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Anomalous scattering of keV neutrons from H_2O and D_2O: I. Single scattering events

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Abstract

Scattering of neutrons in the 24–150 keV incident energy range from H_2O relative to that of D_2O and H_2O–D_2O mixtures was reported recently by Moreh *et al*. This work is related to neutron Compton scattering experiments regarding the 'anomalous' scattering from protons, observed earlier at ISIS by Chatzidimitriou-Dreismann *et al* in the 5–100 eV range. Here we provide the complete data reduction scheme of time-of-flight integrated intensities measured at keV energy transfers, within the impulse approximation of standard theory and for single scattering events. Current investigations of multiple scattering events and the associated preliminary results are mentioned. Direct application of the theoretical results to the new keV scattering data reveals an anomalous ratio of scattering intensity of H_2O relative to that of D_2O of about 20%, thus being in good agreement with the earlier results of the original experiment at ISIS.

1. Introduction

In a recent letter by Moreh *et al* [1], scattering results of neutrons from H_2O relative to those of D_2O and H_2O–D_2O mixtures, in the incident energy range about 24–150 keV, were reported. This work was carried out to search for an anomalous decrease [2] in the neutron scattering intensity from protons at interaction times in the attosecond regime, 10^{-17} s. The energy range here is more than 1000 times larger than that of the original neutron Compton scattering (NCS) experiment carried out with the electron volt spectrometer eVS (newly VESUVIO) at the neutron spallation source ISIS [2]. In this NCS experiment, an anomalous reduction of the neutron scattering intensity from protons relative to that from deuterons was found.

This new phenomenon has been observed at ISIS in a considerable variety of systems, cf [2–6]. However, a full explanation of it remains still the subject of a flurry of theoretical activity [7–14]. Recently, this effect has been confirmed with an independent experimental method, i.e. electron–proton Compton scattering (ECS) from two solid polymers [15–17]; see

also [18]. Note that the data processing of ECS is much simpler than that of NCS [17]; for full details of NCS data analysis, see [19]. Nevertheless, to the great regret of the whole 'neutron community', the necessary conditions for the observation of the considered effect could until now only be realized at the unique time-of-flight (TOF) spectrometer of ISIS, i.e. VESUVIO. Therefore, the novelty of a possible independent *neutron scattering* measurement, like that of [1], is self-evident.

In clear contrast to the NCS and ECS results, Moreh *et al* claimed that the measured neutron scattering intensity ratios in the keV range exhibit no anomalous behaviour. It was concluded that within an overall statistical accuracy of 3% there is no evidence for any deviation from the ratios conventionally calculated on the basis of the tabulated total neutron cross sections [1]. However, only incomplete indications of the used theoretical data-treatment were presented in that paper, and thus an independent assessment of the above claims and/or physical implications was not possible. Nevertheless, it was correctly argued [1, 18] that one would have to shake some well established notions in physics to explain the aforementioned scattering anomaly.

Bearing in mind the possible importance of these keV experimental results, we analysed in detail the data processing scheme indicated in [1] on the basis of standard scattering theory at large energy transfers, where the impulse approximation (IA) is valid; cf [19, 20]. In the present paper, we present the analytical treatment of *single scattering events* in the keV regime and compare the derived analytical results with the experimental data. To our knowledge, this analytical treatment does not exist in the literature thus far. The important issue of *multiple scattering* is shortly mentioned, together with first associated results of current calculations (work in progress) in section 3.

As a result, our theoretical analysis leads to revision of the main finding and conclusion of [1]. It is demonstrated that the correct keV data reduction reveals a strongly anomalous ratio of scattering intensity of H_2O with that of D_2O of about 20%, thus being in good agreement with the associated results of the original ISIS experiment [2]. The calculations presented below contain no fitting parameter.

1.1. Comparison of experimental techniques

To start with, it is important to note that both set-ups of the new keV neutron experiment at the Rensselaer Polytechnic Institute (RPI) [1] and that of VESUVIO at ISIS are essentially similar and the interpretation of their results ought to be based on the same basic theory. The following related remarks are in order.

