

DE LA RECHERCHE À L'INDUSTRIE



NAUSICAA COLLABORATION: FROM EXPERIMENTS TO NUCLEAR APPLICATIONS

Contribution SPRC/LEPH, CEA Cadarache

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<https://www.ill.eu/instruments-support/computing-for-science/data-analysis/nausicaa/>

Nausicaa

Nausicaa collaboration



The NAUSICAA (**N**eutron **AU**gmented **Sa** β **I**n **C**ross sections **A**lternative **A**ssessment) project is a collaborative research study including the ILL, the IRSN, the CEA, the TUM, the ESS, the University of Florence and the Ecole Polytechnique de Montréal. This project started mid-2014, and aims at improving the accuracy of the international neutron cross section libraries for reactor physics by introducing direct measurements. The most direct consequence of this project will be the tremendous improvement heavy water reactors and cold sources modelling. This project is organized under the auspices of the OECD/NEA, which will bring us a strong support, and in collaboration with the IAEA.

One caveat of the neutron cross section libraries is indeed the evaluation process of thermal neutron cross sections in liquids, especially in hydrogenated liquids in which inaccurate approximations are employed. This problem could be solved by the direct use of measured structure factors $S(Q, \omega)$, where Q is the neutron momentum transfer and ω is the neutron energy transfer. Until now all evaluations related to thermal neutron were based upon experiments performed with a momentum transfer $Q=0$, like IR or Raman. The extension on the whole Q domain is carried out by approximate laws which become clearly wrong in the case of liquids like water. This means that measurements of a real $S(Q, \omega)$ enable to get rid of the extension laws approximations and thus to significantly enhance the accuracy of the cross sections.

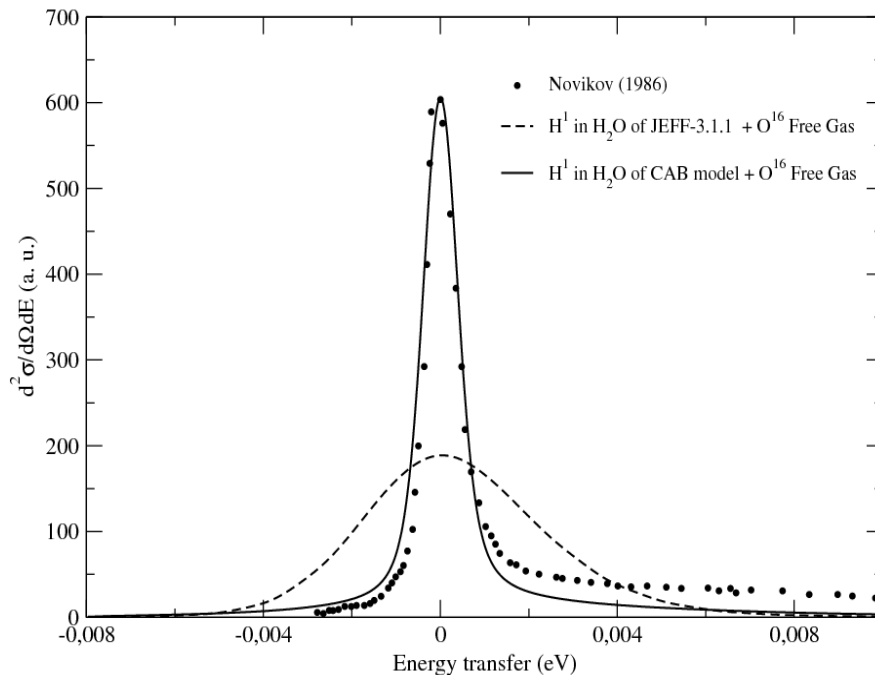
The first step of the study is now completed. A paper has been submitted for light and heavy water and a detailed report has been published in the framework of the CRISP project. We have demonstrated the feasibility and the reliability of this method. Two additional steps are foreseen in the next future and will be carried out in parallel. One is the acquisition and refinement of accurate data on light and heavy water in several conditions of temperature and pressure, from ambient to supercritical conditions. The other is the study of cryogenic liquids like liquid hydrogen and deuterium, which will require several years to carry out the measurements in the best conditions.



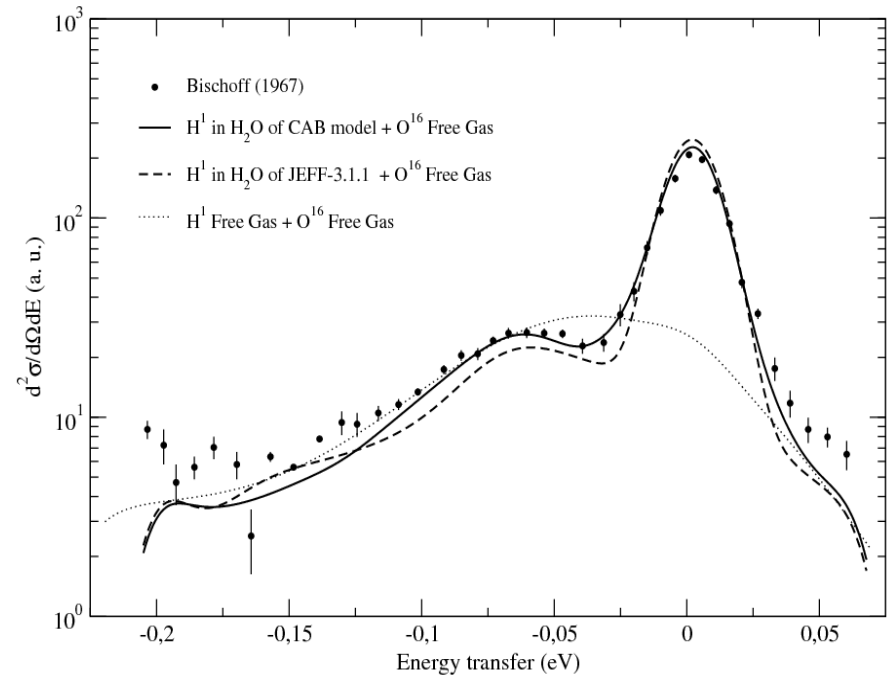
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Next meeting ILL, Grenoble $\Rightarrow$ 3-4 July 2016

Why new experiments are needed ?



