Measurement and evaluation of the neutron scattering cross section for moderator materials in accelerator-based neutron sources

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Introduction

In the development of moderators at neutron sources, the estimation of performance by neutronics calculations using Monte Carlo simulations is important.

Low energy neutron transport calculation

Cross section library
- ✓ Neutron library
- ✓ Thermal neutron scattering law (TSL) library

↓

Monte Carlo simulation code
(PHITS etc.)

→

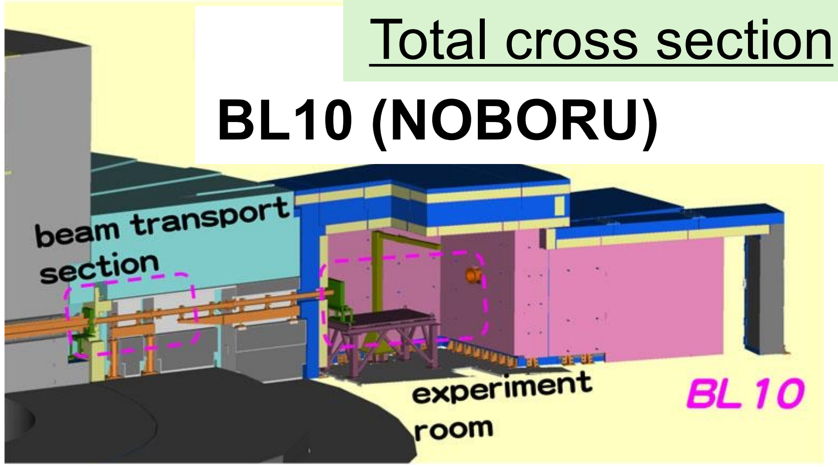
Neutronics evaluation
- ✓ Flux
- ✓ Pulse characteristics

To accurately estimate neutronics of low energy neutrons, TSL data for moderator and reflector materials are important.

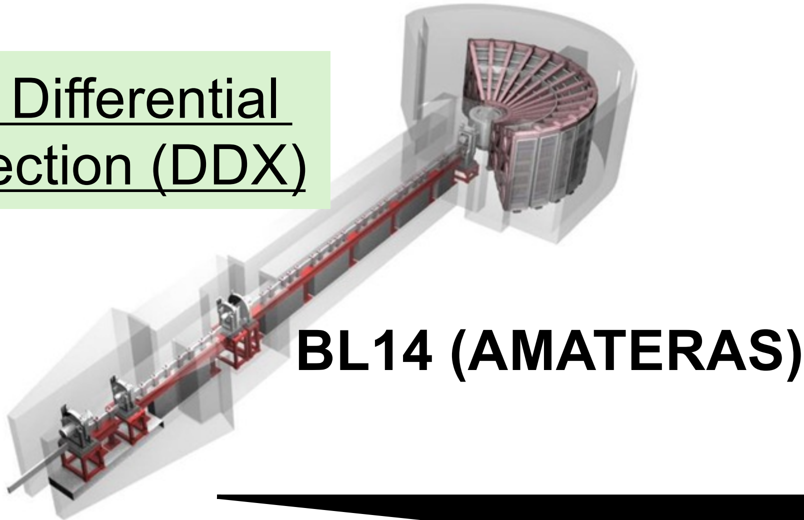
Introduction

Experiment at MLF J-PARC

Total cross section

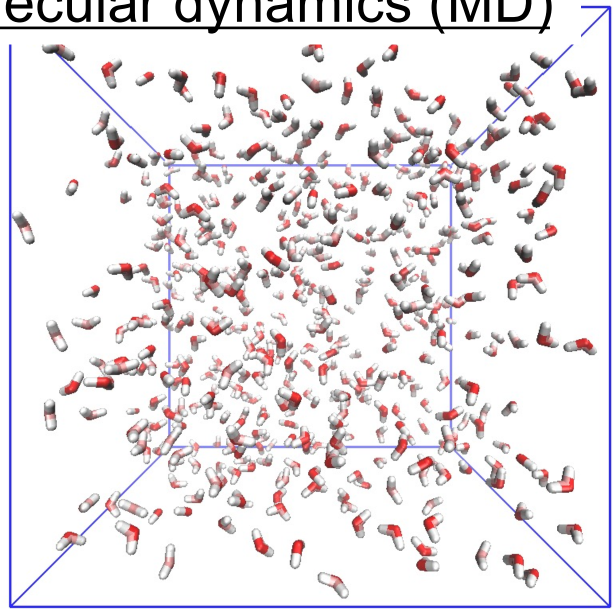


Double Differential cross section (DDX)



Evaluation

Molecular dynamics (MD)



