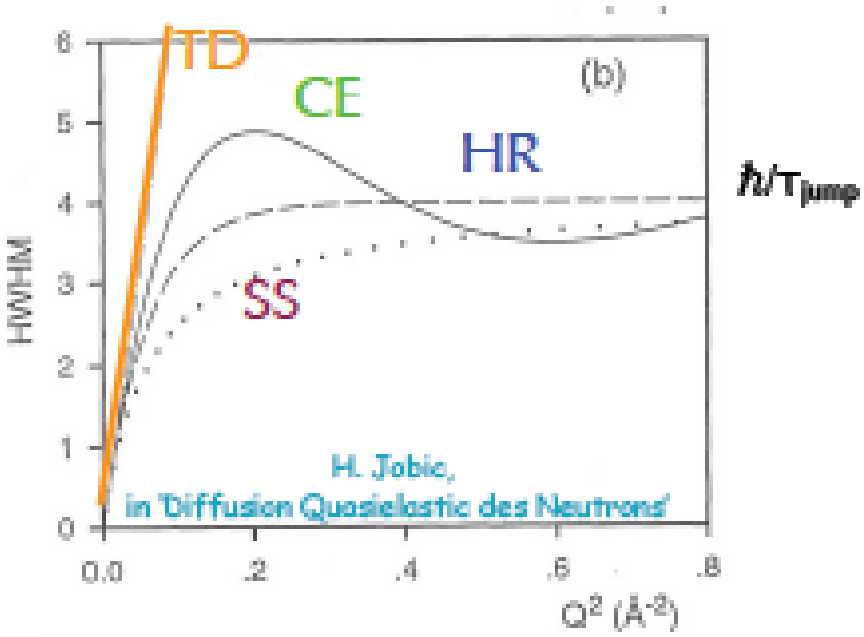
Models for Translational Diffusion

Not all is simple of course, and in many cases **diffusion is restricted** due to confinement (hard or soft), strong interactions, bonding restrictions, or diffusion happens in jumps; ie. deviations from Firk's Law. So we need other models. Here are some examples:

Chudley-Elloitt (CE) – jumps on a lattice

Singwi-Sjölander (SS)- alternation between oscillatory motion and directed motion

Hall-Ross (HR) – jump diffusion within a restricted volume



Residence time in jump and jump length

DQ^2 at low Q and then approaches $1/\tau_{jump}$ at high Q

More models including rotations

$$S_{\mathrm{inc}}(\boldsymbol{Q},\omega) = S_{\mathrm{vib}}(\boldsymbol{Q},\omega) \otimes S_{\mathrm{rot}}(\boldsymbol{Q},\omega) \otimes S_{\mathrm{trans}}(\boldsymbol{Q},\omega)$$

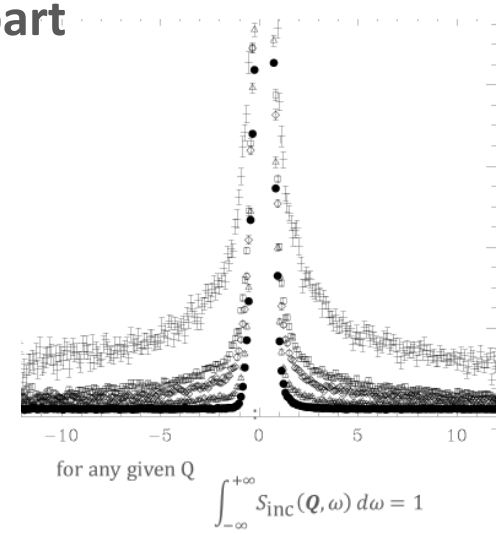
The final part is the case of localised motions such as rotations. In this case we have a stationary part plus a decaying part giving rise to some elastic contribution. This gives rise to a Q-independent line-width and an EISF.

$$S_{\mathrm{inc}}(\boldsymbol{Q},\omega) = \exp(-Q^2\langle u^2\rangle)[A_0(\boldsymbol{Q})\delta(\omega) + \Big(1 - A_0(\boldsymbol{Q})\Big)L(\boldsymbol{Q},\omega)]$$