Double differential scattering cross section for light water calculated with CAB model and JEFF-3.1.1 compared with data measured by Novikov (1986), for **$E_0 = 8$ meV**, $\theta = 37^\circ$ and $T = 293.6$ K



Double differential scattering cross section for light water calculated with CAB model and JEFF-3.1.1 compared with data measured by Bischoff (1967), for **$E_0 = 231$ meV**, $\theta = 25^\circ$ and $T = 293.6$ K

⇒ It is quite difficult to use « old » data of double differential cross sections to precisely validate new TSL

2010

⇒ Light and heavy water in IN5 and IN4 at ILL **in cold operating conditions**

- H₂O: 285 K, 290 K, 294 K, 300 K, 302 K, 311 K, 323 K (P = 1 bar)
- D₂O: 250 K (ice), 295 K, 296 K, 325 K

2015

⇒ Light and heavy water in IN6 and IN4 at ILL **in hot operating conditions**

- T = 300 - 540 K and P = 1 - 600 bar

2016

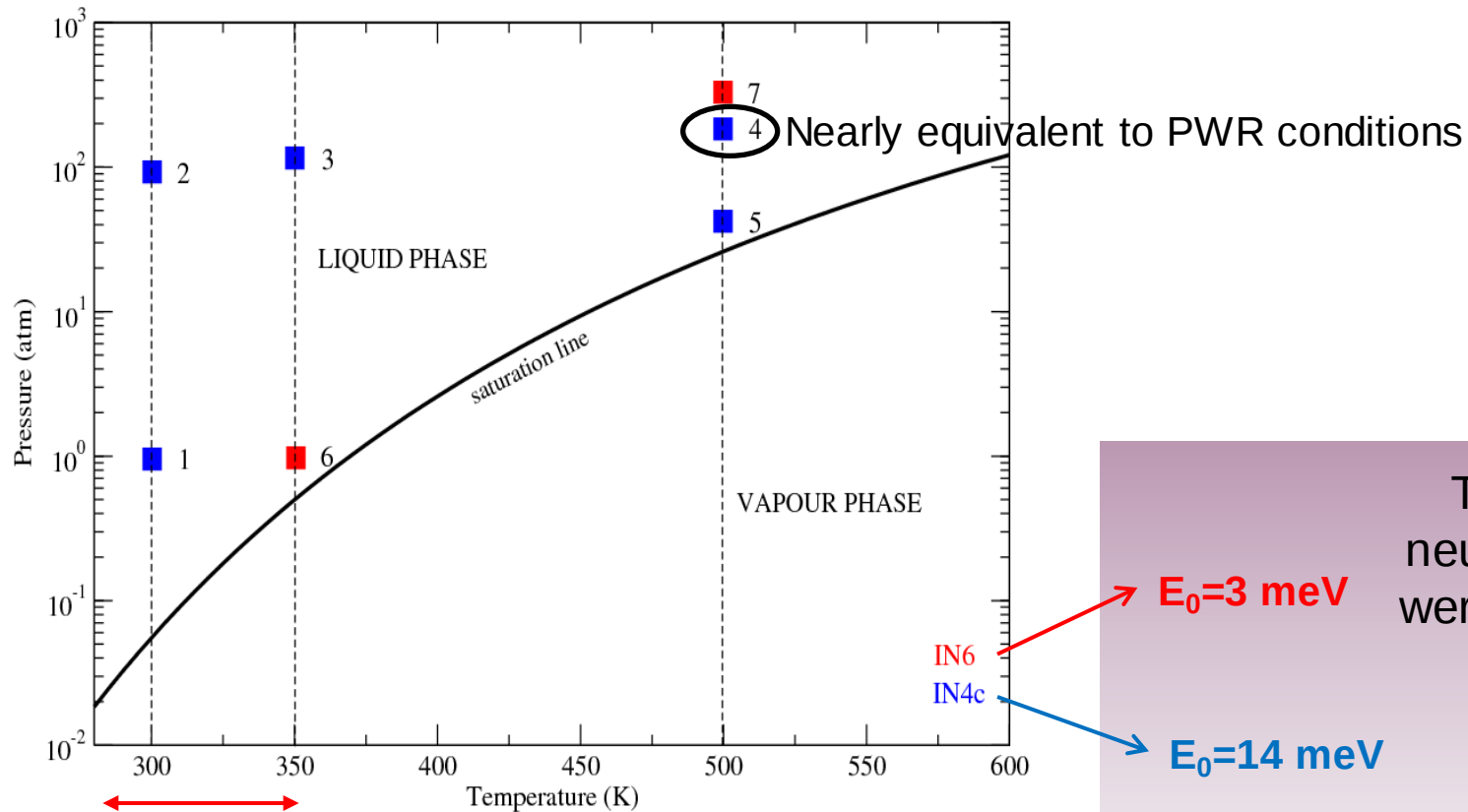
⇒ Measurement of the double-differential neutron cross section of U in UO₂ in IN6 and IN4 **from room temperature to Hot Full Power conditions**

