# Reply to "Comment on 'High-energy neutron scattering from hydrogen using a direct geometry spectrometer'"

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We reply to the comment raised in Mayers *et al.* [Phys. Rev. B **84**, 056301 (2011)]. The comment claims the conclusions by Stock *et al.* [Phys. Rev. B **81**, 024303 (2010)] are not correct owing to the fact that the resolution is not sensitive to detect the changes in the cross section observed using the indirect geometry instrument VESUVIO. We point out several criticisms of this analysis. First, we note that the energy widths measured at large scattering angles on MARI are the same as those measured on VESUVIO (as illustrated in Fig. 6 of Mayers *et al.* [Phys. Rev. B **84**, 056301 (2011)]). We, however, get the same cross section at all other angles and independent of experimental configuration. We also point out that the current data set presented in the Comment is inconsistent with sum rules of neutron scattering. We do not agree with the arguments presented in the Comment and consider that the deficit in the hydrogen cross section measured on VESUVIO is erroneous. Finally, our experiment shows that the impulse approximation is valid over a wide range of energies and momentum transfers.

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Our paper entitled "High-energy neutron scattering from hydrogen using a direct geometry spectrometer" (Ref. 1) describes an investigation of the validity of conventional scattering theory on the cross section of hydrogen using a direct geometry spectrometer. Contrary to previous results using indirect geometry machines, which observe a 20%–40% deficit in the cross section at high (∼100 Å$^{-1}$) momentum transfers, we found the cross section is constant and of the expected magnitude. We therefore consider that the previous results are an experimental artifact from the data analysis procedures for indirect geometry spectrometers. The Comment, Ref. 2, provides a detailed discussion regarding the resolution function in the case of direct and indirect geometry neutron scattering instruments at pulsed sources. Based on this analysis it is claimed that the conclusions obtained with a direct geometry spectrometer (outlined in our publication) are invalid.

In this Reply, we point out several criticisms of the analysis of Ref. 2 and show that the Comment does not change the underlying conclusion presented in Ref. 1—there is no measurable deficit in the scattering cross section of hydrogen. We therefore consider that our original conclusions are correct, namely, that the previous anomalies in the cross section are due to effects related to the use of indirect geometry spectrometers.

## I. HYDROGEN CROSS SECTION IS CONSTANT AS A FUNCTION OF BOTH MOMENTUM AND ENERGY TRANSFER

Reference 1 shows first, that the cross section for all momentum transfers and energy resolutions is constant. Secondly, the absolute value of the cross section is that expected based on the Born and impulse approximations. We obtain the results (Ref. 1) independent of the incident neutron energy, independent of the energy resolution, and independent of the scattering angle.

The basic claim of Ref. 2 is that the energy resolution on MARI is not sensitive enough to observe the changes in the cross section with momentum transfer. However, stating this point, we note that the authors of Ref. 2 agree that the energy widths of the hydrogen recoil line are equal on both direct (MARI) and indirect (VESUVIO) spectrometers at high scattering angles on MARI (see Fig. 6 of Ref. 2). We derive the same cross section at these angles independent of momentum transfer or energy resolution. This marks a clear difference between the results of direct and indirect geometry measurements, however, unlike the case for VEUSVIO, we have performed the analysis at a series of different experimental configurations and obtained identical results. We therefore do not agree with the comments in Ref. 2 as we have found that the hydrogen cross section is constant within the experimental error for all angles and momentum transfer and independent of the incident neutron energy.

## II. IMPULSE APPROXIMATION

The energy widths were calculated in Ref. 2 by assuming that the impulse approximation is valid. This assumption is also made to obtain the energy profiles of a constant momentum scan when using an indirect geometry spectrometer. If, as found in Ref. 2, the hydrogen cross section is not constant with momentum transfer, then the impulse approximation needs to be revaluated as done in several of the theories and papers discussed in the Comment. There are also a series of results obtained with different hydrogen-containing materials and taken with different instrumental configurations which are not self-consistent.[3–5] They are also inconsistent with the impulse approximation which assumes that at high energies all of the atoms respond independently, and therefore the hydrogen recoil scattering should be consistent for all hydrogen-containing materials. The conclusion is that when the impulse approximation is used to analyze the data and a momentum-dependent cross section is obtained, this process shows that the initial assumption about the correctness of the impulse approximation is not valid. We believe that this approach needs to be reconsidered. We note that in Ref. 2, data is illustrated from an upgraded VESUVIO (Ref. 6) for the widths of the hydrogen recoil line, but the intensities are not published yet for this particular configuration.

In contrast with a direct geometry spectrometer, we were able to measure the widths directly from constant angle scans without using the impulse approximation because the momentum transfer was independent of the energy of free hydrogen recoil.

## III. JACOBIAN

We do not agree with the semantics used by the authors when discussing resolution and believe it to be misleading. When discussing resolution applied to neutron inelastic scattering, there are two key points—first, the raw width of the resolution ellipsoid in momentum and energy, and second, how the resolution ellipsoid cuts the dispersion surface of the excitation being measured. The latter point is defined by the Jacobian discussed in Ref. 1. We believe this second point is the origin of the broad peaks observed in a constant angle scan obtained with an indirect spectrometer in Ref. 2.

Reference 2 presents data based on simulated constant momentum scans. The measurements deriving the change in the cross section were obtained from constant angle scans and not by the scans presented (see Fig. 1 of Ref. 1 and the discussion surrounding the width in time and energy in the text).

## IV. INTEGRATED INTENSITY AND SUM RULES

Reference 2 refers to several theories (Refs. 7–9) that state that the measured cross section is tied with the energy resolution. Such a statement may be consistent with sum rules which state that the *integral* over all energies is a constant at different momentum transfers. The data sets presented, however, are not consistent with this sum rule because the integral of the scattered intensity is not independent of the momentum transfer. The data taken on the direct geometry instrument, by MARI, is consistent with this basic notion of neutron scattering up to momentum transfers of $Q \sim 200\ \text{Å}^{-1}$, a momentum range over twice that probed in the indirect geometry experiments (we note that the red curve in Fig. 6 of Ref. 2 extends in momentum transfer well beyond where data has been published on VESUVIO).

If the claim in Ref. 2 that the apparent inconsistency between the results of direct and indirect geometry machines is due to the different energy resolutions of the experiments, then by integrating over all energies (or time) they should be able to find where the missing intensity has reappeared and hence conserve the sum rule described above. This analysis has never been performed to our knowledge.

Theoretical work in Ref. 10 provided a possible explanation and support for the arguments and measurements described in Ref. 2. However, the suggestions in Ref. 10 are inconsistent with our measurements because we observe the same intensity for different incident neutron energies and for a range of scattering angles. If the theory in Ref. 10 was an appropriate description, the changes in the intensity would be observed in our experiment and the missing intensity could be derived from the data taken on VESUVIO.

Based on these four points, we do not agree with the comments described in Ref. 2 and consider that the conclusion that the cross section of hydrogen varies with momentum transfer to be an artifact associated with indirect geometry spectrometers.


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