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Experiments on the Electron Impact Excitation of Hydrogen Molecules Indicate the Presence of the Second Flavor of Hydrogen Atoms

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Abstract: In one of our previous papers, we performed a comparative analysis of the experimental and theoretical cross-sections for the excitation of atomic hydrogen by electrons. We found that the theoretical ratio of the cross-section σ_{2s} of the excitation of the state 2s to the cross-section σ_{2p} of the excitation of the state 2p was systematically higher than the corresponding experimental ratio by about 20% (far beyond the experimental error margins). We showed that this discrepancy can be due to the presence of the Second Flavor of Hydrogen Atoms (SFHA) in the experimental gas and that the share of the SFHA in the mixture, required for removing this discrepancy, was about the same as the share of the usual hydrogen atoms. The theory behind the SFHA was based on the standard quantum mechanics—on the second solution of the Dirac equation for hydrogen atoms—and on the experimental fact that the charge distribution inside the proton has the peak at the center of the proton; the term "flavor" was used by the analogy with flavors of quarks. In the present paper, we used the same guiding principles, as employed in that previous study, for the comparative analysis of the experimental and theoretical cross-sections for the excitation of molecular hydrogen by electrons. We found that presumably the most sophisticated calculations, using the convergent close-coupling method involving 491 states, very significantly underestimate the corresponding experimental cross-sections for the two lowest stable triplet states. We showed that if in some hydrogen molecules one or both atoms would be the SFHA, then the above very significant discrepancy could be eliminated. We estimated that it would take such unusual hydrogen molecules to be represented in the experimental gas by the share of about 0.26. This is just by about 40% smaller than the share 0.45 of the SFHA deduced in our previous analysis of the experiment on the electron impact excitation of hydrogen atoms (rather than hydrogen molecules). It should be emphasized that from the theoretical point of view, the share of the unusual hydrogen molecules in any experimental gas and the share of the unusual hydrogen atoms (SFHA) in any experimental gas should not be expected to coincide (it would be the comparison of "apples to oranges", rather than "apples to apples"). In addition, given the roughness of the above estimates, we can state that the results of the present paper reinforce the main conclusion of our previous papers of the very significant share of the SFHA in the experimental hydrogen gases. Thus, the experiments on the electron impact excitation of hydrogen molecules are the fourth type of atomic experiments that proved the existence of the SFHA.

Keywords: electron impact excitation of hydrogen molecules; discrepancy between theories and experiments; second flavor of hydrogen atoms

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1. Introduction

The theory behind the Second Flavor of Hydrogen Atoms (SFHA) was based on the standard quantum mechanics—on the second solution of the Dirac equation for hydrogen atoms—and on the experimental fact that the charge distribution inside the proton has a peak at the center of the proton [1]. The term "flavor" was used by analogy with flavors of quarks (see Appendix A). In the same paper [1] the first experimental proof of the existence of the SFHA was presented. Namely, the allowance for the SFHA eliminated

a huge discrepancy concerning the linear momentum distribution in the ground state of hydrogen atoms: in its high-energy tail, the distribution derived from the analysis of atomic experiments exceeded the theoretical predictions (made for the usual hydrogen atoms) by several orders of magnitude [1].

The subsequent analysis of the experiments on charge exchange during collisions of low-energy protons with hydrogen atoms yielded the second experimental evidence of the existence of the SFHA [2]. The theoretical cross-sections, calculated with allowance for the SFHA, turned out to agree with the experiments within the experimental error margins—in distinction to the previous calculations made before the theoretical discovery of the SFHA. By the way, this result should be important for atomic codes developed for describing edge plasmas in magnetic fusion devices because charge exchange is a very important atomic process in these plasmas.

The third type of the atomic experiments that proved the existence of the SFHA was the experiments on the electron impact excitation of the n = 2 states of hydrogen atoms [3]. The theoretical ratio of the cross-section σ_{2s} of the excitation of the state 2s to the cross-section σ_{2p} of the excitation of the state 2p turned out to be systematically higher than the corresponding experimental ratio by about 20% (far beyond the experimental error margins). In paper [3] it was shown that this discrepancy can be due to the presence of the SFHA in the experimental gas. The share of the SFHA in the mixture, required for removing this discrepancy, was estimated to be about the same as the share of the usual hydrogen atoms [3].