- T = 294 K, 600 K et 900 K

2018

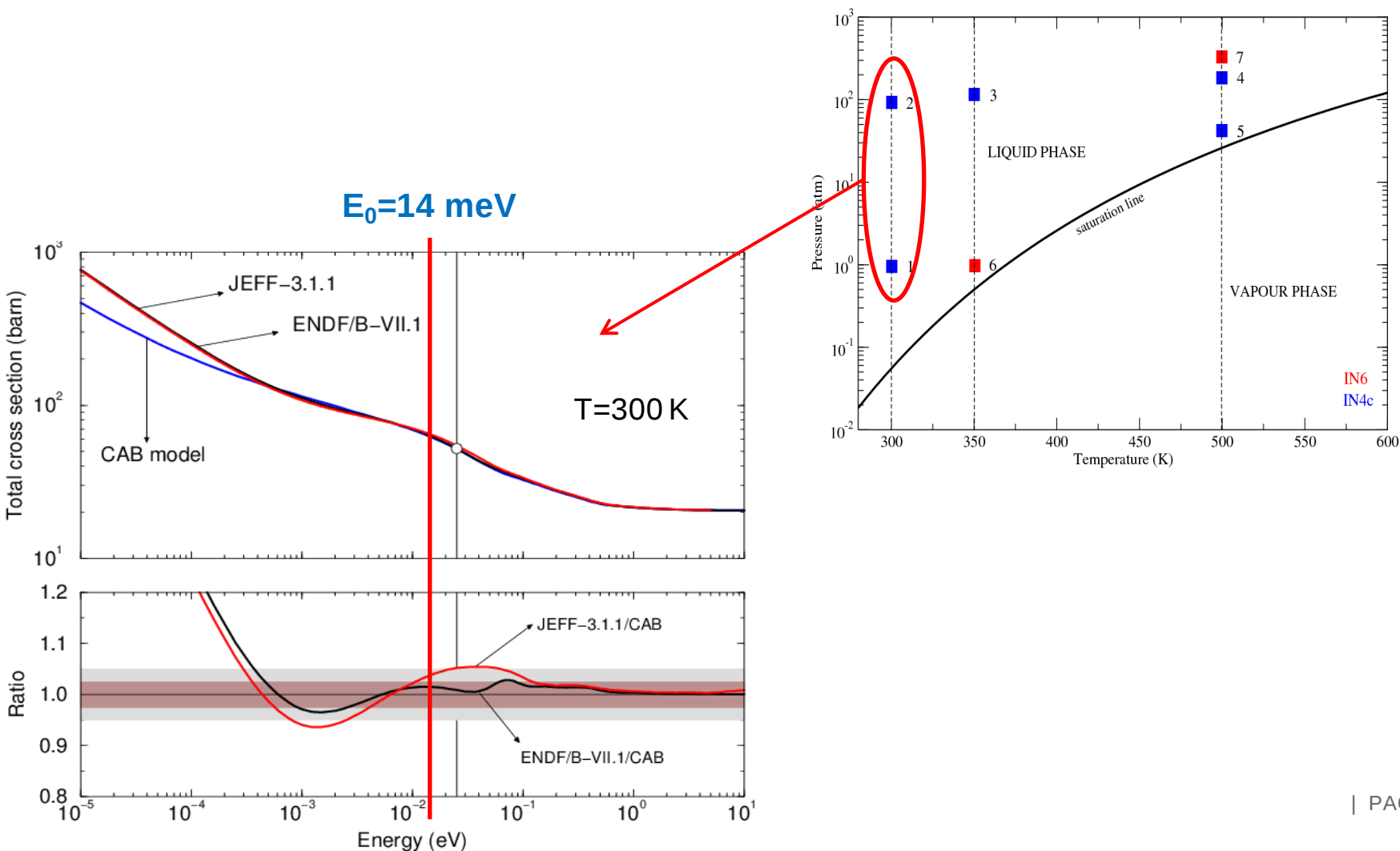
⇒ Measurement of the double-differential neutron cross section of U in UO₂ up to 2000 K

Experimental (P,T) conditions investigated at ILL for light water

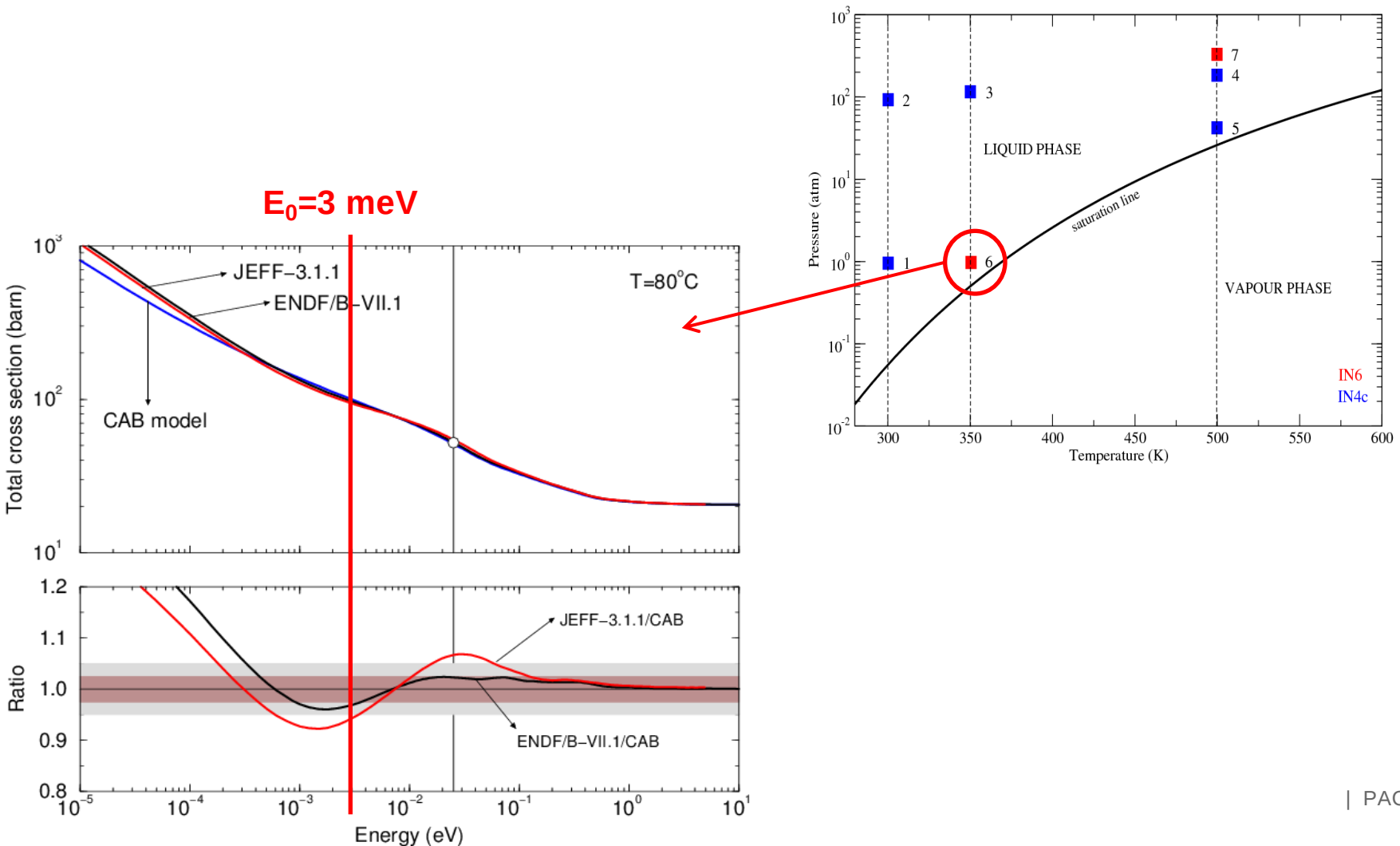


Experimental program 2015 (H₂O)