(i) Both are so-called *inverse geometry* TOF set-ups; i.e., the final energy E_1 of the measured neutrons is fixed, the neutron initial energy E_0 is 'continuous', and the scattered neutrons are analysed using a 'filter' (of Fe at RPI, with $E_1 = 24.3(\pm 1.1)$ keV) or 'analyser foil' (of Au at ISIS, with $E_1 = 4.91(\pm 0.14)$ eV).

(ii) The range of scattering angles θ is similar in both set-ups (i.e. one detector integrating over $\theta = 25°$–$65°$ at RPI; 32 detectors measuring at various scattering angles in the range $35°$–$67°$ at ISIS).

(iii) As a consequence, and according to standard theory [20], the characteristic neutron–proton scattering time in the keV range is shorter by a factor of about 70 [1] as compared to that of the ISIS set-up. In view of some of the mentioned theoretical models [7–15], however, this difference may not preclude the appearance of the considered effect in the keV range.

(iv) As stressed in [1], the IA can be safely assumed to be exact in the keV range, and it is known to be sufficiently fulfilled in the eV range of VESUVIO [19, 20]. In simple terms, each neutron scatters from a single nucleus (of H, D or O).

(v) The set-up at RPI cannot resolve the neutrons scattered from different nuclei, and yields instead an *integrated* scattering signal arising from the (O, H and/or D) nuclei of the liquid samples. The ISIS set-up, however, provides a H-recoil peak well resolved from that of D or O, but this does not represent any significant difference that would prevent comparison of results.

(vi) In the RPI experiment, the scattering intensity, measured by a single detector, is represented by the area of the 24.3 keV line in the TOF spectra, i.e. by adding up the total number of counts in the 24.3 keV peak [1]. An independent fission detector was employed as a neutron flux monitor and served to normalize the TOF spectra. After subtracting the background from each signal, the intensity ratios are taken, as presented in figure 3 of [1]. The measurements were repeated about five times, always giving about the same results within statistics.

(vii) An important difference, however concerns the sample thickness, which, in the RPI experiment, was 18 mm. Obviously, a significant amount of multiple scattering from H_2O must exist (easily estimated to be about 20%). In contrast, the measurements at ISIS are usually made with thin samples exhibiting much less (typically only a few per cent) multiple scattering. This point will be considered further below.

2. Calculation of single scattering events

We now proceed to the derivation of the theoretical expectation for the ratio of scattering intensity of H_2O and D_2O, in the frame of the IA of standard theory; cf [19, 20]. Here we will consider only single scattering effects; cf point (vii) above. The obtained result is interesting in itself, and is also in line with an associated claim of Moreh *et al*, who write 'The effect (of multiple scattering) on the *ratio* of scattering intensities from the two samples is $<1\%$ and was neglected.'; see page 4 of [1].

The starting point is the well established expression for a TOF spectrum as measured with 'inverse geometry' instruments, where the final energy (E_1) of the scattered neutron is fixed and its initial energy (E_0) varies (see e.g. [19], section 2.1). Since in this paper we consider *integrated* intensities only, and to simplify the presentation, we may consider an ideal inverse geometry instrument with precisely defined $E_1 = E_R$ determined by an ideal 'filter' (or resolution) function $D(E_1) = D(E_R)\delta(E_1 - E_R)$.

