



Irreversible hydrogen quantum dynamics and anomalous scattering behavior in liquids and solids

T. Abdul-Redah^{a, b, *}, C.A. Chatzidimitriou-Dreismann^c

^a*School of Physical Sciences, The University, Canterbury CT2 7NR, UK*

^b*ISIS Facility, Rutherford Appleton Laboratory, Chilton/Didcot OX11 0QX, UK*

^c*Institute of Chemistry, Stranski Laboratory ERI, Technical University of Berlin, Str. d. Juni 112, D-10623 Berlin, Germany*

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Abstract

We report on neutron–proton Compton scattering experiments on various hydrogen containing materials like water, an organic polymer and an ionic metal hydride. Furthermore, results of an electron–proton Compton scattering experiment on the polymer are presented. The results reveal a strong decrease of the scattering integral intensities due to the protons in these materials. Thus far these effects have found no common explanation based on existing condensed matter theories. Rather, they invoke the existence of quantum correlations (also called quantum entanglement—QE) and decoherence between the particles. Of particular importance in the present context is the fact that the interaction time of the probe (i.e. neutron or electron) must be of the same order of magnitude as the decay of the coherence (also called decoherence) of the correlated particles. The found experimental effects and their possible explanations may have far reaching consequences for condensed matter physics and in particular for the theoretical treatment of hydrogen containing materials.

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1. Introduction

The importance of hydrogen in materials for technological applications and in natural science is beyond any dispute. The increased awareness of the limitation of the natural fossil fuel reserves (oil, coal, and gas) triggered a rethinking in new directions about energy generation, including solar, wind, and hydrogen energy. The increasing demand on the features of new materials necessitates the application of new production processes and new experimental techniques. Therefore, the engineering aspect of hydrogen energy, storage and hydrogen treatment of materials gives an incentive to develop new and more advanced experimental techniques to reveal more accurate and sophisticated information about

new materials. Thus, the research on these materials reflects in a very impressive way the interconnection between fundamental research and engineering, towards a better understanding of the physical and chemical properties of hydrogen containing materials in order to get more efficient and safer materials.

According to present-day knowledge, chemical bonds are theoretically treated by solving the electronic Schrödinger equation, using the well-known Born–Oppenheimer (BO) scheme and obtaining the wave functions which describe the distribution of electrons in molecules. Furthermore, one describes a chemical reaction as the “movement” of nuclei considered as classical mass points or as quantum mechanical wave packets on electronic BO energy surfaces. Both treatments, however, have in common that the number of particles cannot change. More precisely, in classical mechanics, particles never “disappear” and according to “standard” quantum mechanics, in which the fundamental

* Corresponding author. ISIS Facility, Rutherford Appleton Laboratory, Chilton/Didcot OX11 0QX, UK.

phenomenon of decoherence (see below) is discarded, the time evolution of the wave function of the particles is always unitary, thus conserving the normalization of the wave function and, equivalently, the number of particles.

Here we focus on a new fundamental aspect of the quantum dynamics of hydrogen which goes beyond the conventional theoretical treatment. The novelty of our results from scattering experiments lies in the fact that the protons show an effective number density being different from the one supposed to be according to sample preparation or chemical formula. Pictorially speaking, parts of the protons are invisible for the incoming probe beam (consisting of neutron, electrons or electromagnetic waves). As mentioned above, the conventional theoretical treatment cannot explain this phenomenon. Rather, this behavior is attributed to the existence of short-lived quantum correlations of particles involving mainly the protons in these materials. Due to the low mass of hydrogen and consequently the long de Broglie wavelength representing delocalization, the appearance of quantum features seems to be very conceivable. Already here, it should be mentioned that this anomalous scattering behavior has far reaching consequences, for example for the application of the kinetic gas theory in the context of chemical reaction kinetics and mechanisms in condensed systems.

Interactions between adjacent particles in condensed phases can lead to quantum correlation phenomena also called quantum entanglement (QE). Such effects are theoretically expected to be extremely short-lived, due to decoherence being induced by environmental disturbances. Because of the extremely fast dynamics of decoherence, it has been widely believed that QE effects cannot be experimentally detected in condensed matter. 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 lies in the subfemto–second time range. The first experiments were on H₂O/D₂O mixtures at room temperature [2]. As already mentioned, the effective particle number densities of H and D found in the H₂O/D₂O mixtures were not what one would expect due to sample preparation. Concretely, an “anomalous” decrease of the scattering cross section ratio of H and D, i.e. σ_H/σ_D , with respect to the expected ratio according to the tabulated values has been found [2]. In addition, these “anomalies” showed a strong dependence on the D mole fraction of the sample.

Furthermore, very recently we succeeded to confirm these protonic scattering anomalies (see e.g. [3,4]) with a completely different scattering method, namely electron–proton Compton scattering. This technique is different from the neutron one because it involves Coulomb interaction between the scattered electron and the proton which is in contrast to the strong interaction being involved in the neutron–proton scattering [3,4].

The aim of this paper is to bring fundamental research on hydrogen in condensed systems to the attention of the scientific community working on hydrogen energy in materials and to show new concepts relating modern quantum theory of condensed systems and material sciences.

In Section 2 an outline of the theoretical background of open quantum systems is given in terms of the creation of QE between two particles and its decoherence due to the interaction with the environment. Section 3 is dedicated to a basic description of the used experimental technique, namely NCS. Section 4 which contains the experimental results is followed by the theoretical interpretation of the results in Section 5. The paper concludes with a discussion and outlook part in Section 6.

2. Theoretical background

Physical quantum systems are usually theoretically treated as isolated or closed systems, i.e., they are assumed not to interact with their surroundings. Let A be a quantum particle that is close to another particle B . Since A and B are regarded as closed systems, no interaction between A and B or with any kind of environment is considered. Therefore, their joint state can be assigned a single wave function given by a product state:

$$\Psi(A, B) = \varphi(A) \otimes \phi(B). \quad (1)$$

(If A and B are identical systems, a corresponding symmetrization or antisymmetrization must be considered). Because A and B constitute closed systems, each of them follow Hamiltonian dynamics through the Liouville–von Neumann equation

$$\dot{\varrho}_{A+B} = -i[H, \varrho_{A+B}]. \quad (2)$$

ϱ_{A+B} is the complete system’s density matrix and is block diagonal due to the independence of A and B . Because of the unitarity of this equation—given by the hermiticity of H —non-vanishing off diagonal matrix elements representing phase coherences between degrees of freedom of A and B cannot be created, i.e. ϱ remains block diagonal.

In reality, however, particles do interact with their surroundings and/or with each other and therefore an initially factorizing state will in general not keep this property if interaction is present. To be more specific, consider the Hamiltonian of the complete system $A + B$:

$$H_C = H_A + H_B + V_{A,B} \quad (3)$$

where H_A and H_B are the Hamiltonians of A and B , respectively, and $V_{A,B}$ is the interaction of A and B . Because in general $V_{A,B}$ does not commute with H_A or H_B , respectively, the time evolution operator of the complete system

$$U_{A,B} = \exp(-i(H_A + H_B + V_{A,B})t/\hbar) \quad (4)$$

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