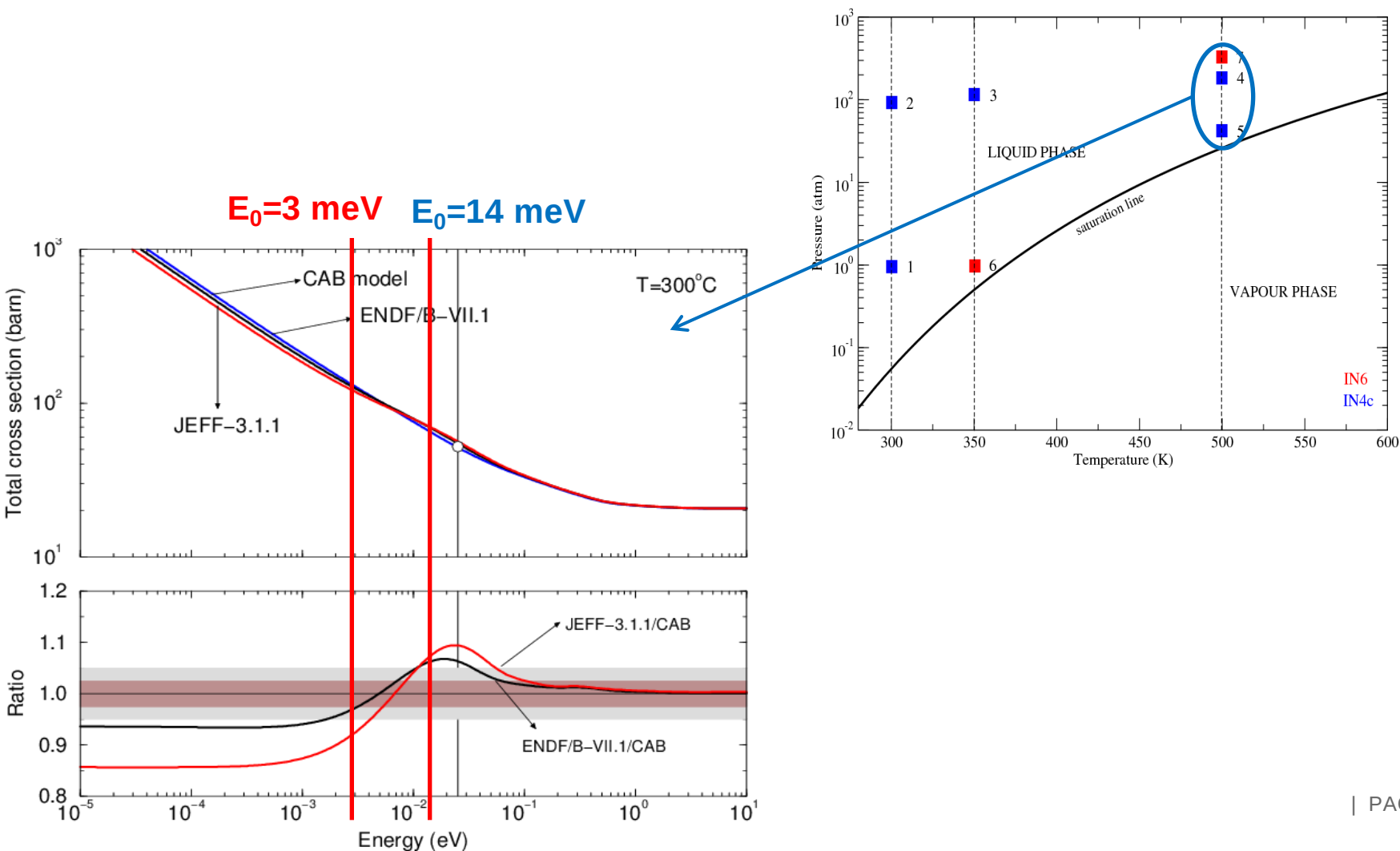
Experimental (P,T) conditions investigated at ILL for light water