KUNSCA

Kyoto **U**niversity **N**eutron **S**cattering **C**ross-section **A**nalyzer [1]

Highly accurate TSL data for moderator materials

[1]Y. Abe, *et al.*, *Annals of Nuclear Energy,* vol **194**, *110101, 2023.*

Outline

■<u>Improvement of scattering cross section for H_2O</u>

- Measurement of DDX
- Comparison with calculation values

■<u>Calculation of scattering cross section for liquid-H_2, -D_2, -HD</u>

- Addition of a new feature in KUNSCA

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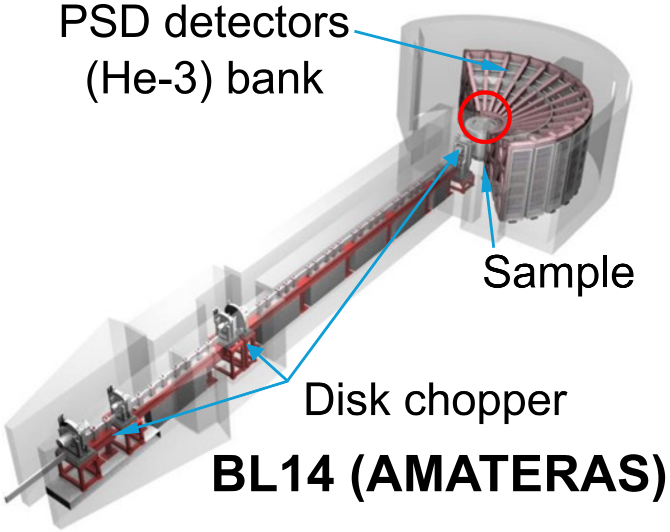
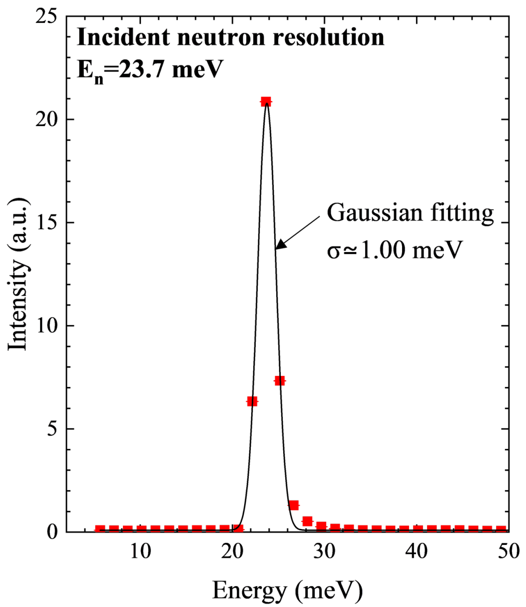
Measurement of DDX

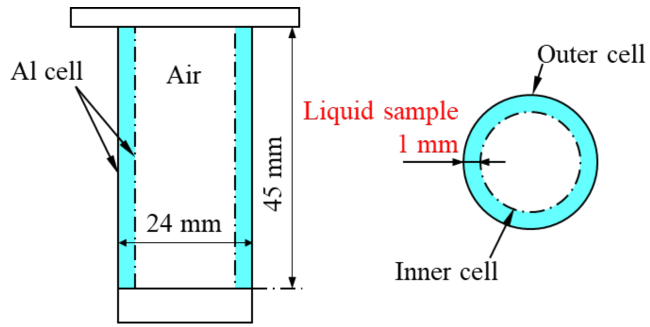
■Experimental setup

- Incident neutron energy : 10.5 meV, **23.7 meV**
- Scattering angle : 30 ~ 110-deg (10-deg interval)





Sample (**H_2O, 300 K**)



