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Short lived protonic quantum entanglement and coupling to the electronic environment in LaH₂ and LaH₃

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Abstract

Very recently, a temperature dependent decrease of the protonic neutron scattering cross section σ_H in LiH using neutron Compton scattering (NCS) has been reported. The decrease of σ_H – which has been found in various materials using different experimental methods – is attributed to short-lived protonic quantum entanglement and it was suggested that the novel temperature dependence is due to the different coupling of the protons to the environment. The exact mechanism of the loss of coherence (i.e. decoherence) of the protonic quantum entangled states due to the interaction with the environment in condensed matter is not fully understood yet. To shed more light onto that, the NCS of LaH₂ and LaH₃ has been measured. While LaH₂ is metallic, LaH₃ is an isolator, thus providing completely different electronic environments the protons are coupled to. The experiment shows that σ_H is smaller for LaH₃ than it is for LaH₂. This result strongly suggest that the different couplings of the protons to the different electronic environments lead to different anomalies.

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1. Introduction

The importance of hydrogen in materials in general and in metals in particular for technological applications and in natural sciences is beyond any dispute. The increased awareness of the limitation of the natural fossil fuel reserves triggered a rethinking in new directions about energy generation. The increasing demand on the features of new materials necessitates the application of new production processes as well as new fundamental research towards a better understanding of the physical and chemical properties of hydrogen containing materials.

In condensed phases interactions of a particle with its environment can lead to quantum entanglement (QE). Such effects are theoretically expected to be extremely short-lived,

due to environmental disturbances. Therefore, it has been widely believed that they cannot be experimentally detected. However, based on previous theoretical work [1], the detection of protonic QE in condensed systems using sufficiently “fast” scattering techniques was proposed. Particularly suitable for this purpose is the neutron Compton scattering (NCS) method the time scale of which lying in the sub-femtosecond range.

In recent years we reported on a new fundamental aspect of the quantum dynamics of hydrogen in various condensed systems like water [2], organic compounds [3–6], and interstitial [7–9] as well as ionic metal hydrides [10]. The novelty of our results lies in the fact that the protons show an effective number density being different from the one supposed to be according to sample preparation. Thus, far these effects have not found a common explanation based on existing condensed matter theories. Rather, these anomalies are attributed to the existence of short-lived quantum entanglement

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of particles involving mainly the protons in these materials [1,11–13].

Very recently, we reported on the measured temperature dependence of the σ_{H} anomaly in LiH [10]. This is an experimental result which is in strong contrast to previous measurements on metallic hydrides like NbH or PdH [7–9]. It has been pointed out [10] that the difference in the experimental results of LiH on the one hand and of NbH and PdH on the other might arise from the fact that while the electronic structures of NbH and PdH, being interstitial hydrides, are similar, the electronic structure in LiH, being an ionic hydride, is completely different.

Following the supposition that the electronic environment might be participating in the dynamic QE effect of reduced protonic scattering cross section, we involved LaH₂ and LaH₃ which differ in their electronic structure completely from each other. Here, we report on our most recent NCS results on these hydrides.

2. Experimental and results

The measurements have been done using the time of flight inverse geometry spectrometer VESUVIO at ISIS, UK. The experimental setup is shown in Fig. 1A. The polychromatic neutrons are scattered by the sample into detectors arranged in an angular range between 30° and 80°. An analyzer foil situated between sample and detectors is cycled in and out of the sample detector axis. The analyzer foil absorbs neutrons at a fixed energy, e.g. 4.9 eV if using gold. The difference of a foil-in and foil-out spectrum gives the final spectrum (see Fig. 1B). The transfers of momentum $\hbar q$ and energy $\hbar\omega$ are so high on VESUVIO that the scattering occurs in the impulse approximation (IA) limit. Under such working conditions, the dynamic structure factor $S(q, \omega)$ of a nucleus of a particular mass M consists of a single peak, i.e., $S(q, \omega) = J_{\text{M}}(y_{\text{M}})M/\hbar q$. Here y_{M} is a scaling variable $y_{\text{M}} = (\hbar\omega - \hbar^2 q^2/2M)M(\hbar q)^{-1}$ [14] and $J_{\text{M}}(y_{\text{M}})$ is the Gaussian shaped neutron Compton profile of the scattering nucleus. Using these quantities, the double differential scattering cross section then reads $d^2\sigma/d\Omega dE_1 = b_{\text{M}}^2 J_{\text{M}}(y_{\text{M}})Mk_1/\hbar qk_0$. The experimentally observed intensity is then proportional to

$J_{\text{M}}(y_{\text{M}})$ convoluted with the instrument resolution function $R_{\text{M}}(y_{\text{M}})$. The peak area A is then proportional to the number density N and to the scattering cross section σ of an isotope in the sample. It follows that

$$\frac{A_i}{A_j} = \frac{N_i\sigma_i}{N_j\sigma_j} \quad \text{or} \quad R_{\text{exp}} = \frac{\sigma_i}{\sigma_j} = \frac{A_i/N_i}{A_j/N_j} \quad (1)$$

Within the IA, it is possible to define a scattering time by $q(\theta)\tau_{\text{sc}}v_0 \approx 1$ [10]. Here, $q(\theta)$ is the scattering angle dependent momentum transfer, and v_0 is the root mean square velocity of the nucleus before scattering. The scattering time is the time range within which the neutron interacts with the scattering nucleus. Therefore, it can be regarded as the time window during which the dynamics of the nucleus is sampled.