Experimental (P,T) conditions investigated at ILL for light water



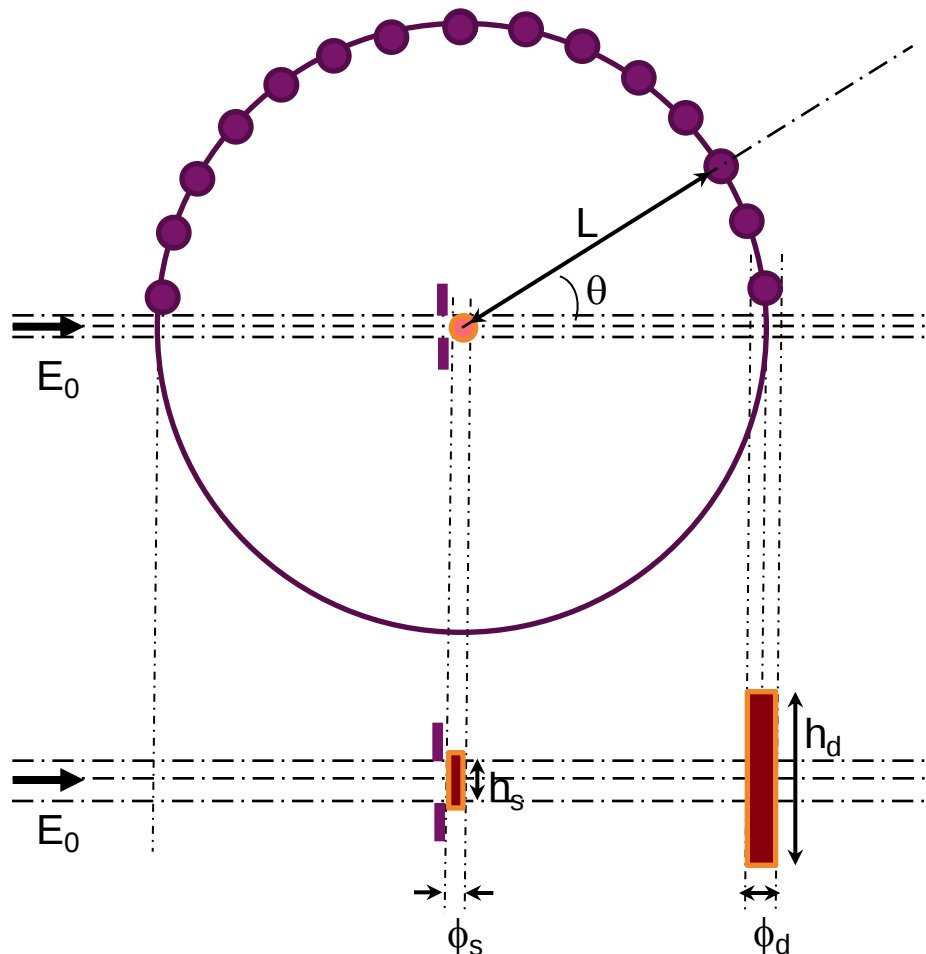
Experimental (P,T) conditions investigated at ILL for light water



Double differential cross section at $T=294$ K

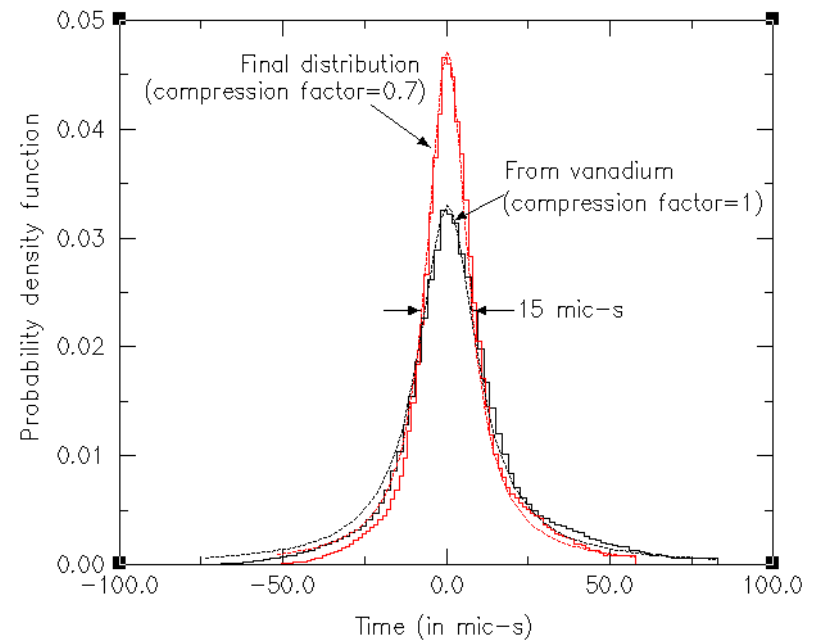
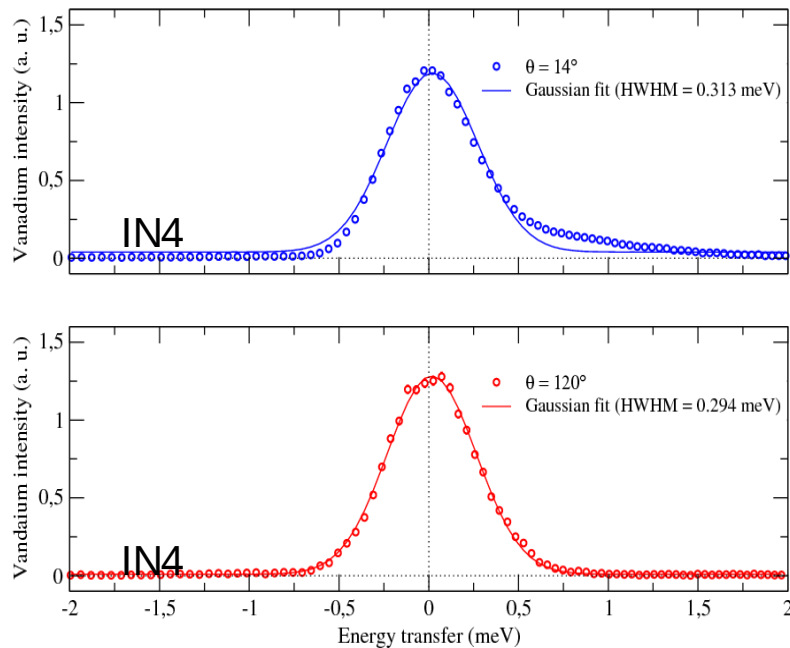
A simplified TRIPOLI4 model (IN4 and IN6) was used for a precise data/theory comparison

- This simplified model can be shared with the community for further tests
- An equivalent MCNP model is in preparation at IRSN



Double differential cross section at T=294 K

The time resolution of the spectrometer is taken into account via the Vanadium peak

