Relaxation of confined water: backscattering experiments and multiple-scattering analysis

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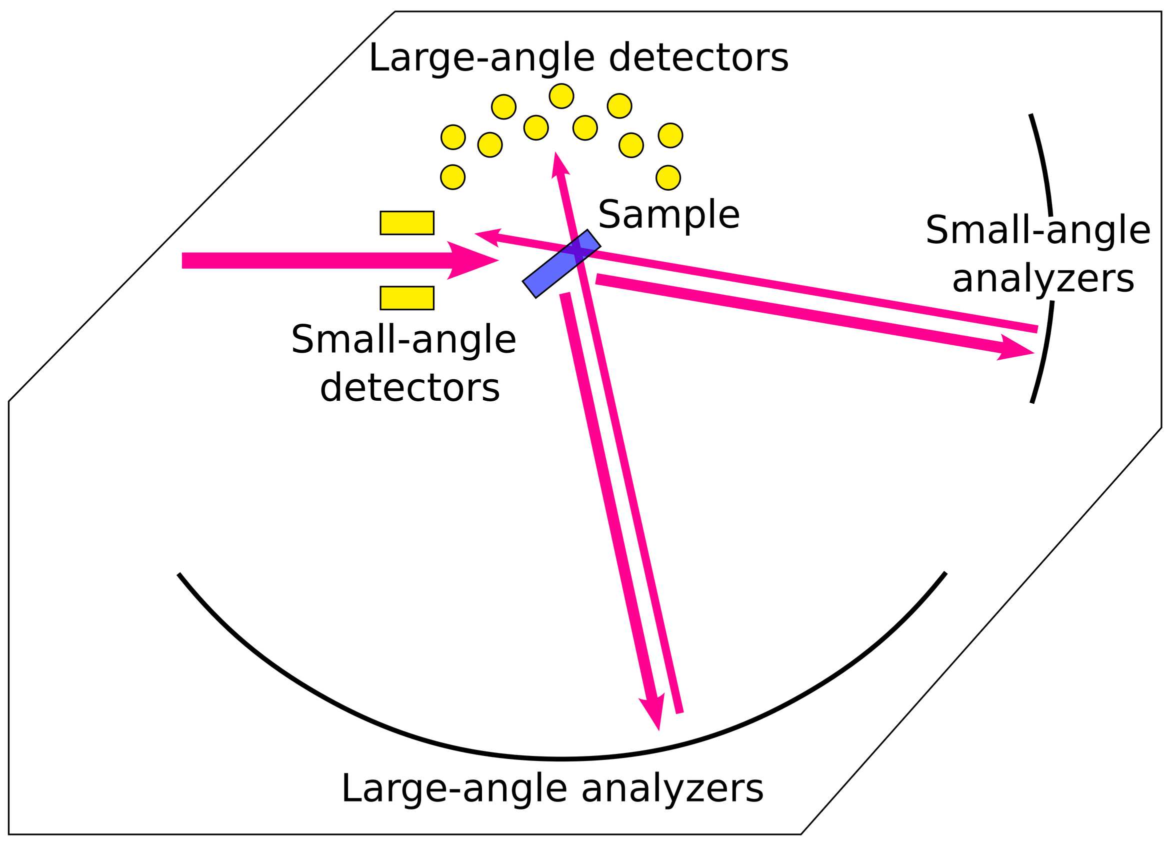
Motivation: MSca - a multiple-scattering simulation package

Experimental data contaminated by multiple-scattering may make data analysis challenging. Being nonlocal in q and ω, multiple-scattering effects are difficult to handle with analytical corrections alone.
To help even the less experienced users to deal with the situation, we have developed a Monte Carlo simulation package **MSca** to resolve multiple-scattering and instrument geometry effects in neutron backscattering instruments, such as SPHERES at MLZ.

In SPHERES, the instrument geometry poses additional challenges. For instance, neutrons pass through the sample a second time on their way from the analyzers to detectors and the small-angle detectors are placed non-ideally around the incoming neutron beam.
As a 'stress test' for MSca, we have applied the simulation to assess multiple scattering effects in neutron backscattering data measured from water confined in carbon nanohorns.