Let us consider scattering from a sample containing atoms of mass M. From basic theory it then follows for the count rate $C_M(t)$ originated from M, at TOF time equal to t,

$$C_M(t) = f' E_0^{3/2} I(E_0) D(E_1) N_M \frac{\mathrm{d}^2\sigma_M}{\mathrm{d}\Omega\,\mathrm{d}E_1}\,\mathrm{d}\Omega. \tag{1}$$

The factor f' contains various instrumental parameters and the neutron mass m; see e.g. [19], section 2. This is the standard expression for the count rate in an inverse geometry TOF spectrometer [19, 21]. For isotropic scattering, the double differential cross section is given by

$$\frac{\mathrm{d}^2\sigma_M}{\mathrm{d}\Omega\,\mathrm{d}E_1} = b_M^2\sqrt{\frac{E_1}{E_0}}S_M\,(\omega, q) \tag{2}$$

($\hbar\omega$ and $\hbar q$: energy and momentum transfers). Defining $f = f' D(E_1)\sqrt{E_1}$, equation (1) yields

$$C_M(t) = f[E_0 I(E_0)]_M N_M b_M^2 S_M(\omega, q). \tag{3}$$

Note that, for fixed final energy E_1, $E_0(t)$ is a function of the (TOF) time t. The intensity $C_M(t)$ of the TOF spectrum is then proportional to $E_0 I(E_0) S_M(\omega, q)$.

The incident neutron flux $I(E_0)$ varies with the incident neutron energy. In the keV experiment one has $I(E_0) \propto E_0^{-0.65}$ [1]. Thus $E_0 I(E_0) \propto (E_0)^{0.35}$.

It should be observed that, while the TOF varies, both ω and q vary, too. As a result, the integrated intensity of a peak in the spectra is not the same as that obtained in a constant-q scan [10], that is easily compared with theory, the latter being due to the well known relation

$$\int S_M(\omega, q = \text{const})\, \mathrm{d}\omega = 1. \tag{4}$$

Namely, a crucial argument by Cowley [10] consists in the fact that the measured intensity $C_M(t)$ is multiplied by a factor of $1/J_M$ compared with the intensity that would be observed in an associated constant-q experiment. J_M is the Jacobian of the transformation from the actually performed TOF scan to the (fictitious) constant-q scan. For an inverse geometry TOF instrument the Jacobian is

$$J_M = 1 - (m/M)\left[1 - \sqrt{E_1/E_0}\cos\theta\right] \tag{5}$$

see equation (9) of [10]. Since the scattering angle θ and the final energy E_1 are kept constant, J_M is a function of E_0 and thus of the TOF t. The relative scattering cross-sections can then be obtained from the intensities of observed peaks if the observed intensities are multiplied by $J_M/[I(E_0)E_0]$ before comparing with the theoretical results [10]. Therefore, it follows from equation (3)

$$C_M(t)\frac{J_M}{[E_0 I(E_0)]_M} = f N_M b_M^2 S_M(\omega, q) J_M. \tag{6}$$

Integrating both sides over ω,

$$\int C_M(t) J_M/[E_0 I(E_0)]_M\, \mathrm{d}\omega = f N_M b_M^2 \int S_M(\omega, q) J_M\, \mathrm{d}\omega = f N_M b_M^2 \tag{7}$$

where equation (4) is used in the last equation.

Since spectral characteristics of the recoil peak are not known, one can approximate $[E_0 I(E_0)]_M$, as well as the Jacobian J_M, with their constant values at the peak centre (corresponding to $\hbar\omega = \hbar^2 q^2/2M$), obtaining

$$J_M/[E_0 I(E_0)]_M \int C_M(t)\, \mathrm{d}\omega = f N_M b_M^2. \tag{8}$$

It is crucial to note that, in the keV range, this approximation is very good, simply because the recoil peaks are very narrow, as compared to those obtained in the eV range of VESUVIO. For illustration, figure 1 shows the simulated TOF spectrum of H_2O, applying standard theory [19] and using the instrumental parameters of the RPI set-up [1].