For atomic physics, the proven existence of the SFHA has fundamental significance in its own right. Nevertheless, it was also found to be important for astrophysics—especially for finding out what is dark matter (i.e., solving the most fundamental cosmological problem). Namely, after Bowman et al. [4] found that the observed absorption signal of the redshifted 21 cm spectral line from the early Universe was about two times more intense than expected from the standard cosmology, meaning that the primordial hydrogen gas was cooler than predicted, Barkana [5] brought up the suggestion that the additional cooling was caused by some unspecified dark matter particles colliding with the hydrogen gas. Then in paper [6] it was shown that the above large discrepancy would be eliminated if it were collisions with the SFHA that caused the additional cooling.

Another astrophysical puzzle was published by Jeffrey et al. [7]: the distribution of dark matter predicted on the basis of Einstein's gravity was not confirmed by the observation—the observed one was smoother. This prompted suggestions on the need for new physical laws that would go beyond Einstein's gravitation. However, in paper [8] it was demonstrated that the perplexing observations by Jeffrey et al. [7] can be explained qualitatively and quantitatively by allowing for the SFHA.

The Occam razor principle favors the SFHA as the possible explanation of dark matter because the SFHA is based on the standard quantum-mechanical Dirac equation and does not resort to new physical laws (in distinction to most other possible explanations of dark matter). Besides, no other hypothesis has the experimental confirmations—in distinction to the SFHA. All of the above reinforced the leading status of the SFHA on explaining dark matter (or at least a part of it).

In the present paper we discuss whether there is yet another experimental proof of the existence of the SFHA—from the fourth type of atomic experiments: the experiments on the electron impact excitation of hydrogen molecules to the lowest triplet states. There are lots of various theoretical approaches on this process—see for example one of the most recent papers [9] and the very extensive list of references therein. We perform our study based on the same principles as in our previous analysis of the experiments on the electron impact excitation of hydrogen atoms [3]. This is explained in the next section.

2. Comparison of the Experimental Cross-Sections with Theories

Let us start by specifying four important points, on which we based our study in paper [3] and which we are going to use in the present study. The first point: in our study

of the experiments on the electron impact excitation of hydrogen atoms [3], we chose the first two excited states: 2s and 2p. This was done because for the first two excited states, calculations are simpler (and therefore more reliable) than for higher states.

The second point: the range of energies relatively close to the excitation threshold was not favorable for determining the presence and the share of the SFHA in the experimental gas mixture. This is because in this range, the excitation cross-sections σ_{2s} and σ_{2p} are strongly dominated by so-called "resonances".

The third point: we considered only the theoretical works where both the cross-sections σ_{2s} and σ_{2p} were calculated in the same theoretical approach. The same about the experiments.

The fourth point: after we found about 20% discrepancy between the theoretical and experimental ratio of the cross-sections σ_{2s}/σ_{2p}, the next task was to estimate the percentage of the SFHA in the hydrogen gas mixture required for eliminating this discrepancy. For this purpose we needed the corresponding theoretical cross-section for the SFHA.

The primary feature of the SFHA distinguishing it from the usual hydrogen atoms is that the SFHA only has states of the zero orbital momentum ($l = 0$) both in the discrete and continuous spectra of energies. Therefore, due to the well-known selection rules, the SFHA does not couple to the electromagnetic radiation: the SFHA remains "dark" (except for the 21 cm spectral line resulting from the radiative transition between the two superfine structure sublevels of the ground state). In the discrete spectrum the states of $l = 0$ are called the s-states. [1,6]. The s-states are spherically symmetric.

Theoretical calculations of the electron impact excitation cross-sections most relevant to the SFHA were performed by Poet [10], who considered such excitation for a model hydrogen atom having only spherically symmetric states. By comparing the theoretical results by Poet [10] with the corresponding theoretical results for the usual hydrogen atoms, and combining this with the above 20% discrepancy, we arrived at the conclusion that the SFHA and the usual hydrogen atoms were present in the experimental gas in about the same shares.

Next, we applied the same principles to the analysis of the experimental and theoretical results on the electron impact excitation of hydrogen molecules. First, we chose the first two stable excited electronic *triplet* states of H_2: the state c $^3\Pi_u$ and the state a $^3\Sigma_g{}^+$. The reason for choosing the triplet states is the following. The singlet states can get populated both by the direct excitation and by exchange between the incident electron and one of the molecular electrons. The triplet states can get populated only by the exchange, so that the corresponding theory is simpler for the triplet states. (This is a generalization of principle number one from the study [3] for the case of H_2.)