Elastic stationary part, EISF

Quasi-elastic decaying part

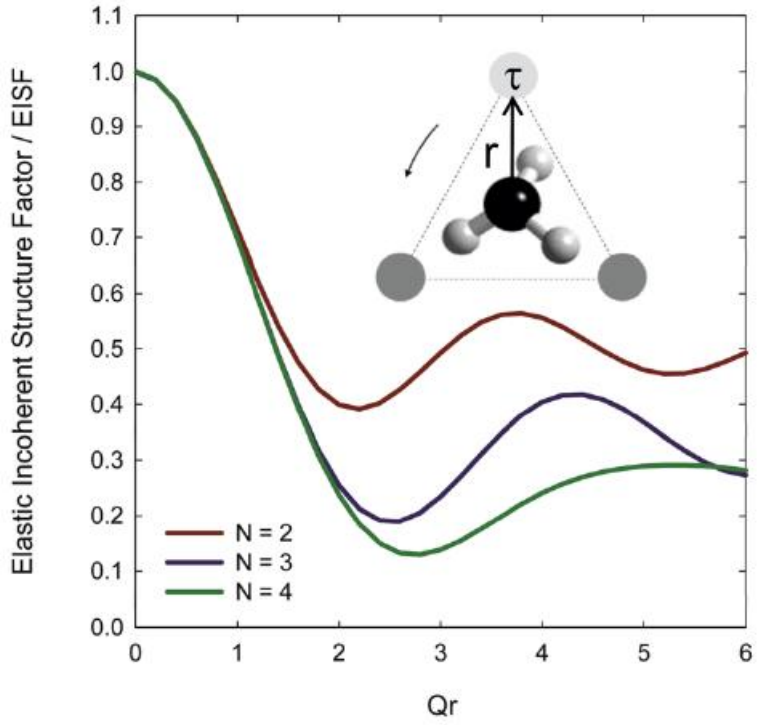
$$EISF = \frac{S_{inc}^{el}(\boldsymbol{Q})}{S_{inc}^{el}(\boldsymbol{Q}) + S_{inc}^{qel}(\boldsymbol{Q})}$$



The **EISF** is the area of the elastic curve divided by the total area, ie. the fraction of elastic contribution.

EISF – Geometry of Motion

Particles move in a restricted space having a specific **geometry of motion**



- Jumps between 2, 3, … *n* sites
- Rotational diffusion on a circle
- Diffusion on a sphere
- Diffusion inside a sphere, cylinder…

For a CH_3 group – site site jumps

$$EISF = \frac{1}{3}\left[1 + 2j_0\left(\sqrt{3}\,Qr\right)\right]$$

Jumps between 2 sites

$$EISF = \frac{1}{2}\left[1 + \frac{\sin(2Qd)}{2Qd}\right]$$

Free diffusion inside a sphere

$$EISF = \left(\frac{3j_1(Qr)}{Qr}\right)^2$$

Summary of Self Scattering Function

$$S(Q,\omega) = S_{vib}(Q,\omega) \otimes S_{trans}(Q,\omega) \otimes S_{rot}(Q,\omega) \otimes ....$$

Translation diffusion

EISF (elastic incoherent structure factor)- motion geometry

$$S(Q,\omega) = e^{-Q^2u^2}\left\{\frac{1}{\pi}\frac{\Gamma(Q)}{\Gamma^2(Q)+\omega^2} + j^2{}_0(Qa)\delta(\omega) + \sum_{l=1}^{\infty} A_l(Q)\frac{1}{\pi}\frac{l(l+1)D_R}{(l(l+1)D_R)^2+\omega^2}\right\} + ...$$

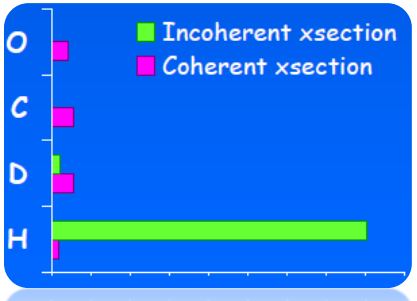
Vibrations [Debye-Waller]

Elastic contribution

Rotations

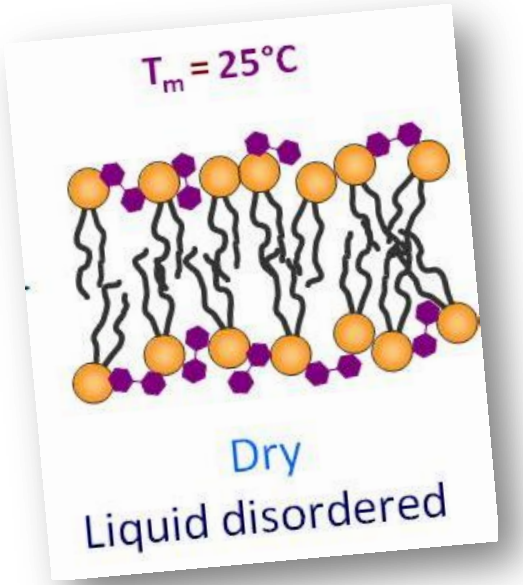
Can't forget the instrumental resolution:

