NAUSICAA : Improved neutron cross sections for reactor physics

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Issues on thermal cross sections

Cross sections libraries use special data for thermal neutrons

Called $S(\alpha,\beta)$ (analogous to $S_{q\omega}$)

Experimental data are old and have a low accuracy

Reliability is low for hydrogenous liquids

Significant impact on hydrogen-based neutron cold sources

Strong effect on cold neutron production modelling

Possible impact on $k_{eff}$ for nuclear facilities (mainly those using heavy water)
The idea

Measurement of $S(q,\omega)$ could lead to a new evaluation of the $S(\alpha,\beta)$ with an improved accuracy!

We propose a new way to evaluate thermal neutron cross sections

Direct input of measurements into THERMR

Basis: neutron scattering laws

$\omega = $ energy transfer

$q = $ wave-vector transfer
The idea

Neutron inelastic scattering experiments are carried out every day at the ILL.

Measurement of structure factor $S(q, \omega)$ for liquids is possible

$$S(Q, \omega) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} dt \ e^{-i\omega t} \frac{1}{N} \sum_{\alpha, \beta=1}^{N} \left< e^{-iQ \cdot R_{\alpha}(0)} e^{iQ \cdot R_{\beta}(t)} \right>$$

Double Differential Cross Section is directly linked to $S(q, \omega)$

$$\frac{d^2\sigma}{d\Omega d\omega} = \frac{k_1}{k_0} \tilde{S}(Q, \omega)$$
The idea

\[ \frac{d^2 \sigma_T}{d\Omega dE'} (E \rightarrow E', \mu) = \frac{\sigma_b}{4\pi kT} \sqrt{\frac{E'}{E}} e^{-\beta/2} S(\alpha, \beta) \]

\[ \frac{d^2 \sigma_T}{d\Omega dE'} (E \rightarrow E', \mu) = \frac{\sigma_b}{4\pi} \sqrt{\frac{E'}{E}} S_{\text{exp}}(q, \omega) \]

\[ \beta = \frac{E' - E}{kT} \]

\[ \alpha = \frac{E + E' - 2\mu \sqrt{EE'}}{AkT} \]

\[ S(\alpha, \beta) = kT e^{\beta/2} S_{\text{exp}}(q, \omega) \]
Project

Project objective: getting reliable $S(\alpha,\beta)$

Project main steps

- Measurement of $S(q,\omega)$ for model systems (heavy and light water)
- Measurement of $S(q,\omega)$ for cryogenic liquids – CRISP project
- Transformation in .ace format for MCNP (thanks to NJOY code)
- Collaboration between the ILL and IRSN and University of Florence
Data processing

Get $S(\alpha,\beta)$ from experimental $S(q,\omega)$ and normalize them against experimental cross sections values.

Measurements on IN5 and IN4C (ILL instruments)
Data processing

Measured \((q, \omega)\) domain limits incident energy to be \(< 50\) meV

We have completed \(S(\alpha, \beta)\) on a larger domain using Molecular Dynamics simulation.

Normalization: EXFOR for thermal neutrons
Data processing

These completed $S(\alpha, \beta)$ corresponds to the whole water molecule, we transform them into $S(\alpha, \beta)$ for a single H or D by removing oxygen $S(\alpha, \beta)$ and dividing by 2.

Then an ENDF file is created with this data and used as an input in NJOY – THERMR.

NJOY – ACER gives us an ACE file.
Process

We change the usual way to get nuclear data

We go directly through THERMR
Light and heavy water

Measurement of $S(q,\omega)$ for heavy water and light water

Experiment carried out in 2012 on IN4C and IN5 instruments at the ILL

Molecular dynamics until 500 meV
D2O cross section

Excellent result

BUT: issue above 200meV

A steep decrease without any physical meaning
H2O cross section

Same case for H2O
Benchmark on RHF

Data were tested with success on the RHF MCNP model

Initial data
Bias : + 350pcm

ILL data
Much better spreading
Cryogenic liquids

Double Differential Cross Section data on liquid $H_2$ are unexpectedly few and partly unreliable.

Total cross section data on liquid $H_2$ need verification.

Calculations can substitute experiments (avoiding difficult measurements on para-$H_2$ for example).

Our calculations based on:
- Ideal gas (Young & Koppel)
- Simul+GA
- Egelstaff-Stofield

$T = 16$ K
expt. Celli et al., 1999
Cryogenic liquids

Few data available

When available: treatment is not clear or reliable
Cryogenic liquids

Situation with ortho-D$_2$ is even worse!

No data available for ortho-D$_2$

Data seem available for normal D$_2$ but in a very limited range

For both D$_2$ and H$_2$: measurements and calculations are highly needed, especially at small q values (for all energies)
Conclusion of CRISP project

Measurement and implementation into MCNP was possible

Benchmark with first results was a success

Liquid hydrogen and deuterium: begun

UNEXPECTED: available data have a poor quality. Further measurements must be carried out
Feasibility has been demonstrated, but a lot of work is still needed.

Proposal: NAUSICAA

Neutron Augmented Saa Cross sections

Alternative Assessment
NAUSICAA

Two main topics

Heavy / light water and data treatment optimization
  Experiments in several conditions of T & P
  MD simulations

Cryogenic Liquids (Hydrogen and Deuterium and...)
  Experiments (need high level of expertise)
  Quantum simulations (challenging)
NAUSICAA

Solution: pool resources

Rely upon PhD students

Need of an international collaboration

We remain open

I’m inviting you to attend to a meeting at the ILL on July 1\textsuperscript{st} and 2\textsuperscript{nd}
Thank you for your attention