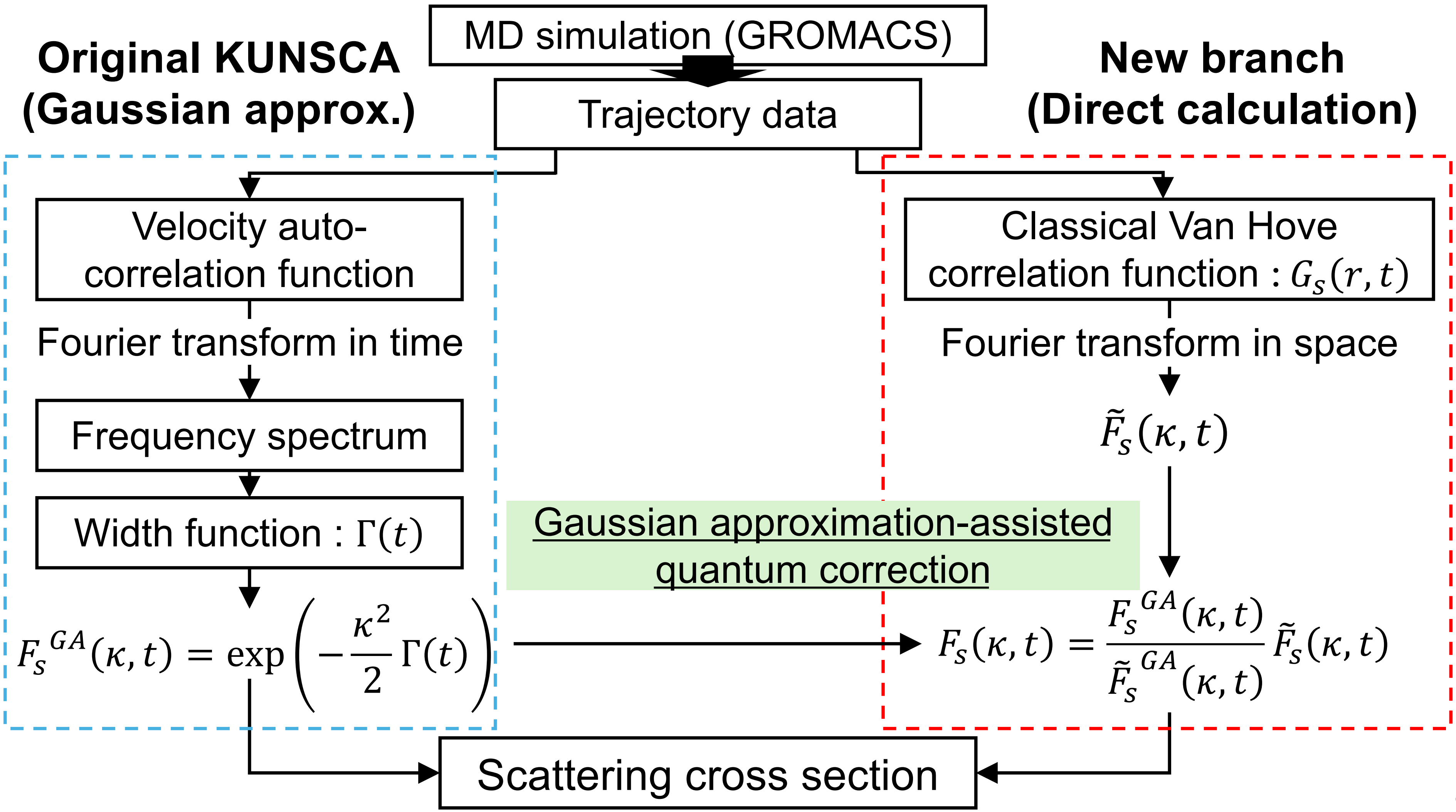
■Data reduction

- The absolute DDX was deduced relative to the incoherent scattering cross section of vanadium.
- Correction factors for multiple scattering and neutron attenuation were calculated by Monte Carlo simulation.

Calculation methodology

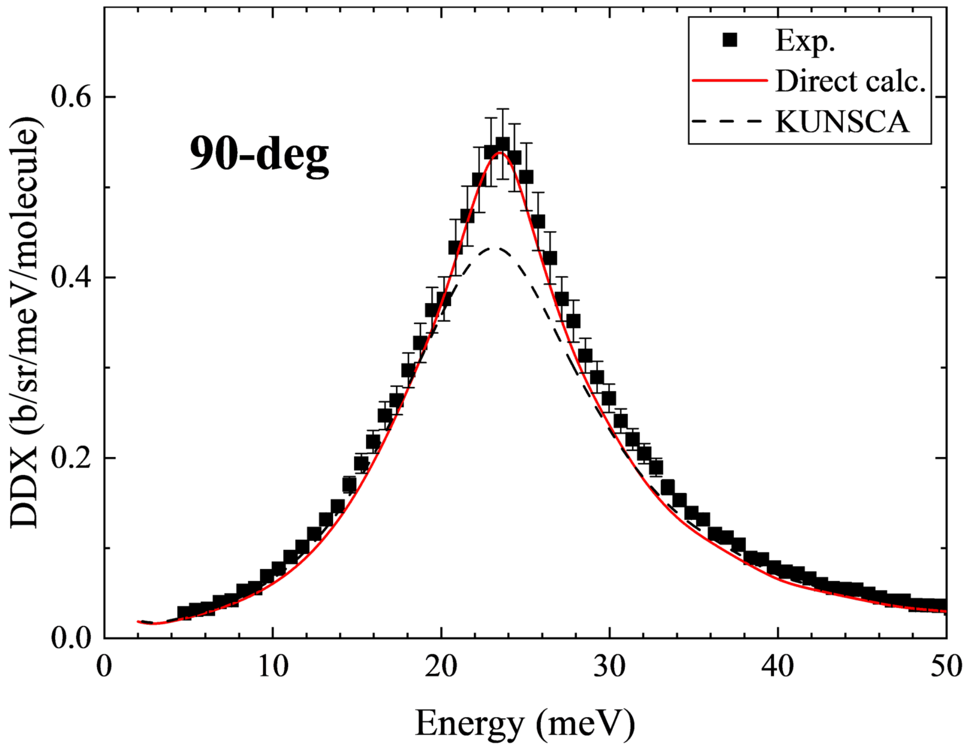
$$\kappa = |\vec{k_0} - \vec{k}|$$
$$\varepsilon = \hbar\omega = E_0 - E$$