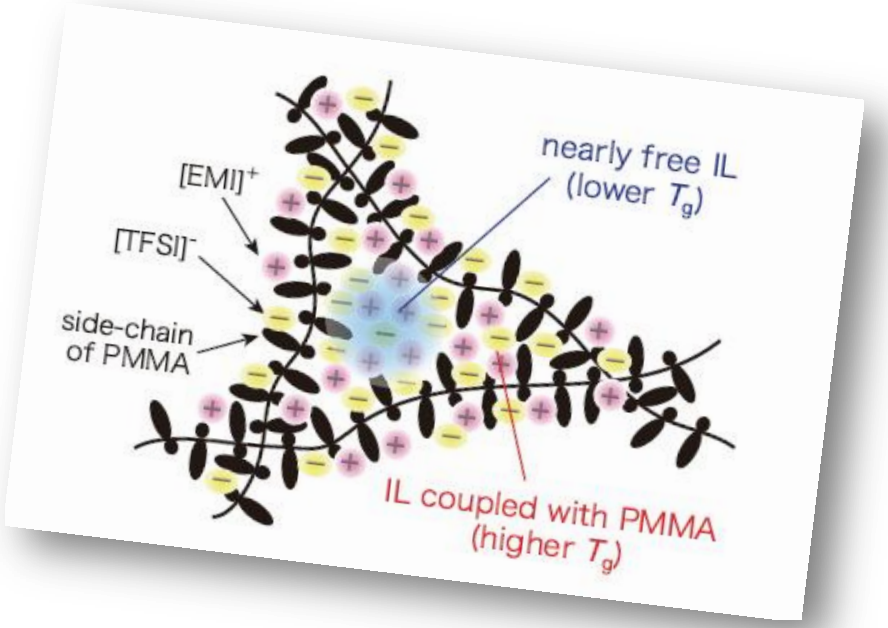
$$S'(Q,\omega) = S(Q,\omega) \otimes R(Q,\omega)$$



A different way to analyse QENS data

Unfortunately things are not quite as easy for some soft matter systems due to their **complexity** (*environments*) and extra **degrees of freedom.** What we are faced with is a distribution of relaxation times (FWHM's), jump lengths, mixture of components, activation energies…



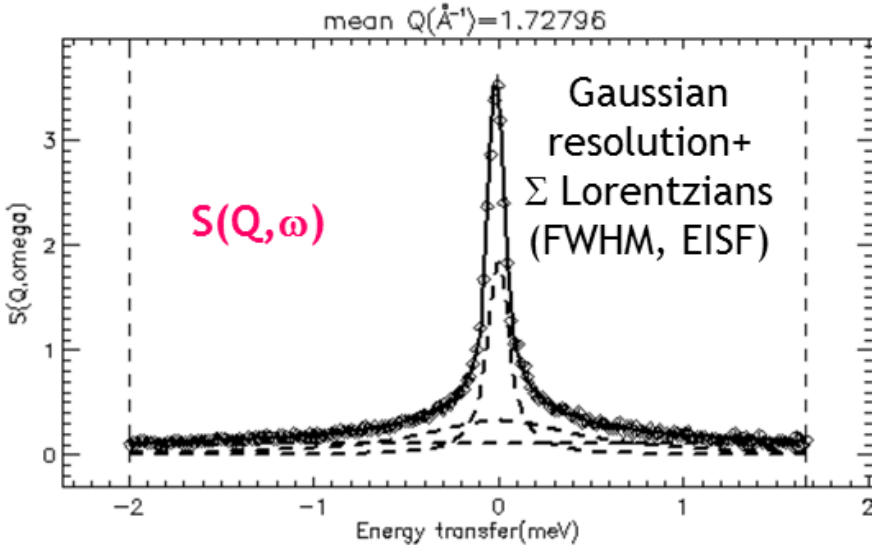


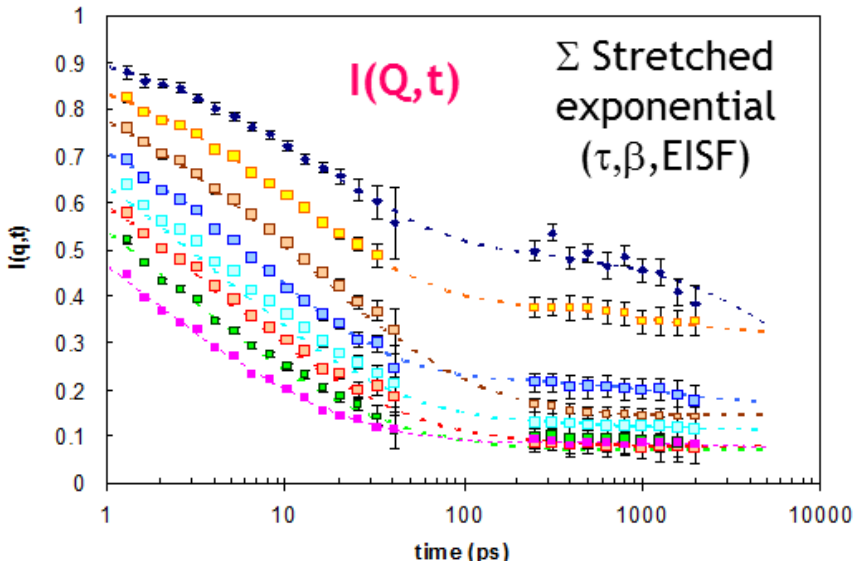
So, many times we cannot simply fit QENS spectra with 1, 2 or even 3 Lorentzians, in fact we need a **distribution of Lorentzians** and since it is easier we move from thinking in the energy space to the time space!