Second: for avoiding resonances, which complicate the calculations and thus complicate determining the presence and the share of the SFHA in the experimental gas mixture, we chose the range of energies starting from 30 eV.

Third: concerning the choice of the experimental and theoretical works. In the experiments by Wrkich et al. [11] (who improved the previous experimental results by Khakoo and Trajmar [12]), both the excitation cross-section to the state c $^3\Pi_u$ and to the state a $^3\Sigma_g{}^+$ were measured, but only up to the energy of 30 eV, so that only their data at 30 eV is relevant for our purposes (according to the second point above). Therefore, we also chose the experiment by Mason and Newell [13], who covered the energies from 30 eV to 60 eV for the excitation to the state c $^3\Pi_u$, as well as the experiment by Ajello and Shemansky [14], who covered the energies from 30 eV to 60 eV for the excitation to the state a $^3\Sigma_g{}^+$. As for the corresponding theoretical work, dealing with the usual (non-SFHA) hydrogen atoms in the molecule H_2, we choose the (presumably most sophisticated) calculations by Zammit et al. (2017) [9]. In that paper, both the excitation cross-section to the state c $^3\Pi_u$ and to the state a $^3\Sigma_g{}^+$ were calculated by the convergent close-coupling (CCC) method with the total number of states equal to 491—they referred to these calculations as CCC(491).

The comparison of the theoretical CCC(491) results from paper [9] (as well as of some theoretical results from paper [15] included for reasons explained later on), with the

experimental results from papers [11,13] in the range from 30 eV to 50 eV (practically the same range as in our study [3]) is presented in Table 1 for the state c $^3\Pi_u$.

Table 1. Comparison of the experimental excitation cross-sections σ (10^{-17} cm^2) to the state c $^3\Pi_u$, deduced from the plots in papers [11,13], with the corresponding theoretical results, deduced from the plots in papers [9,15]. Here N/A stands for "not available".

Energy (eV)	σ Experiment [11]	σ Experiment [13]	σ Theory CCC(491) [9]	σ Theory Lima et al. [15]
30	0.77	0.74	0.38	1.61
40	N/A	0.59	0.19	N/A
50	N/A	0.57	0.10	N/A

From Table 1 it is seen that in the range of incident electron energies from 30 eV to 50 eV, the theoretical CCC(491) results [9] very significantly underestimate the corresponding experimental cross-section: e.g., by a factor of five at 50 eV, by a factor of three at 40 eV, and by a factor of two at 30 eV. At the same time, it is seen that there is a very good agreement between the experimental cross-section by Wkrich et al. [11] at 30 eV (which is the highest energy data point that they measured) with the experimental cross-section by Mason and Newell [13], thus reinforcing the reliability of Mason–Newell results.

Now the question arises: could this huge discrepancy be explained if there were the SFHA in the composition of some hydrogen molecules? (Let's call them "unusual hydrogen molecules"). Physically, what would be the difference in calculating the corresponding theoretical cross-section?

Out of the 491 states, involved in producing the theoretical CCC(491) results, the overwhelming majority of the states would be absent in the unusual hydrogen molecules (because the SFHA has only the s-states). So, how would the dramatic reduction of the states involved in the CCC calculations affect the results? Zammit et al. [9] also provided theoretical results for the CCC involving a lesser number of states. They showed that the decrease of the number of states involved in their calculations yields significantly greater excitation cross-sections than CCC(491).

Here we come to the fourth point in the sequence of steps from paper [3]: the choice of the theoretical calculations of the cross-sections that is the most relevant for the unusual hydrogen molecules. The minimal number of states were used in calculations by Lima et al. [15] (in frames of Schwinger multichannel formulation)—to the best of our knowledge.

From Table 1 it is seen that at the incident electron energy 30 eV (the maximum energy, for which Lima et al. [15] performed their calculations), the CCC(491) result [9] for the usual hydrogen molecules underestimates the corresponding experimental results by a factor of two, while the result from Lima et al. [15] (most relevant for the unusual hydrogen molecules) overestimates the corresponding experimental results by a factor of two. So, if we denote by α the share of the unusual hydrogen molecules in the experimental gas, then from the data at 30 eV it is easy to find that the agreement with the experimental results would be achieved for $\alpha \approx 0.30$ as the solution to the equation $1.61\ \alpha + 0.38\ (1 - \alpha) = 0.755$ (where 0.755 is the experimental value averaged between the corresponding results of the experiments [11,13]).