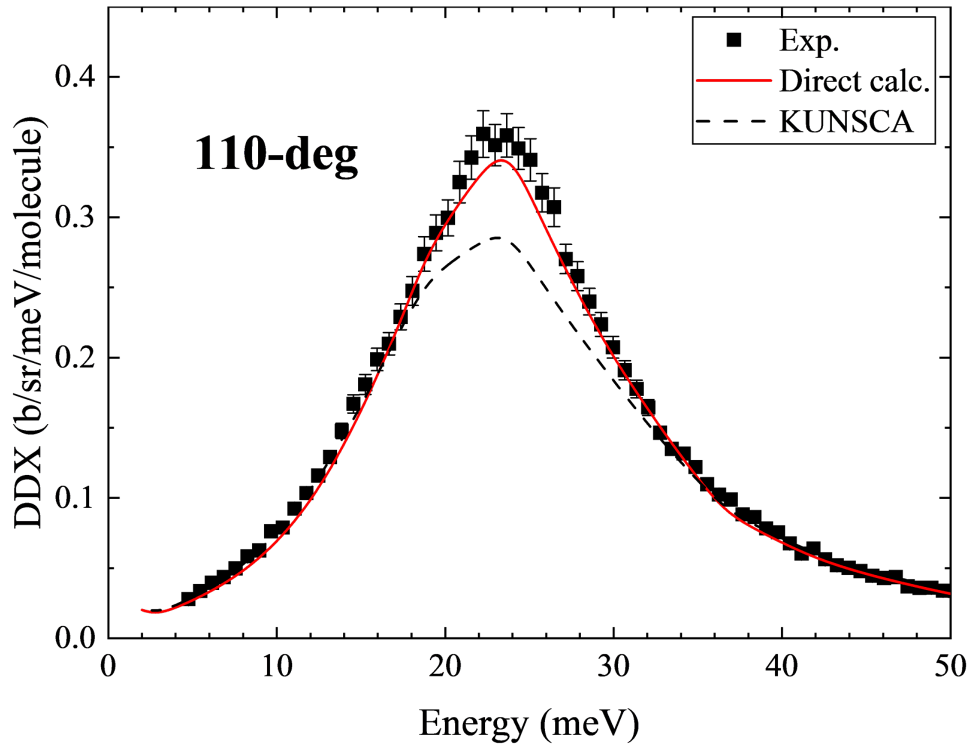
$$\frac{d^2\sigma}{d\Omega d\varepsilon} = \frac{k'}{k}\sum_{x=1}^{N}\frac{\sigma_b^x}{4\pi\hbar}S_s^x(\kappa,\omega) \qquad S_s^x(\kappa,\omega) = \frac{1}{2\pi}\int_{-\infty}^{\infty}F_s(\kappa,t)\exp(-i\omega t)dt$$



Results

Comparison with calculation values





Good agreement with direct calculation results

It is considered that the under estimation of the KUNSCA results from the Gaussian approximation.