The Stretched Exponential (KWW)

$$S_{\mathrm{inc}}(\boldsymbol{Q},\omega) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} I_{\mathrm{self}}(\boldsymbol{Q},t)\exp(-iwt)\,dt$$

Let's take the Fourier Transform





and fit in the time domain

$$I(\boldsymbol{Q},t) = Aexp\left[-\left(\frac{t}{\tau_{\mathrm{KWW}}}\right)^{\beta}\right] = \int_{-\infty}^{+\infty} f(\ln\tau)\exp\left(-\frac{t}{\tau}\right)d(\ln\tau) \qquad \langle\tau\rangle = \frac{\Gamma(1/\beta)}{\beta}\tau_{\mathrm{KWW}}$$

Heterogeneity in Some Systems

$$I(\boldsymbol{Q},t) = Aexp\left[-\left(\frac{t}{\tau_{\mathrm{KWW}}}\right)^{\beta}\right] + (1-A)$$

What do the parameters mean?

$\langle\boldsymbol{\tau}\rangle$ = average **relaxation time** = f(T, Q)

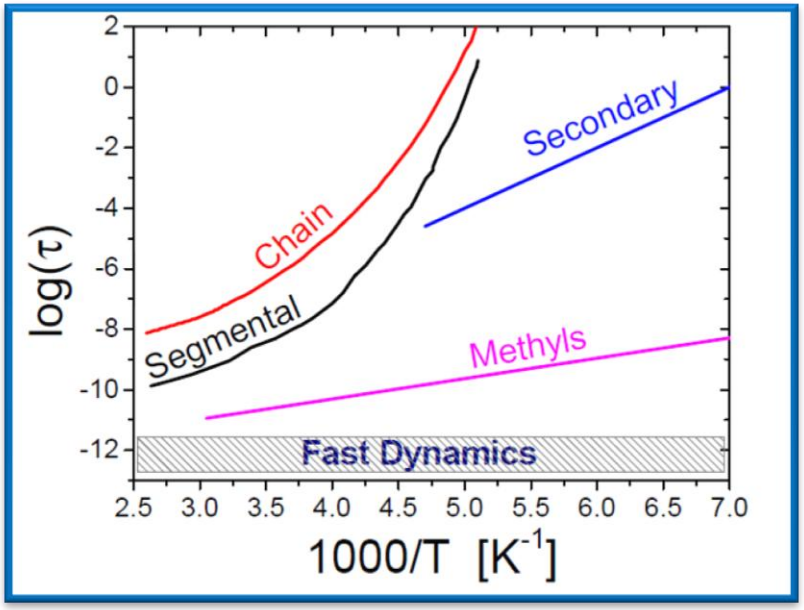
$\boldsymbol{\beta}$ = **stretching exponent** = f(T, Q) If β = 1, all particles move alike

If β < 1, there is heterogeneity in the system. For pure macromolecules 0.4 < β < 0.6 is typical. For polymer blends, confined systems, biological molecules, it can be lower

$\boldsymbol{A}$ = fraction of moving (or **relaxing molecules**) = f(T, Q)

It is the ***Q* and *T* dependence of these parameters** that give us information about the homogeneity or heterogeneity in the system.

Dynamics: Activation energy & Geometry

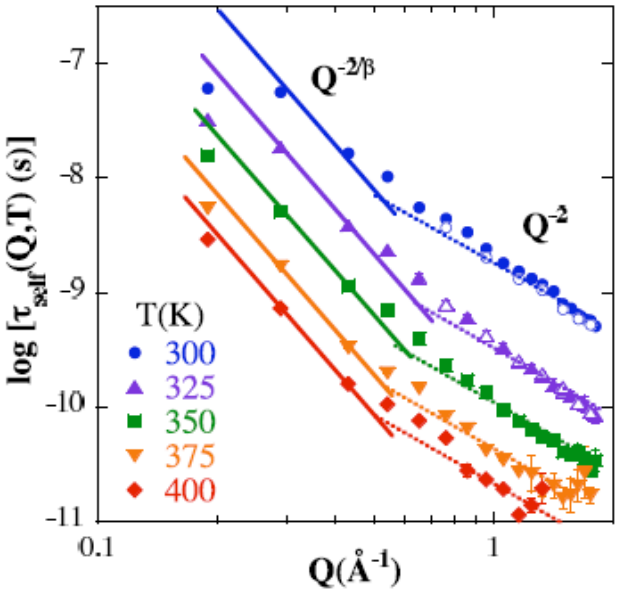


Temperature dependence of the relaxation time

- α-relaxation in polymers (related to Tg) follows a so-called VFT curve
- β-relaxation and other localised modes follow Arrhenius dependence