Recall now that with Moreh's experimental set-up one can only measure *integrated* intensities. It is important to note that the scattering intensity is represented by the area of the 24.3 keV line in the TOF spectra [1]. Thus one must calculate the integral $\int C_M(t)\, \mathrm{d}t$ over the TOF window of the peak corresponding to the 24.3 keV Fe filter, i.e., over the TOF interval about 11–14 μs (cf figure 2 of [1]), before any comparison with the experiment can be done. To achieve this integration, we multiply both sides of this equation with the Jacobian $[\mathrm{d}t/\mathrm{d}\omega]$ of the transformation from TOF to energy transfer, and use the relation $[\mathrm{d}t/\mathrm{d}\omega]\, \mathrm{d}\omega = \mathrm{d}t$. Thus we obtain

$$\frac{J_M}{[E_0 I(E_0)]_M} \int C_M(t)[\mathrm{d}t/\mathrm{d}\omega]_M\, \mathrm{d}\omega = f\, N_M b_M^2 [\mathrm{d}t/\mathrm{d}\omega]_M \tag{9}$$

and rearrangement of factors yields

$$\overline{C_M} \equiv \int C_M(t)\, \mathrm{d}t = f\, [E_0 I(E_0)]_M J_M^{-1} \left[\frac{\mathrm{d}t}{\mathrm{d}\omega}\right]_M N_M b_M^2. \tag{10}$$

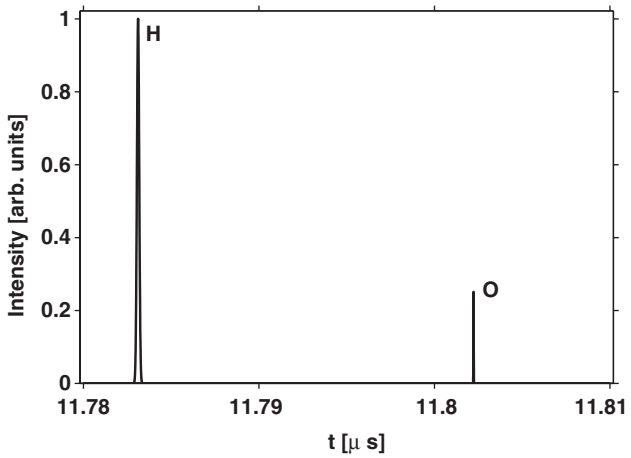

Figure 1. Simulated TOF spectrum of H_2O using the instrumental parameters of the keV experiment [1]. The widths (FWHM) of the two peaks are 15.21×10^{-5} μs for H and 2.22×10^{-5} μs for O.

Again, the Jacobian $[\mathrm{d}t/\mathrm{d}\omega]_M$ in the rhs is taken at the peak centre. This Jacobian is well known in TOF spectroscopy [21]. E.g. it may be obtained by

$$\frac{\mathrm{d}t}{\mathrm{d}\omega} = \frac{\mathrm{d}t}{\mathrm{d}E_0} = \frac{1}{\mathrm{d}E_0/\mathrm{d}t} = cE_0^{-3/2} \tag{11}$$

(c: constant). The latter equation is derived explicitly in [19], equation (2.9).

An additional point to be considered is the numerical value of b_M^2. Note that the scattering length b_M is a parameter of the Fermi pseudo-potential, $V(r) = (2\pi\hbar^2/m)\, b_M\, \delta(r)$. It can be deduced from the associated measured 'free atom' total cross section σ_M [22], by noting the important result

$$\int \frac{\mathrm{d}^2\sigma_M}{\mathrm{d}\Omega\, \mathrm{d}E_1}\, \mathrm{d}\Omega\, \mathrm{d}E_1 = \frac{4\pi b_M^2}{(1+m/M)^2} = \sigma_M \tag{12}$$

see e.g. [19], equation (2.16). It is crucial to note that, in the keV range under consideration, σ_M and thus also b_M^2 depend on the initial energy E_0. This dependence is particularly important for σ_{H} [22].

