Theoretical and Experimental Studies of S(α,β) Thermal Scattering Kernel

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Introduction & Objective of the PhD thesis

IRSN is working on the improvement of thermal scattering cross section data of light water at high temperature and pressure (normal operating conditions of nuclear power reactors) for criticality safety studies and reactor physics applications.

What is S(α,β)? Nuclear cross section data libraries use derived thermal neutron scattering represented by S(α,β) scattering kernel where α and β stand for the unit-less momentum and energy transfers respectively.

What do we have? The available S(α,β) of light water in the evaluated nuclear data libraries are based on experimental data measured in the sixties with a low accuracy due to the limitations of the experimental and computational capabilities at that time.

What do we want? Study the structure and dynamics of light water incorporating both theory (molecular dynamics simulations) and perform new experiments to enhance the reliability of S(α,β) and estimate the associated systematic and statistical uncertainties.

Theoretical Modelling of S(α,β)

The double differential thermal scattering cross section for neutrons with incident energ E_i, secondary energy E_f, scattering angle Ω, bound scattering cross section σ_b and at temperature T can be written as:

$$\frac{\partial^2\sigma_T}{\partial\Omega\partial E_f}(E_i \rightarrow E_f,\Omega) = \frac{\sigma_b}{4\pi k_B T}\sqrt{\frac{E_f}{E_i}}\, e^{-\frac{\beta}{2}} S(\alpha,\beta)$$

Momentum transfer $\alpha = \frac{E_f + E_i - 2\sqrt{E_f E_i}\cos\theta}{A k_B T} = \frac{q^2\hbar^2}{2 M k_B T};\quad \vec{q} = \vec{k_f} - \vec{k_i}$

Energy transfer $\beta = \frac{E_f - E_i}{k_B T} = \frac{-\hbar\omega}{k_B T};\quad \hbar\omega = E_f - E_i$