Spatial (Q) dependence of the relaxation time

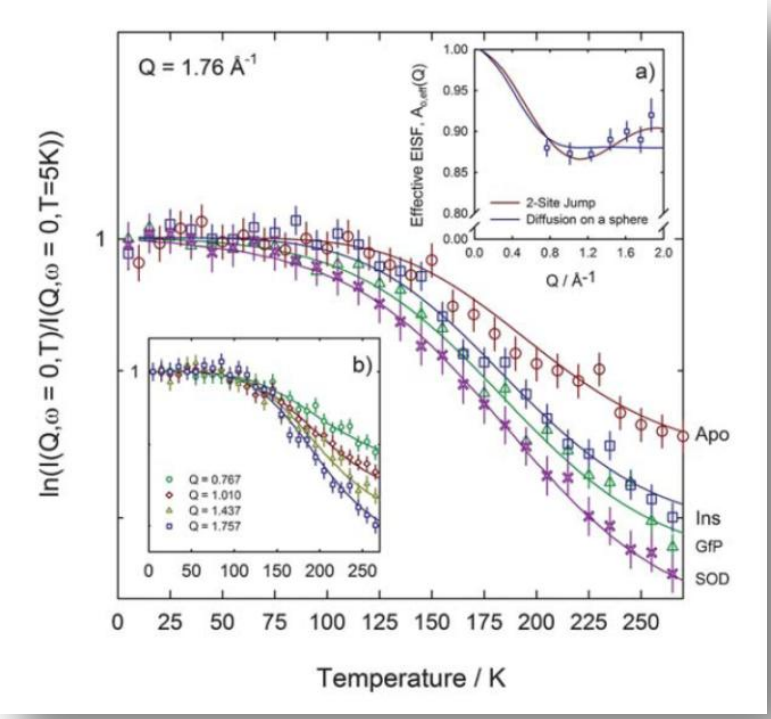
- if $\tau \propto Q^{-2}$ then heterogeneous
- if $\tau \propto Q^{-2/\beta}$ then homogeneous



Dynamics in Soft Matter Systems

$$I(\boldsymbol{Q}, t \approx 0, T) = DWF \times (EISF(Q) + \frac{2}{\pi}\big(1 - EISF(Q)\big)\arctan\left(\frac{\Gamma_{\text{res}}}{\Gamma}\right))$$

where Γ_{res} is the energy resolution of the spectrometer, and Γ is the width if the Lorentzian line characterising the QENS broadening.



In this model we assume that the QENS broadening follows an Arrhenius relationship:

$$\frac{\Gamma}{\Gamma_0} = \exp\left(-\frac{E_a}{kT}\right)$$

For a distribution of Ea's with weighting g_i

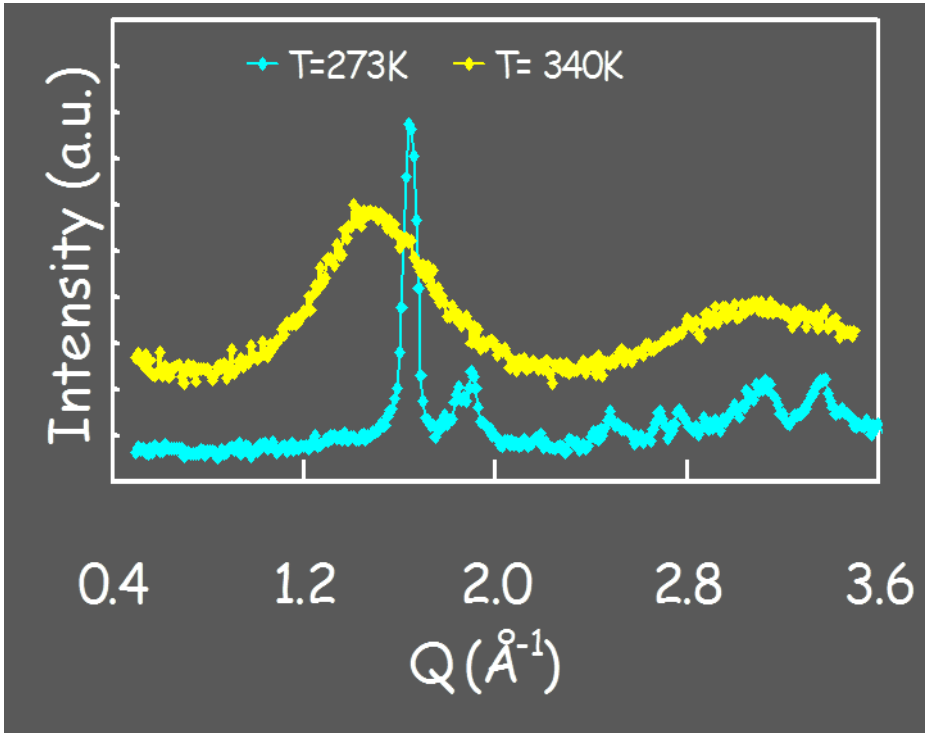
$$\sum g_i \arctan\left(\frac{\Gamma_{\text{res}}}{\Gamma_i}\right)$$

In addition, not all atoms might be mobile and contribute to the fall of elastic intensity:

$$EISF' = p_f + p_m EISF \quad \text{where} \quad p_f + p_m = 1$$

Collective Dynamics (at structure peaks)

Up to now we have only been talking of the self dynamic structure factor and have said nothing about collective modes, the **coherent part of the correlation function**. This is because QENS is mostly used for measurements where the incoherent signal dominates. Also they are trickier to interpret and you need to take into account the **structure factor**, ***S*(*Q*)**, ie. how atoms are distributed in space.



