

Anomalous neutron scattering in metallic hydrides and the validity of the convolution formalism

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Abstract

Recently, we reported the ‘anomalous’ neutron scattering behavior of protons in condensed systems, e.g. water, metallic hydrides, and organic materials as observed on the eVS instrument at ISIS. Very recently, Blostein et al. [Physica B 304 (2001) 357] presented a theoretical investigation criticizing the convolution method used for the analysis of the data obtained on eVS. In particular, they criticize the expression of the experimentally observed spectral intensity as a convolution with the absorption peak of the analyzer foil. They conclude that the usually employed data analysis procedure fails in determining the inferred momentum distribution widths of the peaks and leads to incorrect values of peak areas in the case of two (or more) overlapping recoil peaks, in particular those of H and D. However, experimental results on metallic hydrides show very clearly that the objections concerning the peak areas are not relevant for the results and for the associated subfemtosecond quantum entanglement effect under consideration, thus supporting the validity of the convolution formalism for investigating peak areas on the eVS instrument.

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1. Introduction

Deep inelastic neutron scattering, also known as neutron Compton scattering (NCS), has proven to be a powerful technique for the determination of the nuclear ground state momentum distributions $n(p)$ reflecting the dynamics of the atoms in condensed matter systems. Among others the dynamics of hydrogen in metallic hydrides like ZrH₂, NbH, TiH₂ and CaH₂ have been successfully investigated [1].

For measurements of the nuclear momentum distribution $n(p)$, high values of momenta q and energies ω must be transferred to the recoiling nuclei during the scattering process and this requires high intensities of incident high energy neutrons. These conditions are fulfilled by the inverse geometry time of flight (tof) instrument eVS of ISIS at the Rutherford Appleton Laboratory. In the impulse approximation (IA) limit, i.e. infinite q , the dynamic structure factor $S(q, \omega)$ reduces to a single peak centered at the recoil energy of the corresponding nucleus

$$S(q, \omega) = \frac{M}{\hbar q} J_M(y_M)$$

where y_M is the scaling variable [2,3]

$$y_M = \frac{M}{\hbar^2 q} \left(\hbar \omega - \frac{\hbar^2 q^2}{2M} \right)$$

and $J_M(y_M)$ is the neutron Compton profile of the scattering nucleus of mass M . The experimentally observed intensity is then proportional to $J_M(y_M)$ convoluted with the instrument resolution function $R_M(y_M)$, i.e.

$$c(t) \Delta t \propto J_M(y_M) \otimes R_M(y_M).$$

The resolution function $R_M(y_M)$ contains all geometrical uncertainties of the instrument but is mainly determined by the energy resolution of the analyzer foil that is positioned between the sample and the detector. The foil that absorbs neutrons over a narrow range of energies gives spectra such as those shown in Fig. 1. The energy resolution is determined via calibration runs using a lead sample while the general shape of the energy resolution function is

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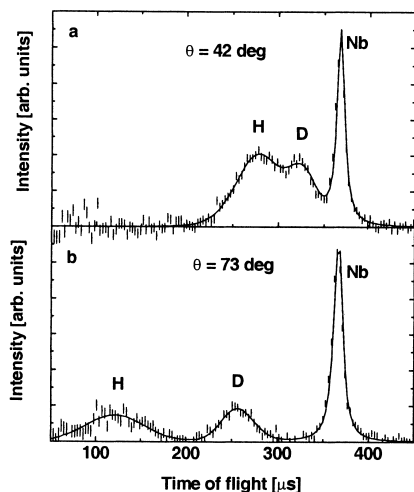


Fig. 1. Shown are the time of flight spectra of $\text{NbH}_{0.16}\text{D}_{0.70}$ (or $x_D = 0.8$) at two different scattering angles. The error bars indicate the measured spectrum, while the solid line shows the fitted spectrum using the convolution formalism (see text). Note that the H and D peaks overlap strongly in the small angle ($\theta = 42^\circ$) spectrum, while they are almost completely separated in the high angle one ($\theta = 73^\circ$).

assumed to be Gaussian for the U (uranium) foil and to be Lorentzian for the Au (gold) foil analyzer. The geometrical uncertainties are Gaussian distributed so that the overall resolution function $R_M(y_M)$ is Gaussian in the case of U and a Voigt function when the Au foil is used. The final shape of the neutron Compton profile $J_M(y_M)$ of the scattering nucleus is determined from the deconvolution of the measured peak from the instrument resolution function.

In contrast to the work dedicated to the determination of the momentum distributions, our experimental work focuses on the determination of integrated intensities, e.g. of H, D, O or Nb while assuming the momentum distribution of the considered nuclei to be of Gaussian shape. In previous experiments on $\text{H}_2\text{O}/\text{D}_2\text{O}$ mixtures at room temperature, an ‘anomalous’ decrease of the scattering cross-section ratio of H to that of D, i.e. σ_H/σ_D , with respect to the conventionally expected ratio (10.7) have been found [4,5]. In addition, these ‘anomalies’ showed a strong dependence on the D mole fraction of the sample. These experiments were motivated by theoretical work on short-lived quantum entangled particles in condensed matter at room temperature [6,7]. Later experiments on metallic hydrides, e.g. NbH_xD_y , have also shown cross-section ‘anomalies’ [8,9]. All these ‘anomalies’ are attributed to the existence of short-lived quantum entangled particles involving mainly the protons. A special feature of the metallic hydride results—which are the focus of this paper—is that the scattering cross-section ratio of H and Nb, i.e. $\sigma_H/\sigma_{\text{Nb}}$, possesses a strong angular dependence; see Fig. 2 (this figure is adapted from Ref. [8]). Various experimental as well as theoretical tests have been conducted and have shown that the ‘anomalous’ results are of real physical origin [4,5,8–12,14]. However, very recently, Blostein et al. [13] presented a theoretical investigation