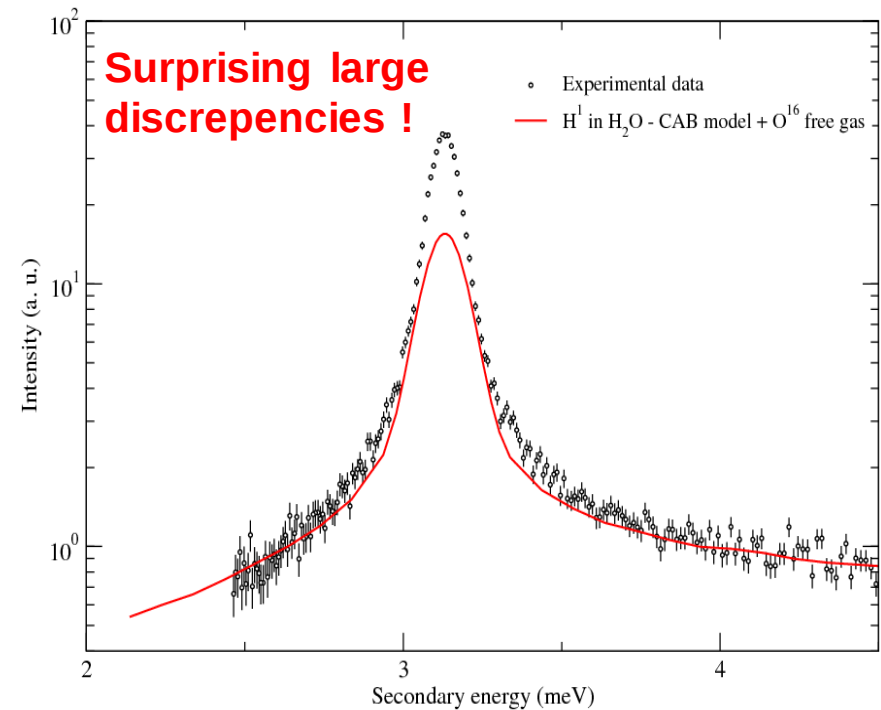
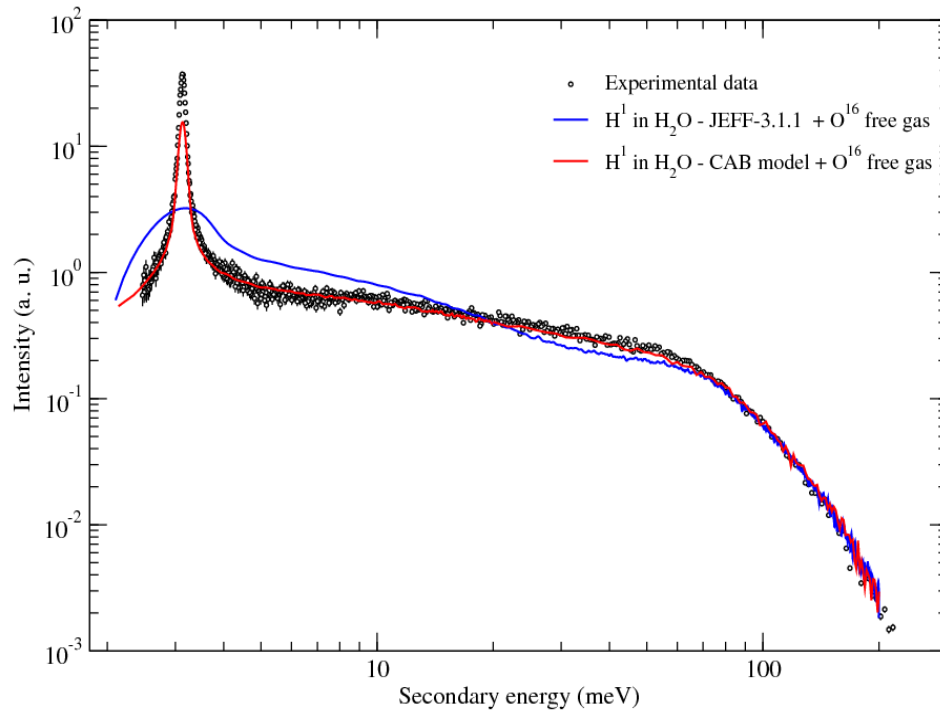


Experimental Vanadium peak $\Rightarrow$ converted in pdf

Double differential cross section at T=294 K

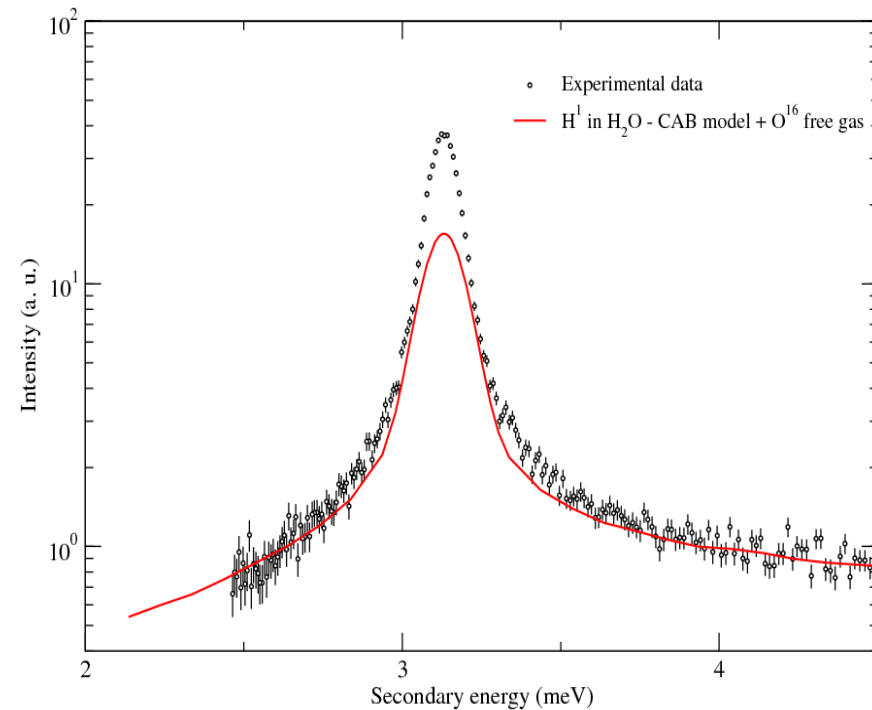
Comparison with TRIPOLI4 results: IN6 data, 3 meV, $\theta = 15^\circ$

The diffusion model of Egelstaff and Schofiel improved the description of the elastic peak (compared to the free gas diffusion model in JEFF-3.1.1)