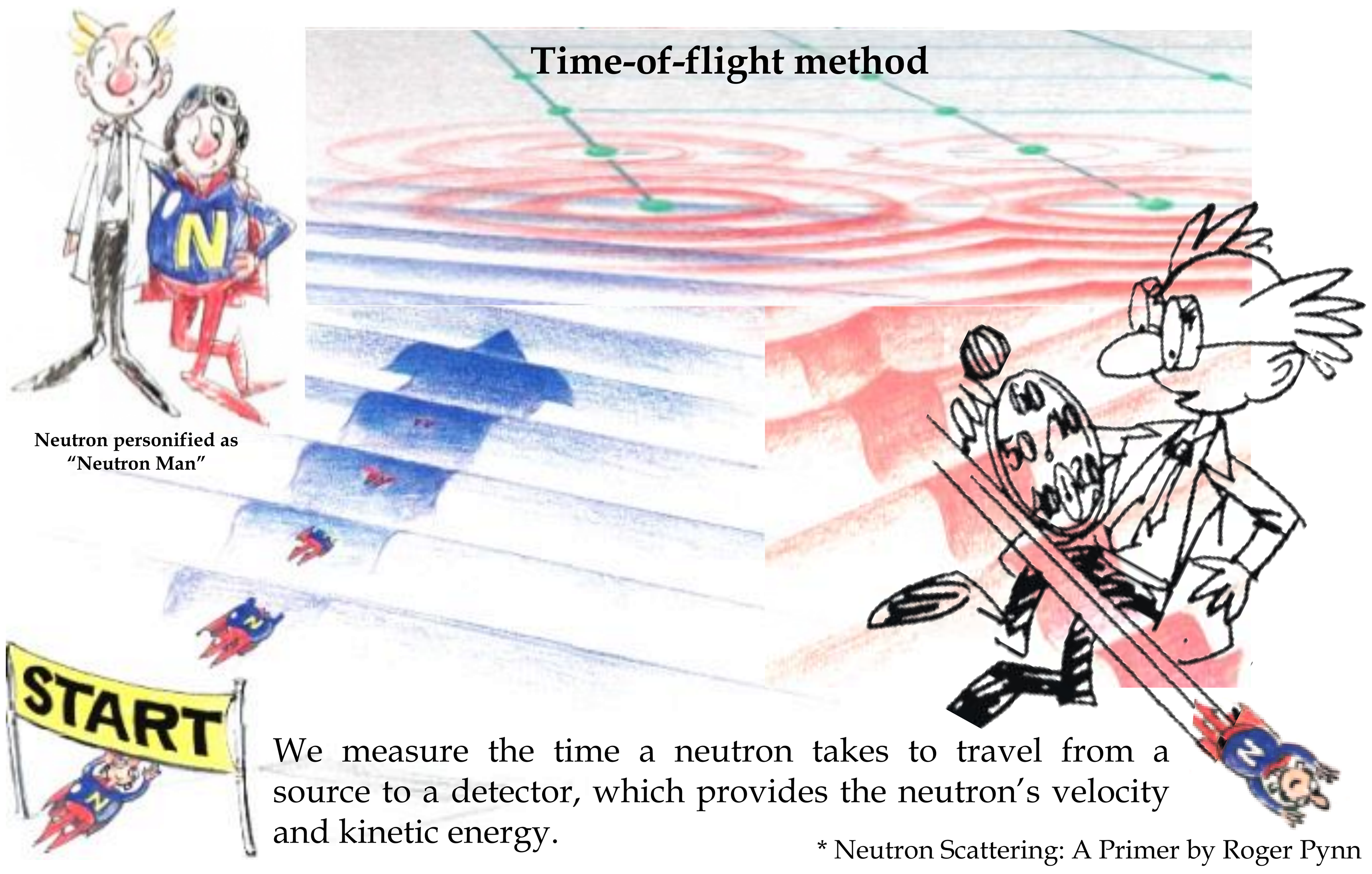
S(α, β) | **$S(\vec{q},\omega)$**

S(α, β) is analogous to the scattering function **$S(\vec{q},\omega)$** where $\vec{q}$ and **ω** stand for the neutron wave vector and energy transfers respectively. **$S(\vec{q},\omega)$** can be measured by performing time-of-flight inelastic neutron scattering experiments with light water, at desired temperature and pressure.

Experiments

IN4c experimental facility

Two consecutive inelastic thermal neutron scattering experiments with light water at high temperature and pressure have been carried out at the Institut Laue-Langevin (ILL, Grenoble) in December 2015, using the **IN4c** and **IN6** time-of-flight spectrometers.



* Neutron Scattering: A Primer by Roger Pynn

IN6 experimental facility

Experimental conditions with IN4c
Wavelength= 2.4 Å; E_i= 14.20 meV

Temperature (Kelvin)	Pressure (bar)
300	1
300	88-100
350	115
392-466	128-165
479-485	172-180
490-497	185
517	42

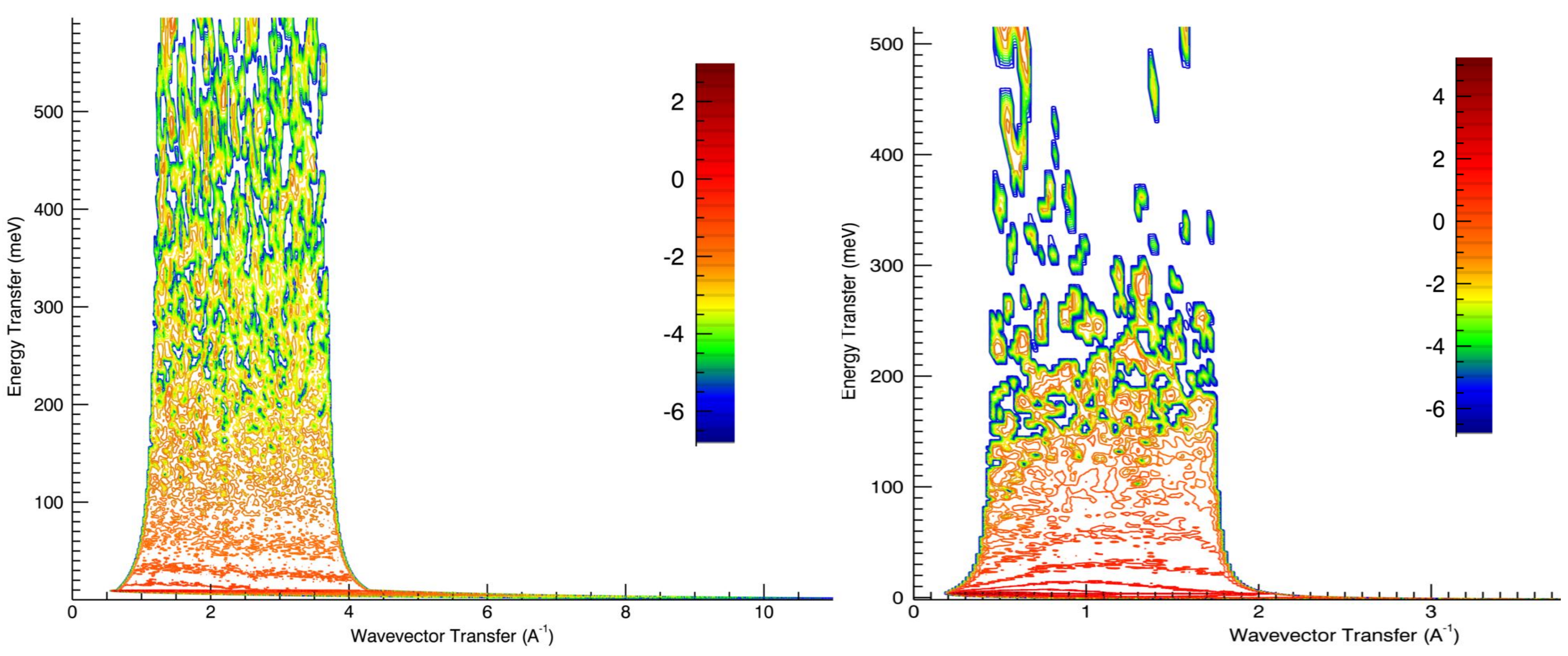
Experimental conditions with IN6
Wavelength= 5.1Å; E_i= 3.14 meV