Geometry of the neutron backscattering spectrometer SPHERES at MLZ.

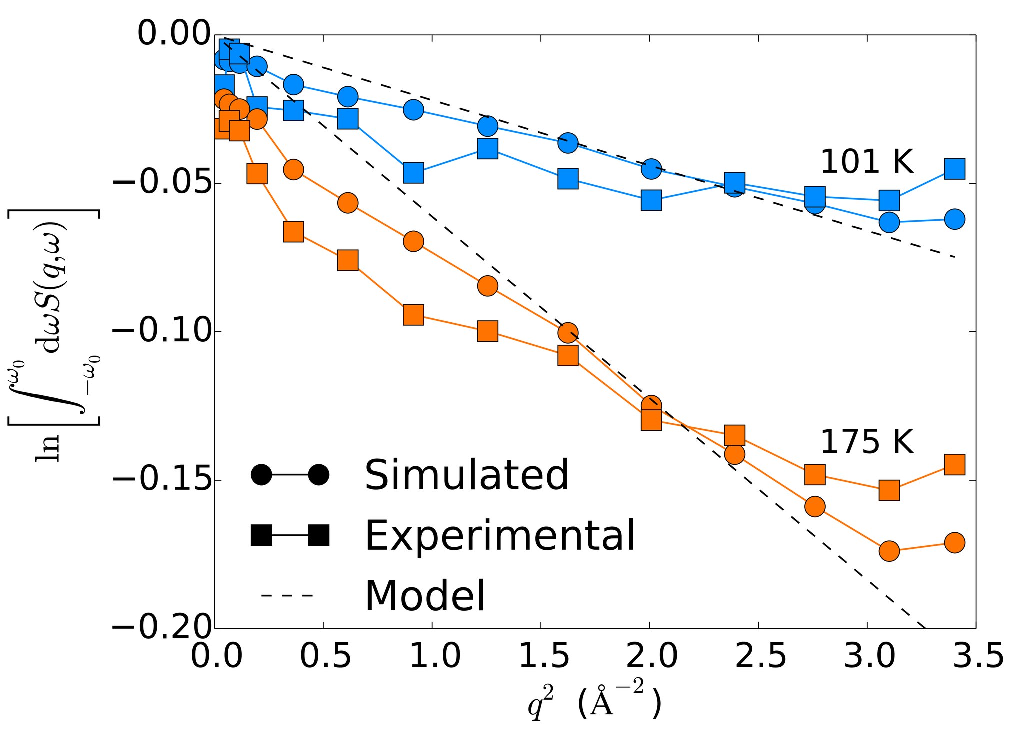
Results: multiple-scattering in elastic and inelastic scans

To analyse the multiple-scattering effects in the experimental data, we used a simple least-squares fitting algorithm: an analytical model was used as an input for the simulation, results of which were then compared with experimental data. By varying the parameters of the input model the simulation was repeated until the best fit was found.