Outline

- Improvement of scattering cross section for H_2O
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- Calculation of scattering cross section for liquid-H_2, -D_2, -HD
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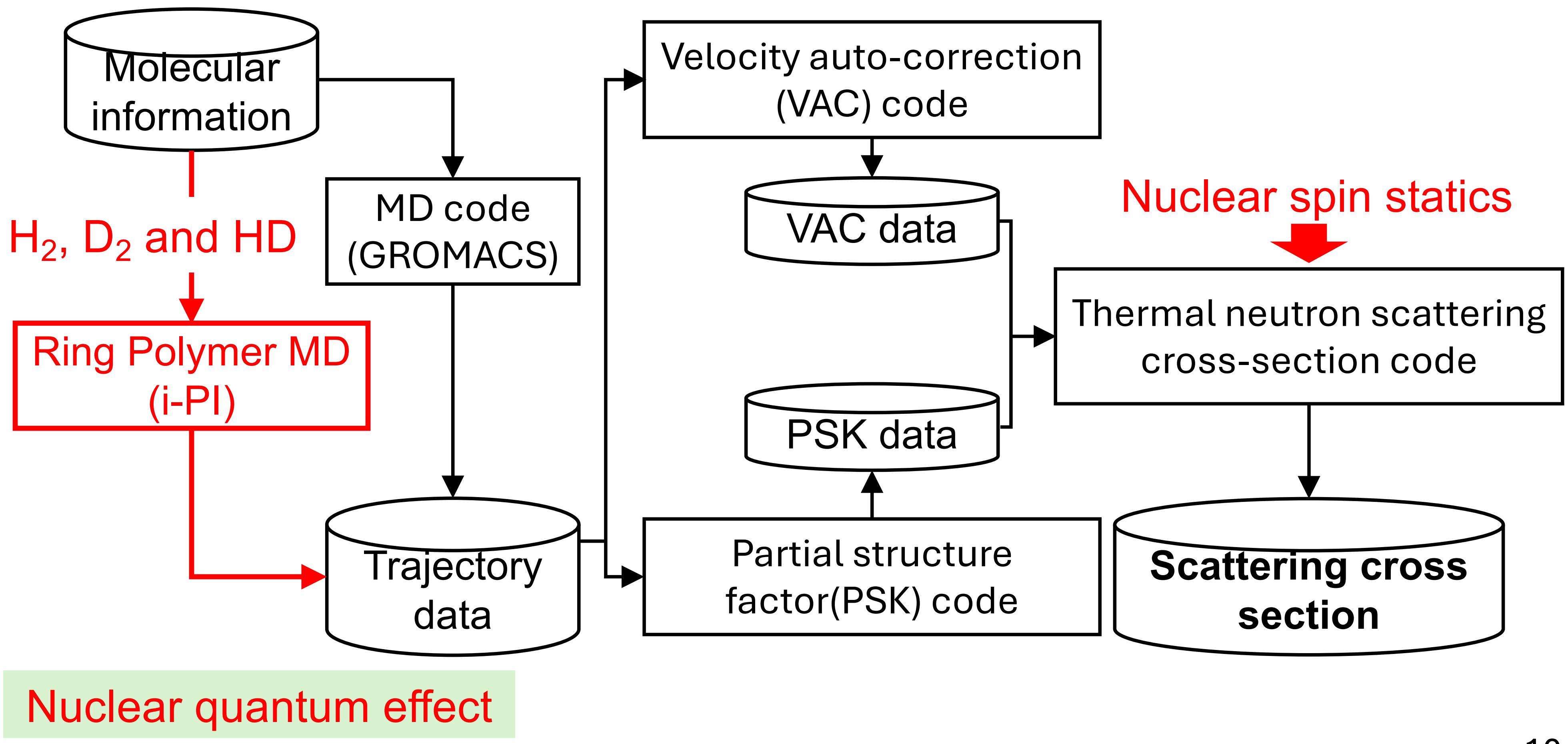
Calculation for cryogenic moderators

■ New feature in KUNSCA

- Scattering cross section for **Liquid-H_2, -D_2 and -HD**
- KUNSCA couldn't calculate scattering cross section for them.



Calculation methodology

$$\frac{d^2\sigma}{d\Omega d\varepsilon} = \frac{k'}{k}\left[u(k)S_d(\kappa,\omega) + \sum_{J_0J_1\nu_1} F(\kappa,J_0,J_1,\nu_1)S_s\left(\kappa,\omega-\omega_{J_0J_1}-\omega_{\nu_0\nu_1}\right)\right]$$

u, F

- Nuclear spin statics
  - Spin correlation (ortho/para-H_2, -D_2)
- $\sigma_{b,coherent/incoherent}$

J : Rotational quantum number
ν : Vibrational quantum number

$\nu_1 = \nu_0$ (Ground state)

Dynamic structure factor

- Self part : $S_s(\kappa,\omega)$
  Gaussian approximation
- Distinct part : $S_d(\kappa,\omega)$
  Sköld approximation
  $$S_d(\kappa,\omega) = S(\kappa)S_s\left(\frac{\kappa}{\sqrt{S(\kappa)}},\omega\right) - S_s(\kappa,\omega)$$