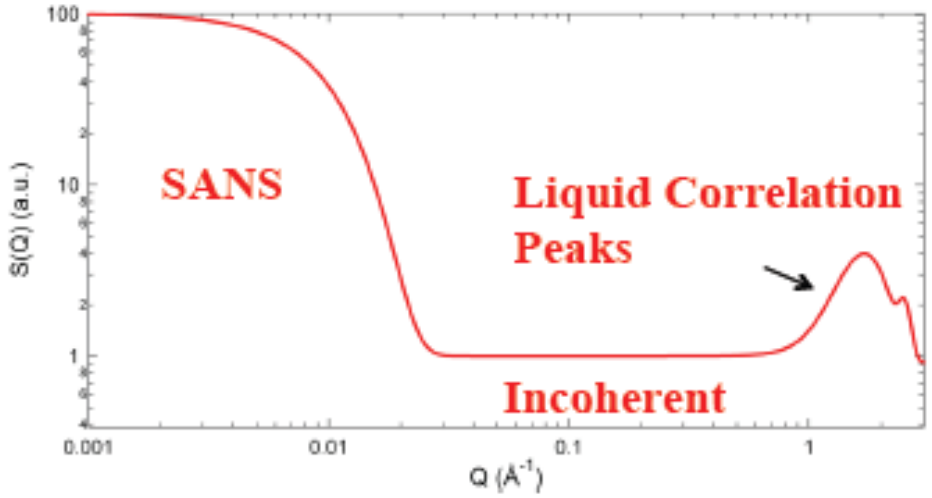
Poly(ethylene oxide) $-(CH_2-CH_2-O)-$

$$I_{\text{coll}}(Q,t) \approx I_{\text{self}}(Q,t)\left(\frac{Q}{\sqrt{S(Q)}},t\right)$$

$$\tau_{\text{coll}}(Q,T) \approx a(T)\tau_{\text{self}}(Q,T)S(Q)^{1/\beta}$$

Neutron Spin-Echo

Although we can measure collective dynamics on any QENS machine, the timescale of motions for soft matter systems are more suited to doing this at a type of neutron spectrometer called **Neutron Spin Echo (NSE**). One advantage is that it gives us the intermediate scattering function, **I(Q,t), directly** and there is no need to FT the data, but the technique is a little trickier!



The best signal in NSE is at the peaks and is very complementary to the SANS structural information.

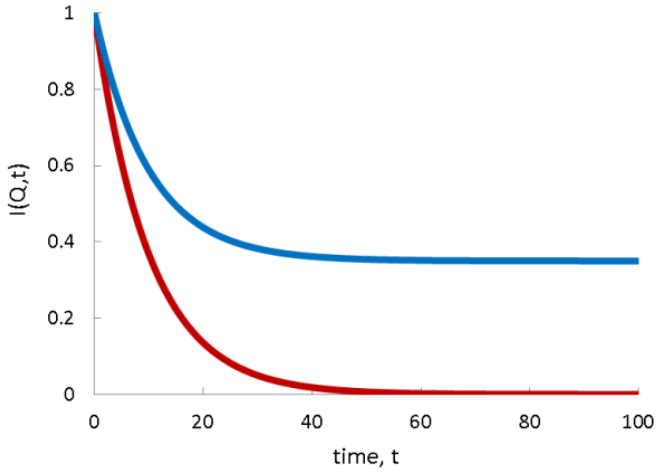
$$I_{\mathrm{NSE}}(Q,t) = \frac{I_{\mathrm{coh}}(Q,t) - \frac{1}{3}I_{\mathrm{inc}}(Q,t)}{I_{\mathrm{coh}}(Q,0) - \frac{1}{3}I_{\mathrm{inc}}(Q,0)}$$

Neutron Spin-Echo

- NSE measures in the time domain – intermediate scattering function
- Primarily use to look at the coherent signal, i.e. collective dynamics
- Incoherent dynamics are possible but still rather slow
- Best NSE in the world is IN15 @ ILL that can measure Fourier times of between 1ps and 1usec

