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Experimental corrections in neutron scattering experiments: A modern theoretical and computational approach

J. Dawidowski[a], L. A. Rodríguez Palomino[a], J. J. Blostein[a] & G. J. Cuello[b]
[a] Centro Atómico Bariloche and Instituto Balseiro, Avenida Ezequiel Bustillo 9500, (R8402AGP) San Carlos de Bariloche, Río Negro, Argentina
[b] Institut Laue Langevin, 71, Av. des Martyrs, 38042 Grenoble, France
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Experimental corrections in neutron scattering experiments: A modern theoretical and computational approach

J. Dawidowski[1], L. A. Rodríguez Palomino[1], J. J. Blostein[1], and G. J. Cuello[2]
[1]Centro Atómico Bariloche and Instituto Balseiro, Avenida Ezequiel Bustillo 9500, (R8402AGP) San Carlos de Bariloche, Río Negro, Argentina
[2]Institut Laue Langevin, 71, Av. des Martyrs, 38042 Grenoble, France

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Experimental corrections in neutron scattering are a longstanding issue that has been addressed in different ways according to the resources available in each age. Since computational resources are not a constraint at present, the early approaches based on theoretical approximations have led to today's computational methods based on numerical simulations. At the base of all the corrections, we must find a numerical method and a suitable model of the neutron interaction with the system. With regard to simulations, the demands posed by different experimental techniques, should lead to the design of specific solutions for each particular case, while models describing the interaction should include a wide variety of systems. In the Neutron Physics Department at Bariloche Atomic Center (Argentina), both issues were addressed for more than two decades. On the one hand, the development of models describing the interaction of neutrons with molecular and solid systems, has helped to strengthen the methods of analysis of various neutron techniques, and has fed nuclear data libraries of extensive employment in the area of Nuclear Engineering. On the other hand, the numerical simulation methods developed were applied in the analysis of very diverse experiments such as diffraction, inelastic neutron scattering, spectroscopy and electron-volt spectroscopy, and were successfully applied in experiments performed at Bariloche, as well as at ILL and ISIS. Moreover, we have validated the role of the technique of neutron transmission (to obtain the total cross section), as a reference tool in the process of absolute normalization of the experimental data, a rarely stated goal in the context of modern neutron scattering techniques.

Introduction

The progress experienced by neutron scattering techniques in recent decades in the experimental plane has reached a high degree of sophistication thanks to the increased intensity of modern sources, and the improved resolution and effectiveness of the instruments. However, this significant progress has not been accompanied by developments equivalently evolved in the aspect of data treatment. Moreover, at present there are large volumes of information, constantly produced in the most advanced international neutron sources, that end up being not properly processed and are underused, and new experiments are planned on subjects that have already been addressed.

Considering this situation, and given the long experience accumulated in the field of neutron scattering techniques, in the Department of Neutron Physics at the Bariloche Neutron Atomic Center (Argentina), for many years we have addressed the problem of experimental corrections, often in collaboration with international laboratories.

In this paper we show an overview of the work done in different lines of work in stationary and pulsed sources, some of them with experimental basis in the Bariloche Neutron Physics Laboratory. We will focus on the data treatment of diffraction, inelastic, and deep inelastic neutron scattering.

Diffraction

Multiple scattering and attenuation effects in diffraction experiments are crucial when one wants to accurately analyze the structure by neutron diffraction experiments. Customary procedures developed for X-rays techniques were imported by neutron users [1,2], even though the working conditions of the former technique are clearly different. In effect, the inelasticity is a dominant effect (particularly in liquids) with neutrons, since their energy is comparable to those of the vibrational excitations. A modern approach to the problem must consider the mul-

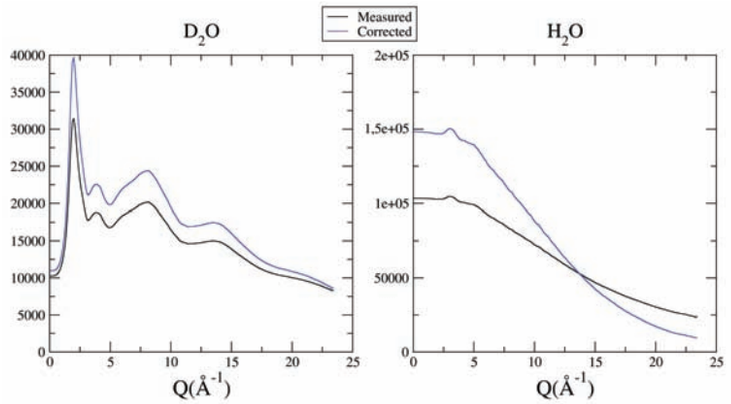

Figure 1. Effects of multiple scattering and attenuation in the diffractograms of D_2O (left) and H_2O (right). In both the measured spectrum is compared with the corrected one.

tiple scattering processes and the energy transferred to the sample in the context of a numerical simulation to describe the system. Copley was a pioneer in developing a multiple scattering code [3], while Granada obtained a reliable description of the inelastic effects with the Synthetic Model [4], that provides a means to perform fast calculations making it ideal to be included in a computer code.