RPMD simulation condition

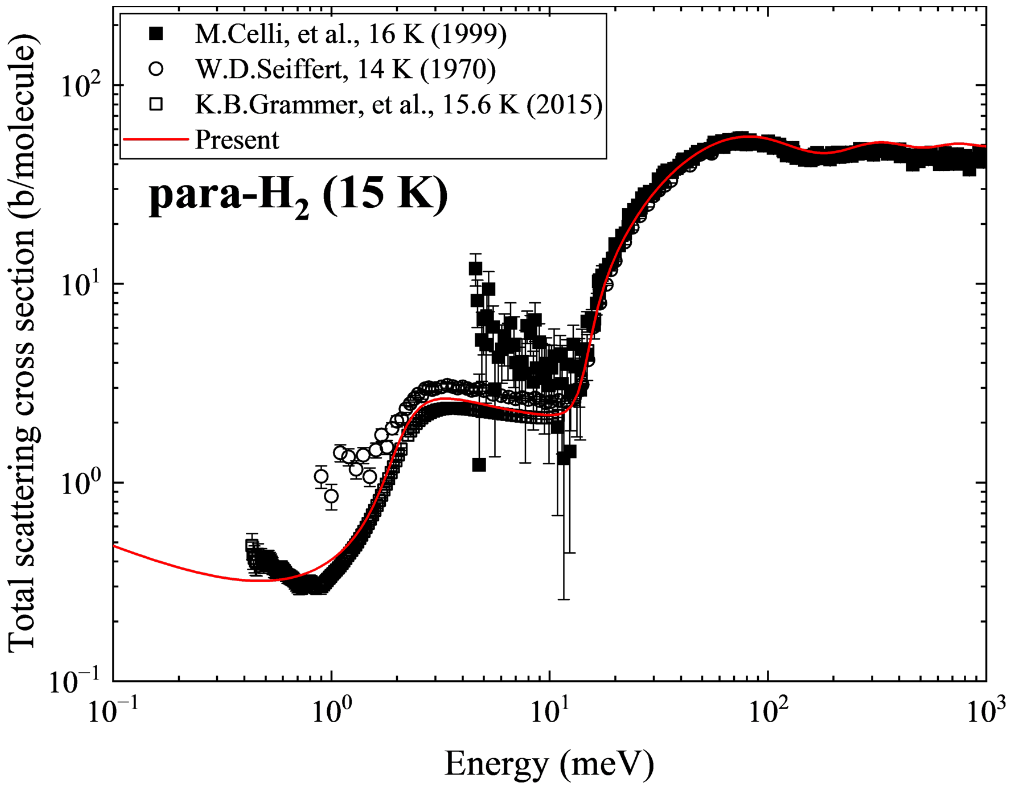
Potential	Silvera-Goldman (SG)
Number of molecules	512
Ensemble	(NVT → NPT →) NVT
Number of beads	62
Boundary condition	Periodic boundary
Temperature (K)	15 (H_2), 19 (D_2), 17 (HD)
Time step (fs)	0.1
Number of steps	10^5