Double differential cross section at $T=294\text{ K}$

Comparison with TRIPOLI4 results: IN6 data, 3 meV, $\theta = 15^\circ$

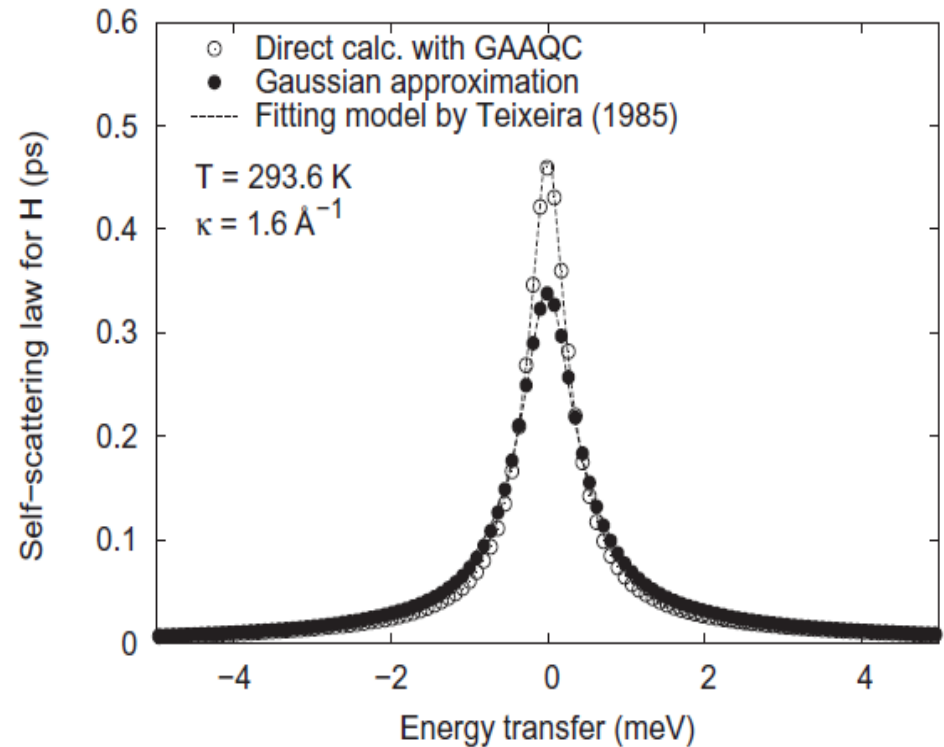
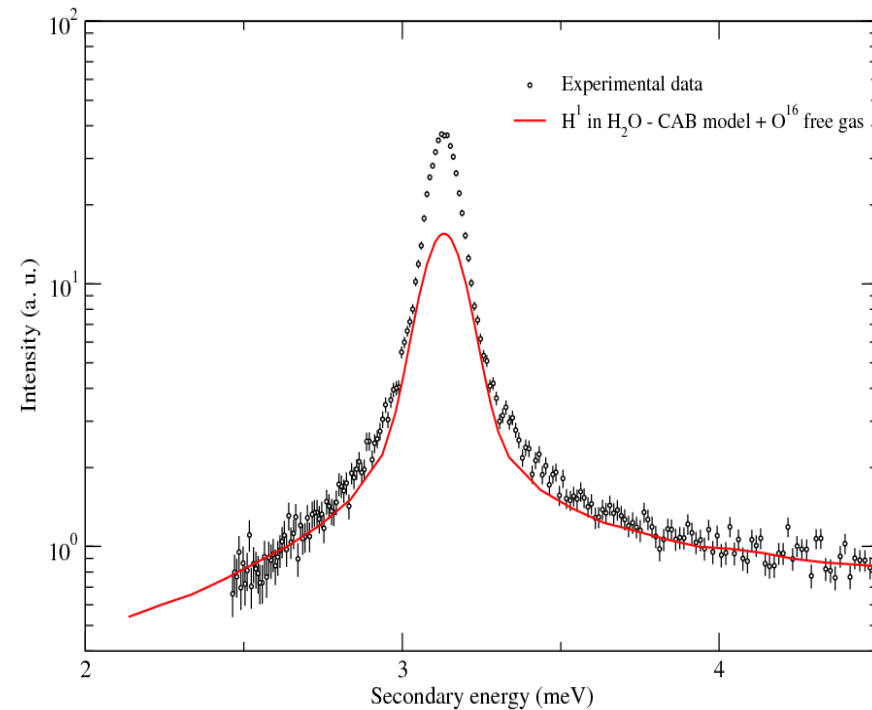


Origin of the discrepancies ?

- Processing of CAB files for TRIPOLI4
- Simplified TRIPOLI4 model
- Diffusion model (Egelstaff and Schofield)
- Background subtraction
-