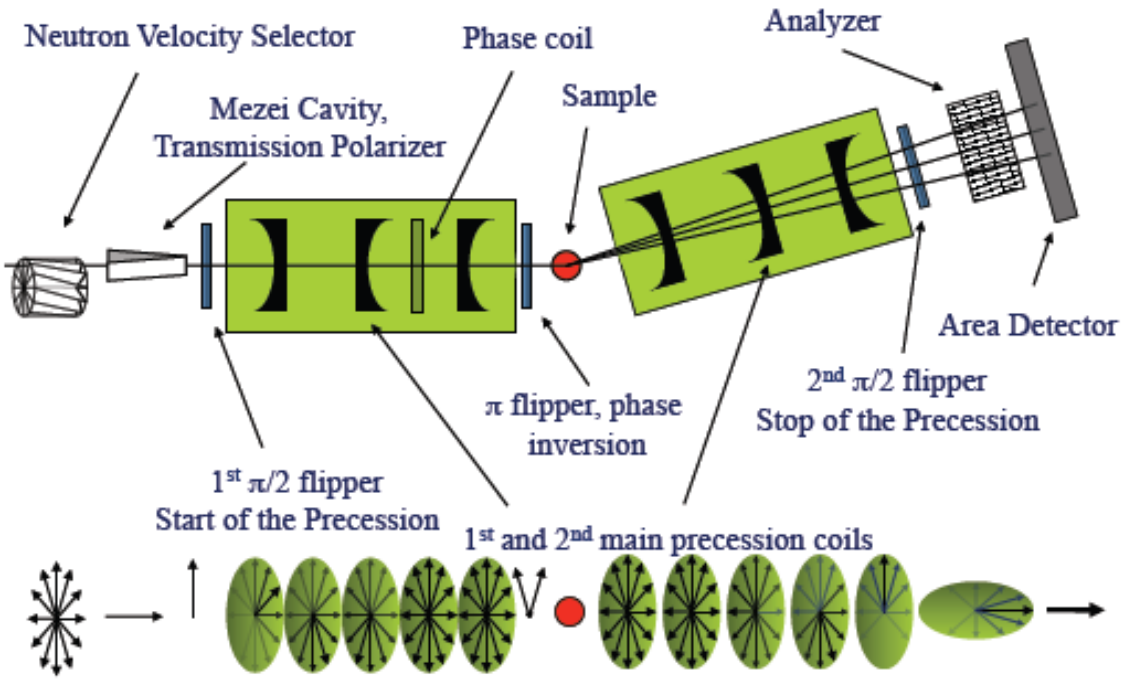
$$S_{\mathrm{inc}}(\boldsymbol{Q},\omega) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} I_{\mathrm{self}}(\boldsymbol{Q},t)\exp(-iwt)\,dt$$

$$S_{\mathrm{coh}}(\boldsymbol{Q},\omega) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} I_{\mathrm{coll}}(\boldsymbol{Q},t)\exp(-iwt)\,dt$$

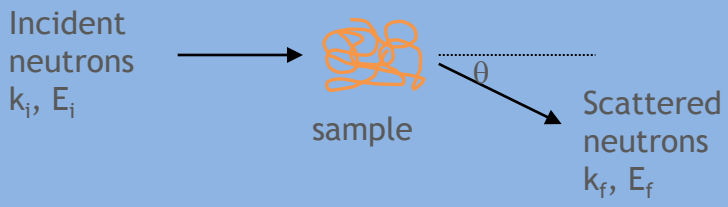


Neutron Spin-Echo

- NSE uses the neutron's **spin polarisation** to encode the difference in energies between incident and scattered beams. Very high energy resolution.
- Neutron perform **Larmor precessions** in two antiparallel magnetic fields, before and after the sample, resulting in polarization of the neutrons.
- Precession angles are equal and opposite and the difference is analysed at the detector. Small energy transfers lead to a change in the precession angle and thus a decrease in measured polarization.



QENS Summary

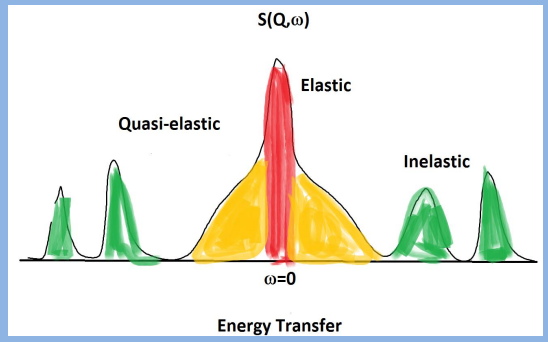


We measure S(Q,ω), the number of scattered neutrons as a function of Q and ω.
What information does S(Q,ω) give us?