We performed new NCS measurements on LaH₂ and LaH₃ at room temperature. The samples were put in standard flat Al cans. An example spectrum of LaH₃ is shown in Fig. 1B. It consists of two peaks: one at 200 μs is due to H and another peak at ca. 375 μs is due to scattering from Al and La. The latter two peaks can not be resolved in the forward scattering spectra. However, due to the much higher $\hbar q$ and $\hbar\omega$ achieved in backscattering, it is indeed possible to resolve the La peak from the Al one. This peak separation facilitates the determination of the area ratio $(A_{\text{La}}/A_{\text{Al}})_{\text{back}}$ which can be used to extract the contribution of the La scattering from $(A_{\text{La}} + A_{\text{Al}})_{\text{for}}$ of the forward scattering. Having determined A_{La} , it is straightforward to determine $R_{\text{exp}} = \sigma_i/\sigma_j = (A_{\text{H}}/N_{\text{H}})/(A_{\text{La}}/N_{\text{La}})$ and to compare it with the tabulated value $R_{\text{tab}} = (\sigma_{\text{H}}/\sigma_{\text{La}})_{\text{tab}} = 9.1$.

The results of this experiment are shown in Fig. 2. As can be seen very easily, R_{exp} is strongly reduced with respect to the tabulated value of R_{tab} for both systems. In addition, a slight angle dependence is visible as well: The anomaly is smaller in the low angle region than it is in the high angle one. However, most importantly for the present context is the fact that the anomaly of LaH₃ is different from the LaH₂ one. It is also visible that these differences are more pronounced in the high angle region.

To summarize, we found for the first time a significant dependence of the dynamical quantum entanglement effect, being manifested by protonic scattering cross section anomaly, on the electronic structure surrounding the protons.

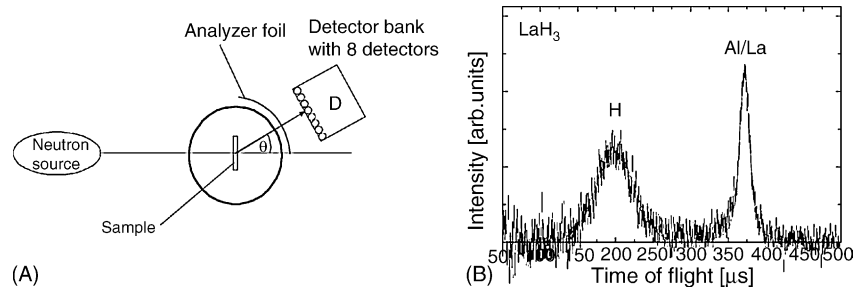


Fig. 1. (A) Schematic instrument setup: The polychromatic neutrons leave the neutron source, are scattered by the sample under the angle θ and are detected in D. The analyzer foils are cycled in and out of the scattered neutron beam. (B) Time of flight difference spectrum of foil in and foil out spectrum of LaH₃.

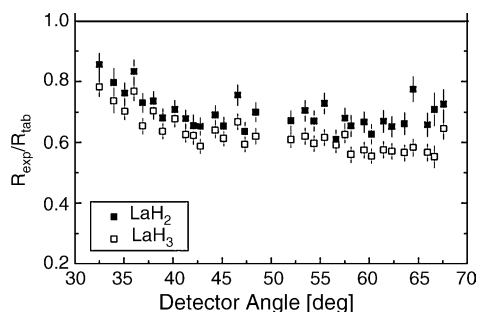


Fig. 2. The experimental ratios $R_{\text{exp}} = (\sigma_{\text{H}}/\sigma_{\text{La}})_{\text{exp}}$ of LaH_2 and LaH_3 , respectively, divided by the tabulated one $R_{\text{tab}} = (\sigma_{\text{H}}/\sigma_{\text{La}})_{\text{tab}} = 9.1$ as a function of scattering angle. $R_{\text{exp}}/R_{\text{tab}}$ is strongly reduced and a slight angle dependence is observed for both systems. Most importantly, however, is that LaH_2 and LaH_3 show different anomalies which is attributed to the coupling of the protons to the different electronic environments – LaH_2 being metallic and LaH_3 being an insulator.

3. Summary and conclusions

The scattering cross section anomalies found in various hydrogen containing materials have found thus far no explanation within existing condensed matter theories. Recently, a neutron transmission experiment showed no cross section anomalies in water [15]. However, its inappropriateness has been discussed by Karlsson and Mayers [16]. Additionally, the NCS data analysis procedure as applied on VESUVIO has been criticized by some authors [15,17]. But, very recently, it has also been shown in a very detailed work that the involved data analysis procedure is indeed correct and that the criticisms outlined in [15,17] do not account for the experimentally found anomalies [18]. Furthermore, we also succeeded to confirm the NCS results by applying an independent method, namely electron-proton Compton scattering (ECS) [6]. This method is completely different from NCS due to the fact that Coulomb interaction is involved in ECS in contrast to the strong interaction involved in NCS. In addition, the ECS instrument is completely different in that the incoming electron beam is continuous as well as monochromatic and the spectra are recorded with respect to energy loss. In the light of these facts, the present experimental results on LaH_2 and LaH_3 as well as the previous ones on LiH [10] indicate that the electronic environment surrounding the

hydrogen atom in the material might be responsible for the different features of the cross section anomalies of the proton and thus for different decoherence mechanisms. This interpretation is supported by the fact that the time scale involved in the NCS process ($<10^{-15}$ s) is of the order of the electronic dynamics. Due to this fact, it is very straightforward to see the importance of the dynamical quantum entanglement effect for chemical processes occurring in condensed systems at room temperature.

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