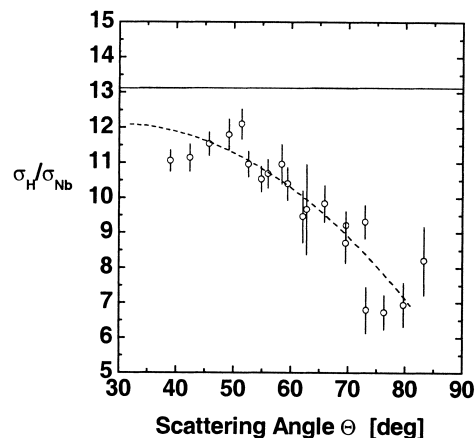


Fig. 2. Shown is the ratio $\sigma_H/\sigma_{\text{Nb}}$ of the scattering cross-section of H to that of Nb of $\text{NbH}_{0.16}\text{D}_{0.70}$ (or $x_D = 0.8$) as a function of scattering angle θ . The conventional value of $\sigma_H/\sigma_{\text{Nb}} = 81.67/6.25$ is indicated by the horizontal line at 13.1. The dashed line is a guide to the eye. Note, that in this sample the H content is much lower than that of D and therefore, the overlapping effect should be very large according to Blostein et al. [13].

concerning the analysis procedure of the data collected on the eVS instrument. They claim that the convolution formalism (see above)—as a procedure which does not take into account the complete absorption cross-section of the analyzer foil—produces errors resulting in incorrect peak positions in the time of flight spectra and, more importantly for the present work, incorrect peak areas. The latter are due to a misrepresentation of the right hand tail of e.g. the H recoil peak in the tof spectrum, thus giving rise to ‘erroneous’ areas due to overlap with the D recoil peak (see Fig. 1a).

The following analysis will show that the argument of Blostein et al. does not affect our experimental results and is thus irrelevant for the quantum entanglement effect under consideration, as observed in metallic hydrides. For a related DINS experimental test using $\text{H}_2\text{O}/\text{D}_2\text{O}$ mixtures, see the very recent Ref. [14].

2. Experimental and results

In order to proceed, the following statement will be the subject of the discussion here:

If the ‘anomalies’ found in the niobium hydrides (see Fig. 2) or the other condensed matter system studied thus far [4,5,8–12,14] are due to the misrepresentation of the right hand tail of the H recoil peak in the time of flight spectrum caused by overlapping, then these ‘anomalies’ should decrease with increasing angle where the peaks are more separated from each other than at smaller angles (see Fig. 1). To be more concrete, we will have a closer look at spectra recorded at two different scattering angles possessing a largely

differing extent of H and D peak overlap and then consider the determined relative H area values.

Here we show two spectra of $\text{NbH}_{0.16}\text{D}_{0.70}$. This sample was hanging freely in the incident neutron beam. Since the peak intensity of H is the subject of the considered quantum entanglement effect [8,9], a relatively high content of D atoms (the D mole fraction in this sample is $x_{\text{D}} = n_{\text{D}}/(n_{\text{H}} + n_{\text{D}}) = 0.8$) was chosen here in order to maximize the effect of the D signal on the right hand tail of the H signal in the tof spectrum.

As given in Fig. 1a, a strong overlap of the H and D peaks can be observed for scattering at $\theta = 42^\circ$, whereas this overlap is negligible at the higher angle of $\theta = 73^\circ$ (Fig. 1b). Therefore, following the argument of Blostein et al. [13], the H peak intensity should be more affected by the presence of the D signal in the spectrum at $\theta = 42^\circ$ than in the spectrum at $\theta = 73^\circ$. As a consequence, $\sigma_{\text{H}}/\sigma_{\text{Nb}}$, i.e. the H peak area normalized by its number density in the sample and divided by the respective quantity of Nb, should show a larger decrease at $\theta = 42^\circ$ with respect to the conventionally expected value of 13.1 than the corresponding one at the higher angle of $\theta = 73^\circ$. However, if one considers Fig. 2, it becomes evident that the opposite is the case, i.e. $\sigma_{\text{H}}/\sigma_{\text{Nb}}$ appears to be significantly smaller at higher angles than at smaller ones.

Summarizing, the better the peaks are resolved from each other, the larger are the found ‘anomalies’ which contradicts the statement given above. Therefore, as concerns the determined areas from the eVS data, the argument of Blostein et al. does not play any role and the associated sub-femtosecond quantum entanglement effect found in the metallic hydride is not affected at all.

3. Summary and conclusions

The experimental results reported above clearly contradict the statement that is given at the beginning of the previous section and that represents a consequence of the conclusions of Blostein et al. [13]. However, this does not mean that the theoretical investigations of Blostein et al. are fundamentally flawed. Rather, the above results along with previous investigations [14] demonstrate that the short-lived quantum entanglement effect revealed in the niobium hydride system as well as in the condensed matter systems studies thus far are real and are not caused by misinterpretation of data. In fact, the calculations of

Blostein et al. [13] might affect the majority of the NCS work on eVS dedicated to the determination of the ground state momentum distributions and the associated determinations of kinetic energies and ground state potentials. While we have shown that the data analysis procedure available on the eVS instrument is correct as concerns the determination of peak areas, the question remains open whether the same is valid for the determination of the shapes of momentum distributions as well. The continued development of the experimental set up of eVS within the VESUVIO project which involves a significant improvement of the energy resolution as well as associated Monte Carlo simulations will shed more light onto the effects of the energy resolution function on the determined shapes of the momentum distributions.

Acknowledgements

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