Summarizing, equation (10) represents the *theoretically predicted value* of the integrated intensity $\overline{C}_M \equiv \int C_M(t)\, \mathrm{d}t$, and the latter is to be compared with the *experimental* results of [1]. E.g., the integral scattering intensity from pure H_2O is simply $\overline{C}_{\mathrm{H_2O}} = 2\,\overline{C}_{\mathrm{H}} + \overline{C}_{\mathrm{O}}$, i.e.

$$\overline{C}_{\mathrm{H_2O}} = F[E_0 I(E_0)]_{\mathrm{H}} J_{\mathrm{H}}^{-1} [\mathrm{d}t/\mathrm{d}\omega]_{\mathrm{H}} 2 \times b_{\mathrm{H}}^2 + F[E_0 I(E_0)]_{\mathrm{O}} J_{\mathrm{O}}^{-1} [\mathrm{d}t/\mathrm{d}\omega]_{\mathrm{O}} 1 \times b_{\mathrm{O}}^2 \tag{13}$$

(F: constant independent of M, E_0 and t). Similarly, one can calculate the integral scattering intensity $\overline{C}_{\mathrm{D_2O}}$ from pure D_2O, as well as the intensity ratio $\overline{C}_{\mathrm{H_2O}}/\overline{C}_{\mathrm{D_2O}}$. Obviously, in the latter the constant F is cancelled out. This ratio contains no fitting parameters at all.

To compare with a calculation in [1], our derived theoretical prediction equation (10) is now applied to integrated scattering intensities at $\theta = 45°$. The corresponding incident energies E_0 for H, D and O are 48.6 keV for H, 32.9 keV for D and 25.2 keV for O [1]. At these incident energies, the measured total cross sections for H, D and O are 15.7, 3.34 and 3.73 barn [22]. From equation (12) we then obtain the associated values of $4\pi b_M^2$ for H, D and O, which are 62.8, 7.515 and 4.21 barn. For $[E_0 I(E_0)] \propto (E_0)^{0.35}$ one obtains numerical values proportional

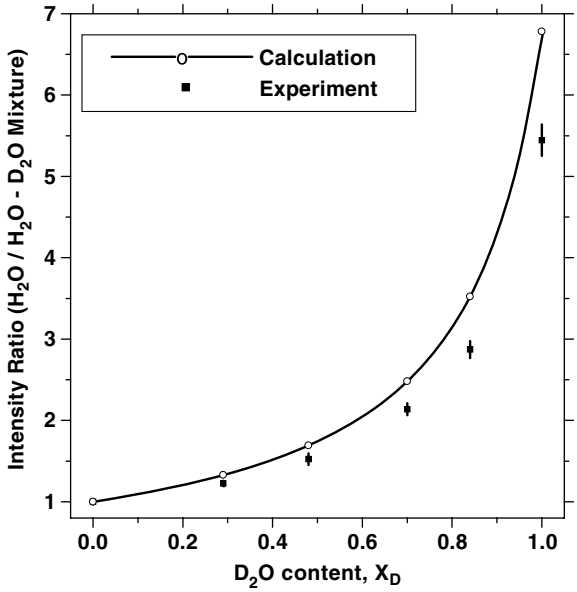

Figure 2. Measured (full squares, with error bars)—taken from figure 3 of [1]—and corrected calculation (solid line, open circles) for $\theta = 45°$ of scattered intensity ratios versus X_D, the D_2O concentration in the H_2O–D_2O mixture. The calculated intensity ratio for pure H_2O and pure D_2O is 23% higher than the experimental one; see the text.

to 3.89 (for H), 3.40 (for D) and 3.09 (for O). (The proportionality constant cancels out in the intensity ratios given below.) The Jacobians J_M, equation (5), are calculated with the aid of the well known equation

$$\sqrt{\frac{E_1}{E_0}} = \frac{\cos\theta + \sqrt{(M/m)^2 - \sin^2\theta}}{M/m + 1} \tag{14}$$

which holds for the peak centre [3, 6, 19]. The J_M-values for H, D and O are equal to 0.5000, 0.8038 and 0.9809. Finally, the numerical values of the Jacobian $d\omega/dt = dE_0/dt$ are proportional to 338.8 (for H), 188.8 (for D) and 126.6 (for O). Thus we obtain for the ratio of integrated intensities from pure H_2O and pure D_2O at $\theta = 45°$ the theoretically expected result

$$\overline{C}_{H_2O}/\overline{C}_{D_2O} \approx 6.78 \tag{15}$$

which is about 23% *larger than the measured* value of 5.5, the latter being given in figure 3 of [1].