Q gives information about structure

ω gives information about dynamics (motion)

- *Elastic*
- *Quasi-elastic*
- *Inelastic*



Elastic Scattering

Structure

$[r_i(0)-r_j(0)]$

-SANS, reflectometry, diffraction
-Coherent scattering
-Contrast due to differences in scattering length densities

Quasi-elastic/Inelastic Scattering

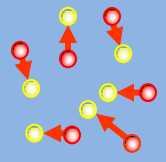
Relative motion

$[r_i(t)-r_j(0)]$

-Neutron spin-echo
-Coherent scattering
-Contrast due to differences in scattering length densities

Self motion

$[r_i(t)-r_i(0)]$



-Backscattering, time-of-flight
-Incoherent scattering
-Contrast provided by large incoherent x-section of H atoms

Further Reading

General QENS books

- M. Bée, “Quasi-elastic Neutron Scattering Principles and Application in Solid State Chemistry, Biology and Materials Science”, Adam Hilger, Bristol (1988)
- R. Hempelmann, “Quasi-elastic neutron scattering and solid state diffusion”, Oxford Series on Neutron Scattering in Condensed Matter 13, Clarendon Press, Oxford (2000)
- T. Springer, “Quasi-elastic neutron scattering for the diffusive motions in solids and liquids”, Springer Tracts in Modern Physics 64, 197, Springer Verlag (1972)
- V. Garcia Sakai and M. T. F. Telling, “A Practical Guide to QENS”, in prep. (tbp 2019)

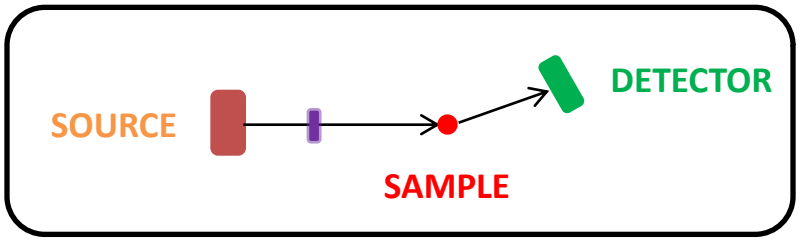
Specific for Soft Matter

- V. Garcia Sakai, C. Alba-Simionesco, S.-H. Chen, “Dynamics in Soft Matter”, Springer (2012)
- V. Garcia Sakai and A. Arbe, “Quasielastic neutron scattering in soft matter”, Current Opinion in Colloid and Interface Science 14, 381-390 (2009)
- J. S. Higgins and H. C. Benoît, “Polymers and Neutron Scattering”, Oxford Science Publications (1994)
- J. Fitter, T. Gutberlet, J. Katsaras (Eds.), “Neutron Scattering in Biology”, Spinger (2006)

Instrumentation

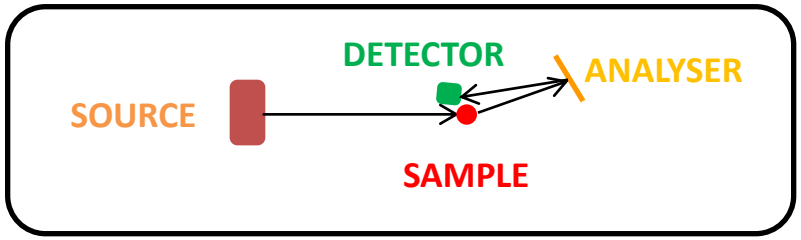
Frequency domain $S(Q,\omega)$

Direct geometry



- Lower energy resolution
- Larger ΔE and Q range
- Flexible in choosing Q-E space
- Repetition Rate Multiplication
- Picosecond
- Self-correlation function (H)
- IN5, LET, CNCS …

Indirect geometry or Backscattering

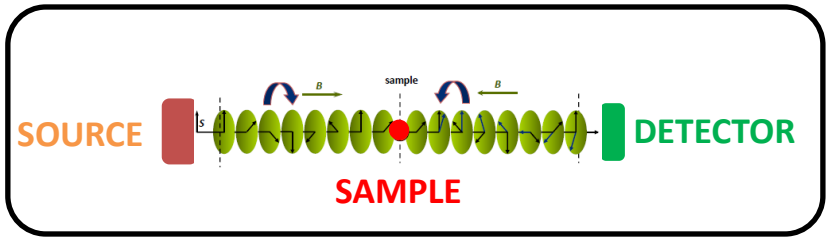


- Higher energy resolution
- Smaller ΔE and Q range
- Fixed Q-E space
- Picosecond-nanosecond
- Self-correlation function (H)
- DNA, IRIS, IN16B, HFBS

Instrumentation

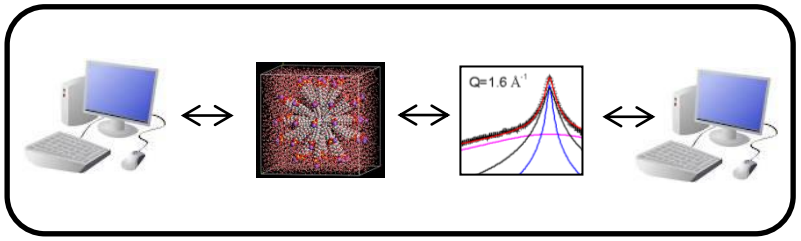
Time domain I(Q,t)

Neutron Spin Echo



- Highest energy resolution
- Typically lower Q range
- Nanosecond
- Collective dynamics (H/D)
- IN15, NIST-NSE

Molecular Dynamics Simulations



- Flexible parameter space
- Large parameter space
- Need to optimize and choose FF
- Directly comparable with neutron data