With these antecedents, the Bariloche neutron group developed a Monte Carlo code that performs a detailed description of the history of the neutron in the sample taking into account its energy changes. We note that at different neutron energies, the mean free paths are different too, a fact often overlooked in current data treatment procedures, and that was an area of expertise of the Bariloche neutron group for decades through the study and measurement of total cross sections.

Figure 1 shows the effect of multiple scattering in the diffractograms of H_2O and D_2O through the comparison of the measured spectra and those corrected by our method [5]. The measurements were performed at diffractometer D4 (ILL, Grenoble, France), with an incident wavelength of 0.5 Å [6]. The significance of the effects is apparent and highlights the importance of appropriate corrections. To illustrate a detail of the corrections, Figure 2 shows the calculated components of the observed diffractogram, due to single and multiple scattering as well as the container contribution. Also shown is the scat-

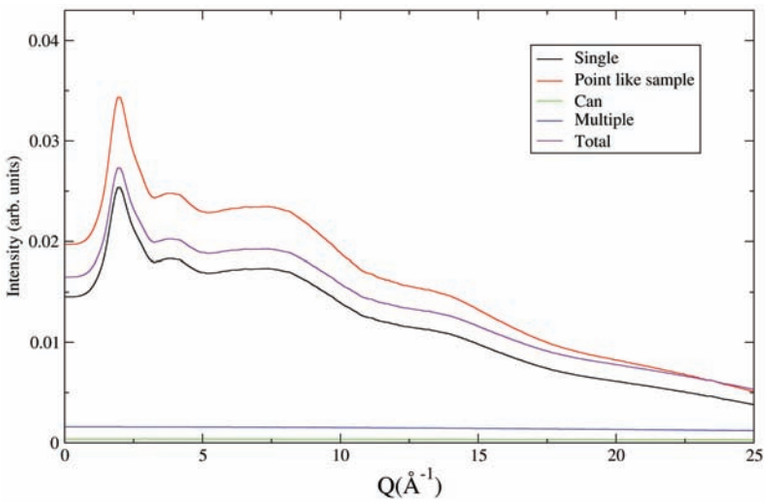

Figure 2. Calculated components of the observed diffractogram: single, multiple scattering and the container contribution. Also shown is the scattering of a point-like sample with the same scattering power of our sample.

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tering due to a point-like sample with the same scattering power of our sample, free of multiple scattering effects.

Inelastic scattering

Even if inelastic scattering experiments are carefully designed to minimize the effects of multiple scattering, there can always be a portion of the diffraction pattern that, because of its low signal, has important corrections for this effect. This highlights the extreme importance of the multiple scattering corrections for these experiments in general.

The general ideas about these corrections were applied to data obtained from the spectrometer MARI (ISIS, RAL, UK), for which we designed specific software, described in references [7] and [8]. A typical spectrum in the *Q*-ω plane is shown in Figure 3, where the experimental data for liquid para-hydrogen at a pressure of 80 bars and a temperature of 16.5 K. Figure 4 shows the details of the different components that contribute to the observed spectum (at a constant *Q*-slice) as revealed by our simulations.

The correction procedure is based upon an iterative scheme that employs Monte Carlo simulations:

- Neutron histories are individually monitored.
- The choice of different energies and flight directions at each step in a neutron history is based upon the experimental raw scattering laws deduced from measurements carried out for the sample and empty-container measurements in the first run and in the corrected distributions in the subsequent runs.