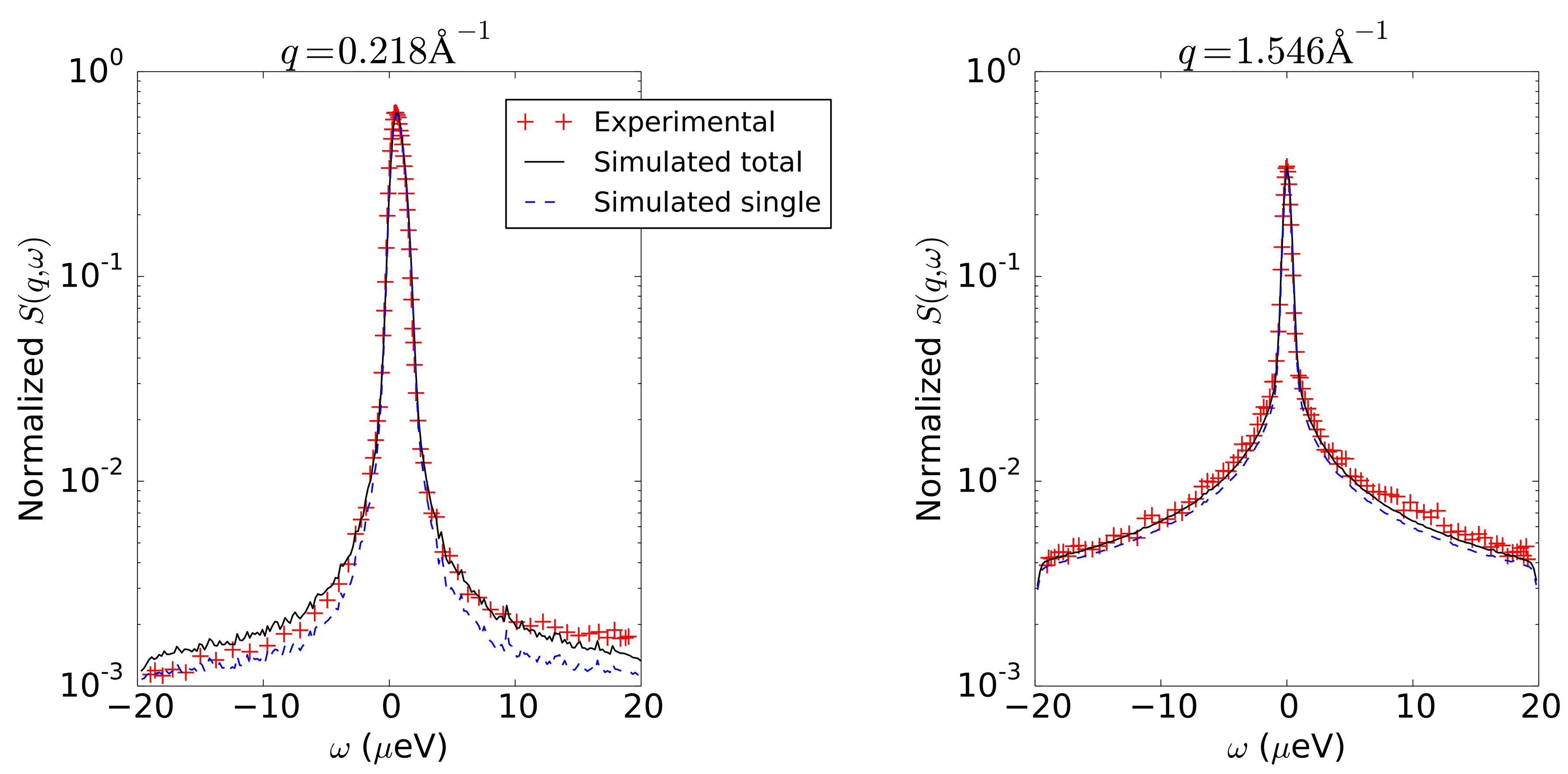
In **elastic scans**, a simple Gaussian approximation model for the elastic incoherent structure factor,

$$A(q)=e^{-\langle u^2\rangle q^2/3},$$

is often used to extract the mean squared displacement $\langle u^2\rangle$. However, plotting the logarithm of the normalized elastic intensity vs. q^2 usually results in non-straight lines due to multiple-scattering. The figure on the right shows the effect in the case of water in carbon nanohorns. Both the slope and the intercept with the y-axis differ from the slope extracted from the input model for the simulation.



The effect of multiple-scattering in elastic scans.



Experimental and simulated spectra at 225 K showing the difference between total and single neutron scattering for detectors at two different *q*.

In the case of **inelastic scans**, we used the Kohlrausch-Williams-Watts function as a model for the relaxation of water molecules. The resulting input model for the simulation was as follows:

$$S(q,\omega)=e^{-\langle u^2\rangle q^2/3}[(1-a)\delta(\omega)+a\,F(e^{(t/\tau)^\beta})]$$

The figures on the left show a comparison between experimental and fitted simulated data at 225 K. At small q, multiple scattering adds a significant contribution to the quasielastic wings while at large q, the effect of multiple-scattering is weaker. Multiple-scattering also becomes less pronounced at higher temperatures.

In summary: Multiple-scattering in neutron backscattering spectrometers can be studied using our MSca software package.

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