Temperature (Kelvin)	Pressure (bar)
350	1
494	70
494	340-600

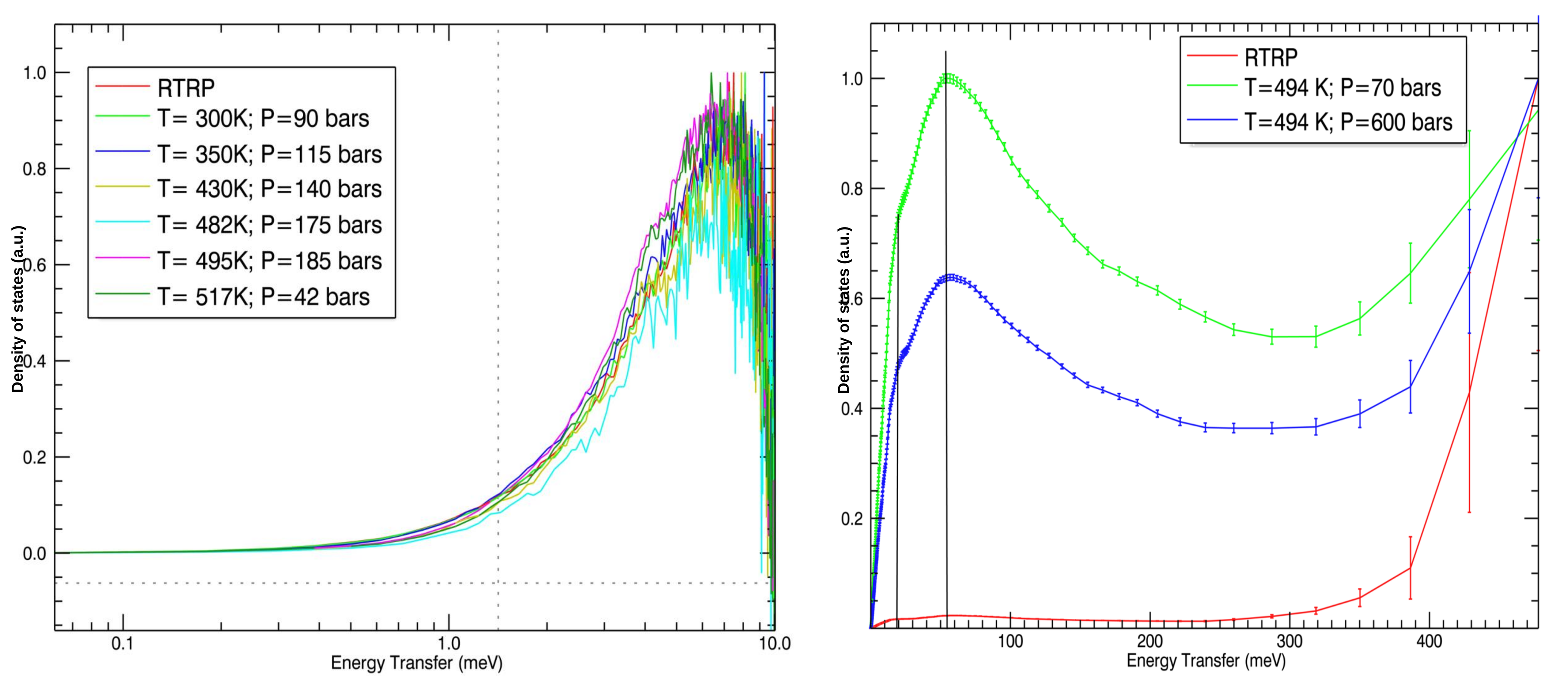
The experimental run may be over but the experiment is not; Raw time-of-flight data, uncorrected and unprocessed, are useless !!

Data Analysis & Preliminary Results

A detailed data reduction of the raw time-of-flight experimental data is done using data analysis tools (LAMP, iFit) to obtain **$S(\vec{q},\omega)$** and **g(ω).**



Symmetrized dynamic structure factor $S_{sym}(\vec{q},\omega)$ of light water measured from IN4c (left) and IN6 (right)



g(ω) (gDOS-Generalized density of states) of light water measured from IN4c (left) and IN6 (right)

Methodology & Future work:

EXPERIMENTS → $S(\vec{q},\omega) = \exp\left(\frac{\hbar\omega}{2k_B T}\right) S_{sym}(\vec{q},\omega)$

→ $S(\alpha,\beta) = k_B T\, S_{sym}(\vec{q},\omega)$ + MOL. DYNAMICS → S(α, β) → COMPARE

→ $g(\omega) \simeq \lim_{q\to 0} \frac{\omega^2}{q^2} S_{sym}(\vec{q},\omega)$ → LEAPR (NJOY) → S(α, β) → COMPARE

MOL. DYNAMICS → g(ω) → LEAPR (NJOY)