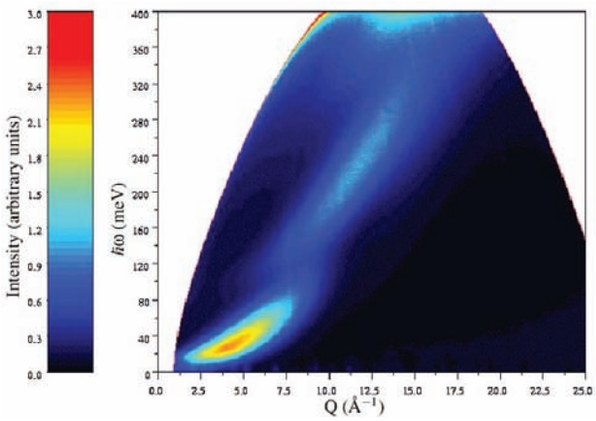

Figure 3. Inelastic neutron scattering spectrum in the *Q*-ω plane from the spectrometer MARI (ISIS, RAL, United Kingdom), for liquid para-hydrogen at a pressure of 80 bars and a temperature of 16.5 K.

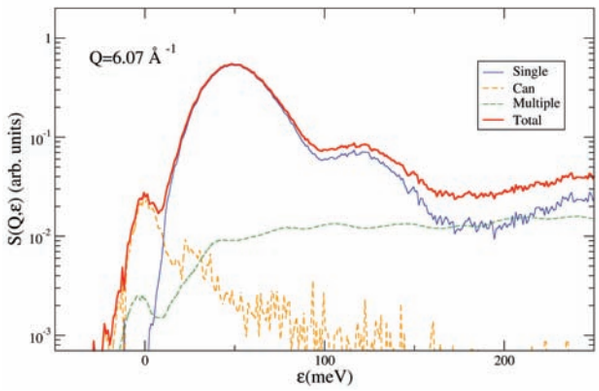

Figure 4. The different components that contribute to the observed inelastic spectum (at a constant *Q*-slice).

Typically, four iterations were needed to reach convergence. We must emphasize the importance of the accuracy of these corrections (shown in [8]), where the detailed shape of the spectrum revealed subtle aspects of the dynamics of hydrogen, which helped to decide in favor of a theory that describes this system.

Deep inelastic neutron scattering

This technique was developed to study the momentum distribution of the atoms composing the condensed matter. Being the main experimental facility that of RAL (United Kingdom) (spectrometer VESUVIO), at the Bariloche neutron laboratory it has been built one in which various experimental tests can be performed [9]. In particular, the multiple scattering corrections procedure developed by our group for this technique was supported by experiments performed in our laboratory [10]. At present, part of our research is also carried out in VESUVIO.

A result that highlights this activity is the investigation of the neutron cross sections of hydrogen and deuterium in H_2O-D_2O mixtures. The interest in this work was to examine the anomalous behavior in the hydrogen neutron cross section reported in the past in similar experiments that raised a longstanding controversy [11]. Indeed, some authors [12] have reported measured values significantly lower than those tabulated for the cross section of hydrogen employing this technique.

The result of our work led us to conclude that the purported anomaly can be ascribed to inaccuracies in the data processing method. Essential to this analysis was the realization of multiple scattering corrections, presented in Figure 5, where measured neutron Compton

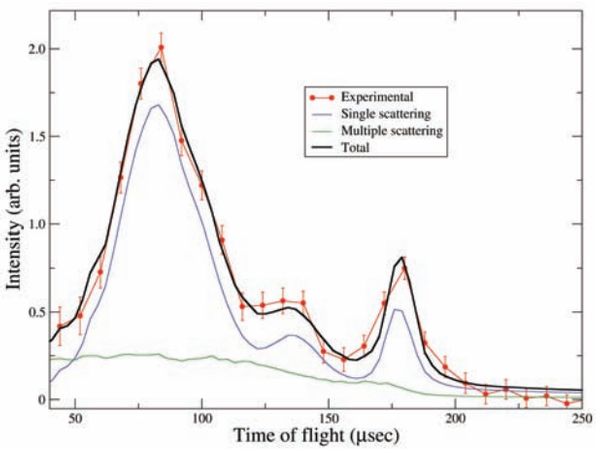

Figure 5. Measured neutron Compton profile for the mixture H_2O-D_2O with 40% deuterium. Results of the Monte Carlo simulations showing the single, multiple, and container contributions, and also the total scattering.

profile for the mixture H_2O-D_2O with 40% deuterium is shown. The results of the Monte Carlo simulations show the single scattering contribution, the multiple scattering, the container contribution, and the total scattering. The determined cross sections of different mixtures were fully compatible with the commonly accepted tabulated values of neutron cross sections of hydrogen, deuterium, and oxygen.

The method of analysis developed highlighted the need to carefully review the general methodology used in neutron techniques to obtain an accurate normalization to account for the cross sections on an absolute scale (in barns). This premise was also employed in the analysis of diffraction experiments as described above, and presently continues in development.

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