The results of our calculations for all intensity ratios investigated in [1] are presented in figure 2, together with the experimental data. As the overall errors of the measurements were about 3% while the actual statistical errors were about 2% [1], one must conclude that the revealed anomaly is significant.

For a further check of the derivations, we repeated the above calculation by introducing the West scaling of the dynamic structure factor,

$$S_M(q,\omega) = \frac{M}{\hbar q} J_M(y_M), \tag{16}$$

where $\hbar y_M = (M/\hbar q)(\hbar\omega - \hbar^2 q^2/2M)$ and $J_M(y_M)$ is the M-nucleus momentum distribution (see [19], section 2). This scaling is commonly applied in NCS investigations [20]. Here, the

Jacobian ($\mathrm{d}y_M/\mathrm{d}t$) is needed, in order to calculate the integrated intensities $\overline{C}_M$, which are obtained from the exact expression (see [19], equation (2.21))

$$C_M(t) = A_M \frac{E_0 I(E_0)}{\hbar q} M J_M(y_M), \tag{17}$$

where the constant A_M is proportional to $N_M b_M^2$.

For $\theta = 45°$, this alternative data processing produced the same result (15). Our results were confirmed independently by calculations of Mayers, applying the routines for NCS-data analysis available at ISIS [28].

To estimate possible errors of result (15) we made additional calculations taking into account the finite widths of the resolution function $D(E_1)$ and of the H-recoil peak; result (15) was found to remain unaffected. Furthermore, we calculated the average of the above ratio over scattering angles between 25° and 65°, i.e. the angular range given in [1]. The E_0-dependence of σ_H was taken into account. A result similar to (15) was obtained: $\overline{C}_{\mathrm{H_2O}}/\overline{C}_{\mathrm{D_2O}} \approx 6.64$, being about 21% larger than the measured value of 5.5.

2.1. Remarks on multiple scattering (MS)

As mentioned above, effects of multiple scattering (MS) were not considered here. This was motivated by findings of Moreh *et al*, who wrote 'The effect (of MS) on the *ratio* of scattering intensities from the two samples is <1% and was neglected.'; see [1], page 4.

Curiously, our preliminary MS calculations [23] seem to support qualitatively this finding, since $R = \overline{C}_{\mathrm{H_2O}}/\overline{C}_{\mathrm{D_2O}}$ appears to depend on MS only weakly. This happens for the following reasons. The large sample thickness (18 mm) of these experiments leads to a considerable *attenuation* of the neutron beam (transmitted through the sample) and associated *decrease* of the single scattering intensity component. This attenuation would have led to a ratio $R \approx 5.5$, if only single scattering events had contributed to the measured (total) intensity—which of course is not true. Obviously, this attenuation is intrinsically connected with a considerable *increase* of the rate of double scattering events from protons. This scattering from protons is not isotropic, but it was shown to be strongly oriented in the 'forward' scattering direction $\theta < 90°$ [23], thus increasing again the total scattering intensity measured by the detector in the angular range $\theta = 25°$–$65°$ of the RPI set-up [1].

More specifically, preliminary calculations [23] of double scattered neutrons from H_2O at $\theta = 45°$ and their contribution to the total scattering intensity from H_2O lead to a slightly reduced value $R = 6.55$ as compared with (15). This value is anomalously larger than the experimentally determined [1] ratio $R_\mathrm{exp} = 5.5$ by about 19%. Further analytical and numerical MS investigations are currently in progress.