Double differential cross section at T=294 K

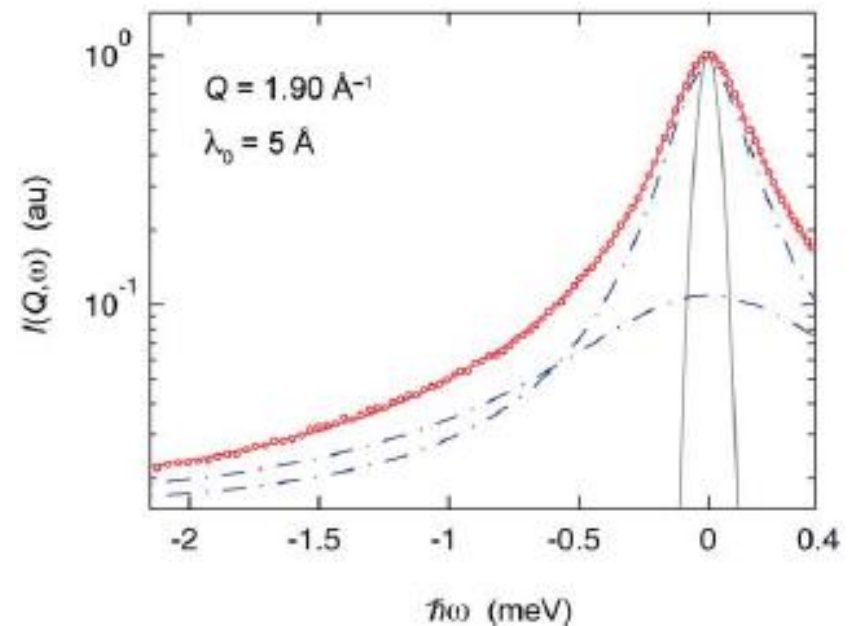
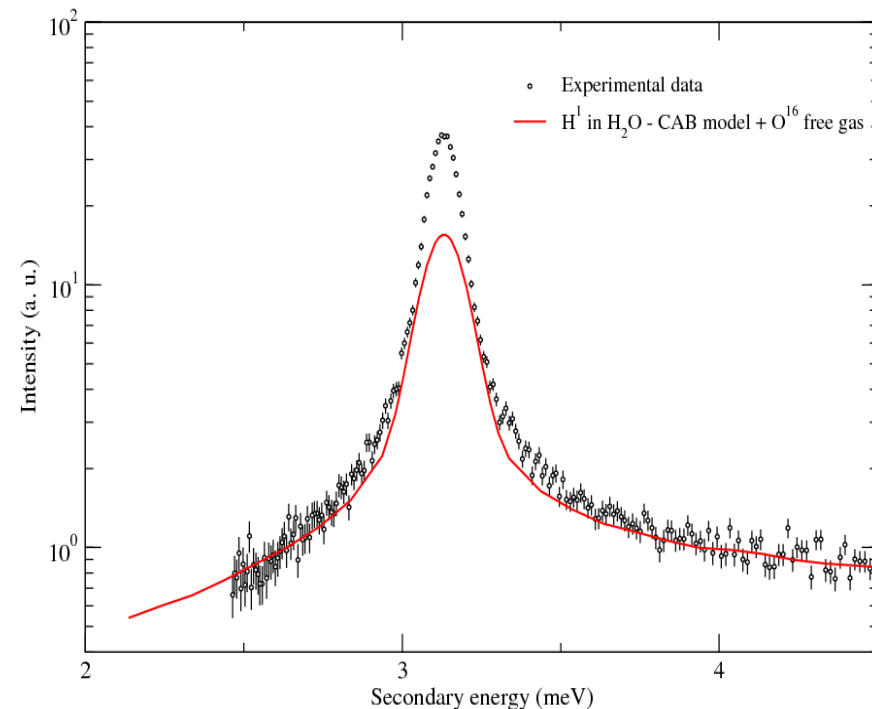
Abe and Tasaki (2015) $\Rightarrow$ Jump-diffusive behavior of the molecular translational motion



The differences seems to be too large $\Rightarrow$ cannot be explained by the Gaussian Approximation-Assisted Quantum Correction (GAAQC) $\Rightarrow$ could support a problem of background substraction

Double differential cross section at T=294 K

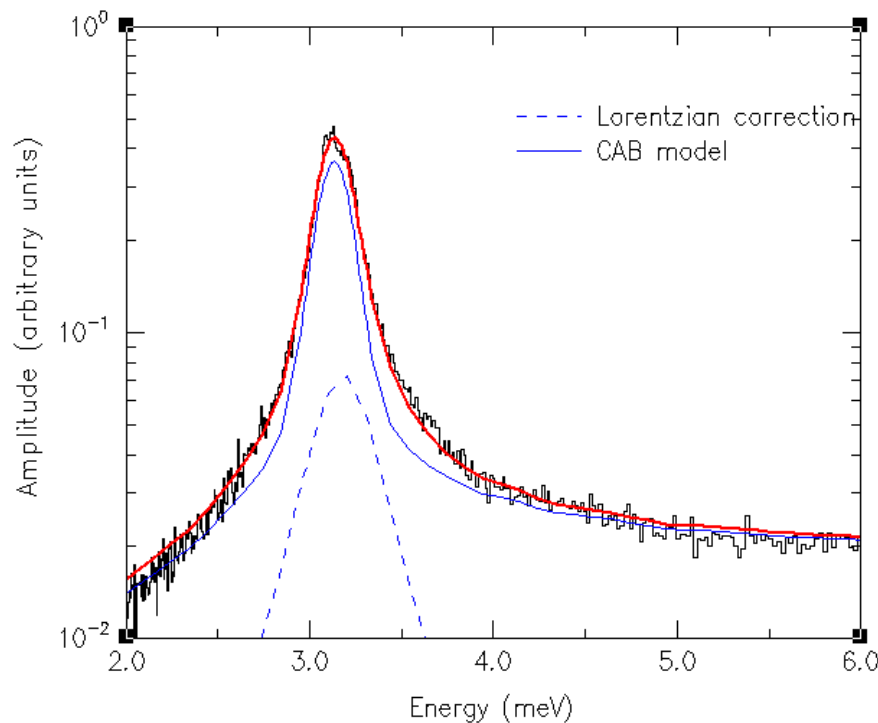
Qvist et al. (2011) $\Rightarrow$ IN5 data could be rather well described by a model that attributes the observed proton dynamics to two independent molecular motions: **continuous rotational diffusion superimposed on jumplike translation**



The large differences could be explained with this phenomenological model, often adopted for the analysis of water and aqueous solutions

Double differential cross section at T=294 K

Qvist et al. (2011) $\Rightarrow$ IN5 data could be rather well described by a model that attributes the observed proton dynamics to two independent molecular motions: **continuous rotational diffusion superimposed on jumplike translation**



Interest of such a « descriptive » model

Addition of a had-hoc Lorentzian correction to reproduce the data $\Rightarrow$ makes possible the extraction of **experimental $S(\alpha\beta)$** corrected from multiple-scattering and resolution broadening

Presentations of the NAUSICAA activities during the WPEC/SG-42 meeting (collaboration ILL/IRSN/CEA Cadarache)

- **Vaibhav JAISWAL**, “Thermal scattering law for light water at high temperature and pressure”
- **Juan Pablo SCOTTA**, “Covariance matrices of the neutron thermal scattering law of light water for reactor applications”
- **Gilles NOGUERE**, “Status of the UO₂ measurements at ILL from room to 900 K”