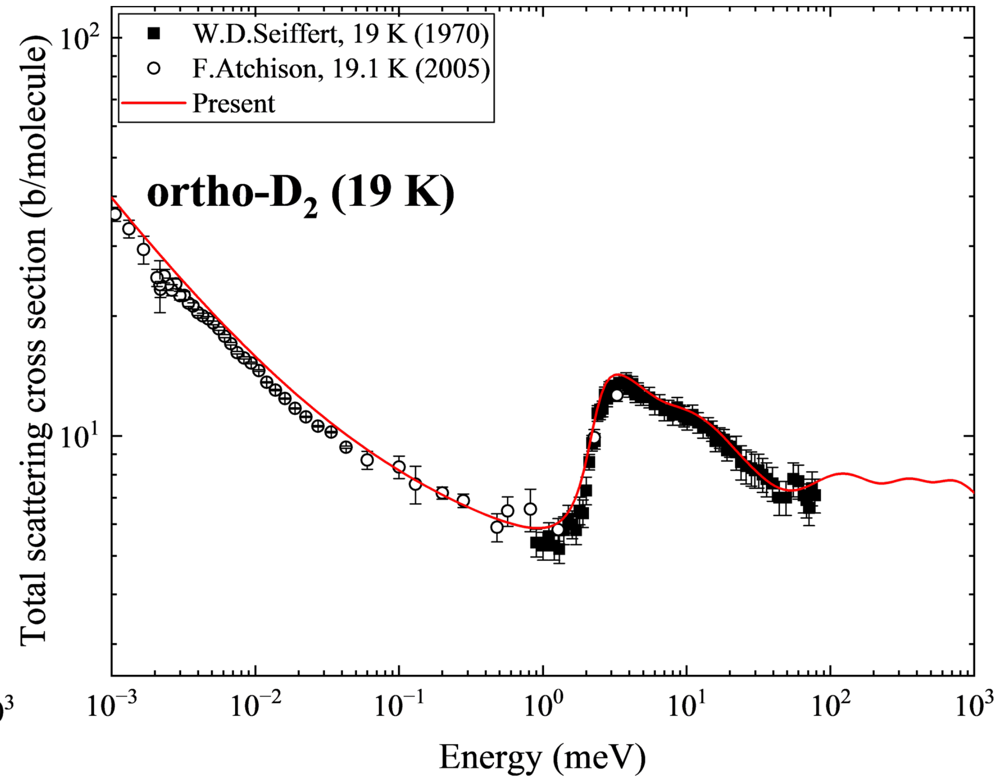
Equilibrium runs

Results

■ Liquid-H_2 and -D_2

Comparison with experimental data obtained from EXFOR

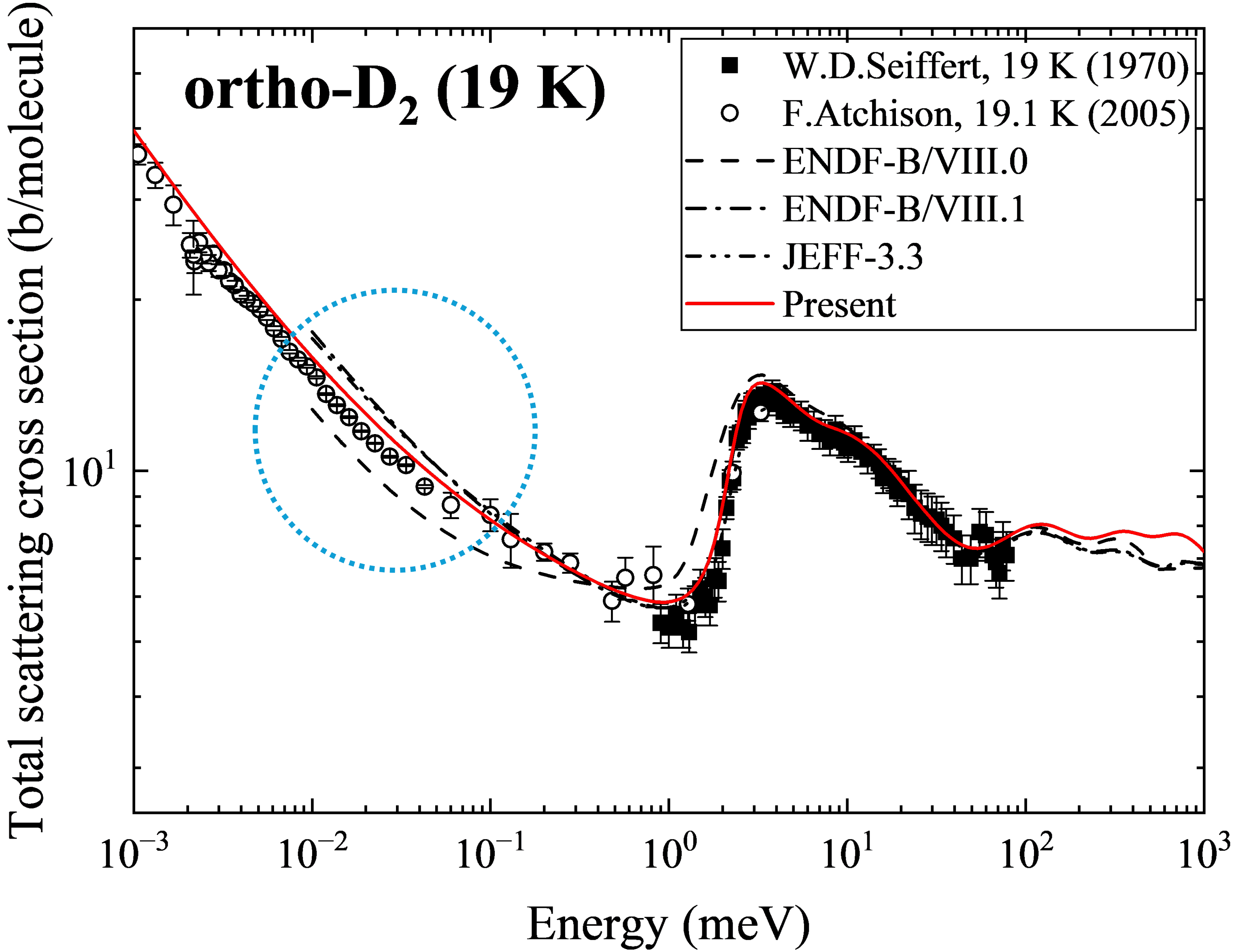




Good agreement with experimental data

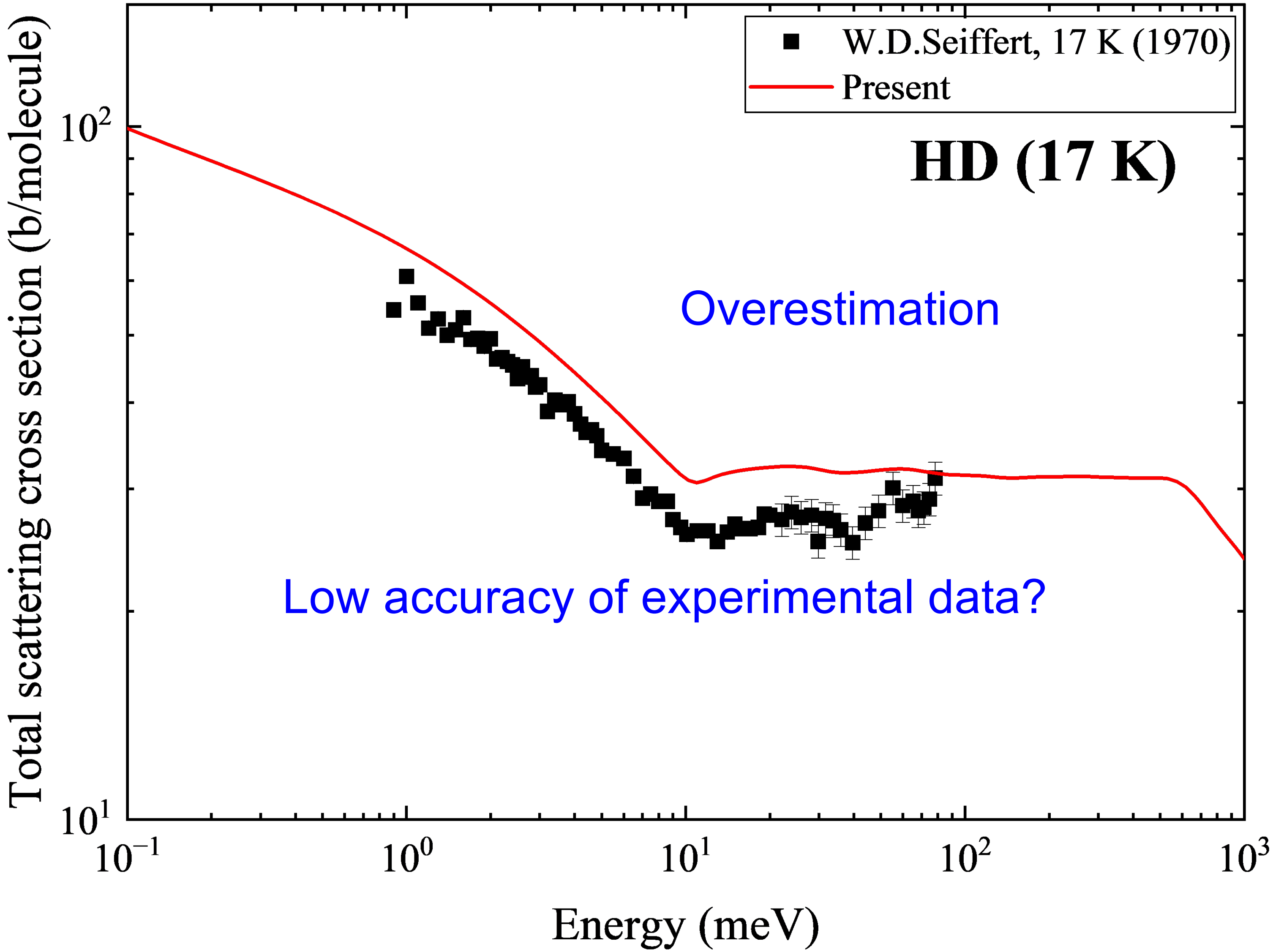
Results

Comparison with nuclear data libraries



Results

■<u>Liquid-HD</u>



Summary

■ Improvement of scattering cross section for H_2O

The direct calculation results agreed better with experimental DDX values obtained at MLF J-PARC than the KUNSCA results．

■ Calculation of scattering cross section for liquid-H_2, -D_2 and -HD

New feature in KUNSCA

- H_2 and D_2 : Good agreement with experimental data
- HD : Overestimation

Future perspective

Measurement of total cross section and DDX for liquid-H_2, -D_2 and -HD at MLF, J-PARC