3. Discussion

The detailed calculation of intensity ratios presented above, based on single scattering events, is in contrast to that indicated in [1]. In particular, Moreh *et al* calculated for $\theta = 45°$ the laboratory scattering cross sections (say, $\mathrm{d}\sigma/\mathrm{d}\Omega$) of neutrons from H, D and O, which are 3.5, 0.47 and 0.33 barn sr^{-1}; see [1] for details. (These values were deduced using standard theory and the ENDF tabulated data [22] of the total neutron cross sections.) Based on these values, a straightforward calculation of the ratio comparing scattering from H_2O and D_2O then yields

$$\frac{(\mathrm{d}\sigma/\mathrm{d}\Omega)_{\mathrm{H_2O}}}{(\mathrm{d}\sigma/\mathrm{d}\Omega)_{\mathrm{D_2O}}} = \frac{2 \times 3.5 + 1 \times 0.33}{2 \times 0.47 + 1 \times 0.33} = 5.77 \tag{18}$$

which might appear to be in good agreement with the measured ratio (=5.5) of integrated intensities. However, this result does not prove such an agreement, for the trivial reason that the proportionality factor between $(\mathrm{d}\sigma/\mathrm{d}\Omega)_M$ and integrated scattering intensity $\overline{C}_M \equiv \int C_M(t)\,\mathrm{d}t$ is *not* independent of M, and thus the first equality in (18) is erroneous.

The preceding derivations and the corrected interpretation of Moreh's experimental results [1] have various far-reaching theoretical and experimental consequences. A few related remarks are in order.

First, it should be stressed that the intensity ratios determined in this experiment can only provide information about a possible *difference* between the scattering behaviour of H and D, and not about that of H alone. In view of several theoretical works [9, 11, 12], it may be expected that, in the keV range, both protons and deuterons should violate the Born–Oppenheimer (BO) approximation, leading to the above 'anomaly' for both H and D.

Second, earlier NCS from D-containing materials has already shown that D also exhibits a small anomalous shortfall of scattering intensity. E.g., in [3] it was reported that this shortfall in $NbD_{0.8}$ was about 10%. Several NCS measurements on pure D_2O showed a shortfall of the cross sections ratio σ_D/σ_O of about 10–15% [24]. Based on these experimental findings and the 20% anomaly of the ratio (15), one thus may conclude that $\overline{C}_{H_2O}$ exhibits an anomalous shortfall of the order of 25%.

Third, as noticed by Cowley [10], the considered intensity shortfall is inconsistent with the sum rules of standard theory. However, the fast neutron–proton collision is governed by a *non-unitary* time evolution, due to the decoherence effect [9]. Note that such a time evolution is not taken into account in the proof of the sum rules, which are based on the standard *unitary* quantum dynamics of closed quantum systems.

Additionally, the following point should be mentioned. The possible 'divergence' [25] of the integral of $S(q,\omega)$ over ω for a constant scattering angle θ does not affect the results presented above. This is because the scattering angular range $\theta = 25°$–$65°$ of the keV experiment is well within the range of validity of data analysis based on the impulse approximation, as discussed by Cowley and Mayers [25]. Moreover, according to the recent study by Dorner [26], the aforementioned 'divergence' does not exist, even at scattering angles larger than 65°, if all TOF-dependent factors in (10) are applied 'pointwise' for all TOF values, instead of using the single TOF values calculated at the peak centres; see also [27]. However, due to the narrowness of the TOF peaks (see figure 1), the difference between the above two approaches, as far as the ratio R is concerned, is negligible.

Summarizing, we conclude that the considered scattering anomaly is present at both 5–100 eV [2] and 24–150 keV [1] ranges of incident energies. Thus, and using a terminology of [1, 18], we may say that, within the neutron–proton interaction times of $\sim 10^{-17}$ s, the water molecule chemical formula still remains $H_{1.5}O$. Obviously, the novel experiment [1] and its correct analysis established above open up new perspectives for neutron research on the above attosecond effect, and thus they may have far reaching consequences for current and future experimental and theoretical investigations.

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