Experimental report

02/08/2017

Proposal: 6-02-551 **Council:** 10/2014

Title: Dynamics of liquid para-hydrogen: a low-Q determination of its doubledifferential cross section

Research area: Physics

This proposal is a new proposal

Main proposer: Eleonora GUARINI

Experimental team: Emmanuel FARHI
Ferdinando FORMISANO
Ubaldo BAFILE
Vladyslav ROMANKOV
Eleonora GUARINI

Local contacts: Alessio LALONI
Alessio DE FRANCESCO

Samples: para hydrogen (p-H2)

Instrument	Requested days	Allocated days	From	To
BRISP	8	8	05/09/2016	13/09/2016

Abstract:

We propose to investigate the collective dynamics of liquid para-H2 at T = 16 K i.e. close to the triple point. These measurements are mainly suggested by the present need of achieving much more accurate determinations of the dynamic response to neutrons of several crucial materials in reactor-industry and neutron production facilities. Cryogenic liquids still miss a quantitative assessment of the coherent scattering properties in the low-Q neutron range. The quantum nature of the hydrogen liquids (H2, D2) further suggests detailed experimental investigations of the total (inter and intra-molecular) dynamics, yet out of reach of simulation or modeling capabilities as soon as the classical approximation becomes inapplicable, and in the presence of existing pioneering data which, unfortunately, do not match the accuracy required nowadays

The experiment (proposal 69408) was planned to investigate the low-*Q* collective dynamics of liquid para-H_2 at 16 K and at the lower bounds of the thermal energy range (20 meV). A similar experiment, with identical scientific and applicative aims, was proposed in parallel on liquid D_2 (proposal 69488) and accepted for the Brisp CRG beamtime. Use of a catalyst is mandatory to convert normal hydrogen to para-hydrogen, however the cell prepared in Florence and containing the catalyst turned out to slightly misfit the cryostat tail for an unexpected defect in construction. Other available cells were not appropriate for insertion of the catalyst and for the scattering properties of H_2. To avoid losing precious beamtime we therefore decided to perform the D_2 experiment (for which absence of the catalyst is far less critical) by using one of the available slab aluminum cells fairly matching the scattering properties of liquid deuterium.

The liquid D_2 sample was prepared by condensing the gas in the cell at 20 K, using the gas handling circuit of the ILL under the management of the ILL technician expert of the circuit. Sample preparation took several hours, as expected, but went on without any difficulty, reaching stable thermodynamic conditions (20.4 K, 0.5 bars, approximately) that were easily maintained for the whole duration (days) of the sample measurements. It was our first time we didn't use our own gas-circuits (built and tested in Florence), but we report a **complete satisfaction** about the equipments available now at ILL and masterly managed by the ILL technician that followed our experiment with lots of attention and care. A similar **full satisfaction** concerns the instrument performance and the enthusiastic assistance of the Brisp Instrument scientists and technician.

Spectra were collected for empty cell, sample, vanadium, absorber, both at 2 and 1 Å incident neutron wavelength, with the aim of comparing two independent data sets with different energy resolutions. In both cases, the signal aspect looked extremely 'clean' and with the marked features that are exactly those motivating our proposals, and which need the absolute-scale comparisons with models and quantum-MD calculations [1-4]. A better, quantitative, assessment of the response to neutrons of liquid hydrogens at small *Q* is therefore strongly promised by the performed experiment. Analysis is in progress.

[1] E. Guarini, M. Neumann, U. Bafile, M. Celli, D. Colognesi, S. Bellissima, E. Farhi, Y. Calzavara "Velocity autocorrelation by quantum simulations for direct parameter-free computations of the neutron cross sections: II. Liquid Deuterium"
Phys. Rev. B **93**, 224302 (2016). 2-s2.0-84974817781

[2] E. Guarini, "The neutron cross section of the hydrogen liquids", CRISP - WP11: Moderator neutron cross-section data, Final Report on Cryogenic Liquids, ILL (2014).

[3] E. Guarini, M. Neumann, U. Bafile, M. Celli, D. Colognesi, E. Farhi, and Y. Calzavara "Velocity autocorrelation in liquid para-hydrogen by quantum simulations for direct, parameter free, computations of the neutron cross sections"
Phys. Rev. B **92**, 104303 (2015). 2-s2.0-84942447101

[4] This experiment was part of the experimental programme of the *Nausicaa* consortium (https://www.ill.eu/?id=15488), gathering the ILL, IRSN, CEA, TUM, ESS, the University of Florence and the *Ecole Polytechnique de Montréal,* as well as ANL, AECL, IAEA, NEA/OECD and other observers. The core of this project is to measure or properly calculate the double differential cross section of crucial neutron moderators (including water and cryogenic liquids) to produce largely improved $S(Q,\omega)$-kernels finally available to the nuclear-reactor industry.