Now let us proceed to the situation with the excitation to the state a $^3\Sigma_g^+$. Table 2 presents the comparison of the experimental results from papers [13,14] with the corresponding theoretical result CCC(491) from paper [9] and with the corresponding theoretical result from paper [15]. It is seen that at the incident electron energy 30 eV (the maximum energy, for which Lima et al. [15] performed their calculations), the CCC(491) result [9] for the usual hydrogen molecules underestimates the corresponding experimental results by a factor of about 1.5, while the result from Lima et al. [15] (most relevant for the unusual hydrogen molecules) overestimates the corresponding experimental results by a factor of about 1.5.

Table 2. Comparison of the experimental excitation cross-sections $\sigma(10^{-17}$ cm$^2)$ to the state a $^3\Sigma_g^+$, deduced from the plots in papers [11,14], with the corresponding theoretical results, deduced from the plots in papers [9,15]. Here N/A stands for "not available".

Energy (eV)	σ Experiment [11]	σ Experiment [14]	σ Theory ccc(491) [9]	σ Theory Lima et al. [15]
30	0.18	0.33	0.18	0.52
40	N/A	0.15	0.081	N/A
50	N/A	0.10	0.054	N/A

The share α of the unusual hydrogen molecules in the experimental gas necessary for achieving the agreement with the corresponding experimental results can be easily estimated from the data at 30 eV as the solution of the equation $0.52\ \alpha + 0.18\ (1 - \alpha) = 0.255$ (where 0.255 is the experimental value averaged between the corresponding results of the experiments [11,14]). It yields $\alpha \approx 0.22$.

For estimating the share of the unusual hydrogen molecules we could not use the data at 40 eV and 50 eV because for these energies there is no data from Lima et al. [15] representing the corresponding theoretical cross-sections for unusual hydrogen molecules.

Both for the state c $^3\Pi_u$ and for the state a $^3\Sigma_g^+$, these are rough estimates. The value of α averaged over the corresponding results for the states state c $^3\Pi_u$ and a $^3\Sigma_g^+$ is $\alpha = 0.26 \pm 0.04$, so that the scatter is just about 15%. The above results can be interpreted as the possible evidence that in the experimental gas, the shares of the usual and unusual (i.e., the SFHA-based) hydrogen molecules differed just by a factor of three.

In paper [3] where we compared the experimental and theoretical results on the electron impact excitation of hydrogen atoms, the share of the SFHA was found to be approximately 0.45. The corresponding value of 0.26 for the experiments on the electron impact excitation of hydrogen molecules (rather than hydrogen atoms) is less than 0.45 by just about 40%. It should be emphasized that from the theoretical point of view, the share of the unusual hydrogen molecules in any experimental gas and the share of the unusual hydrogen atoms (SFHA) in any experimental gas should not be expected to coincide (it would be the comparison of "apples to oranges", rather than "apples to apples"). In addition, given the roughness of the above estimates, we can state that the results of the present paper reinforce the main conclusion of paper [3] of the very significant share of the SFHA in the experimental hydrogen gases.

3. Conclusions

We performed a comparative analysis of the experimental and theoretical cross-sections for the excitation of molecular hydrogen by electrons. We employed the same set of guiding principles as in our previous analogous study of the electron impact excitation of hydrogen atoms [3]. We found that presumably the most sophisticated calculations by Zammit et al. [9], using the convergent close-coupling method involving 491 states, very significantly underestimate the corresponding experimental cross-sections.

We showed that if in some hydrogen molecules one or both atoms would be the SFHA, then the above very significant discrepancy could be eliminated. We estimated that it would take such unusual hydrogen molecules to be represented in the experimental gas in the share of about 0.26. This is about 40% smaller than the share 0.45 of the SFHA deduced by the corresponding analysis (in paper [3]) of the experiments on the electron impact excitation of hydrogen atoms (rather than hydrogen molecules). It should be emphasized that from a theoretical point of view, the share of the unusual hydrogen molecules in any experimental gas and the share of the unusual hydrogen atoms (SFHA) in any experimental gas should not be expected to coincide. Given the roughness of the above estimates, we can state that the results of the present paper reinforce the main conclusion of paper [3] of the very significant share of the SFHA in the experimental hydrogen gases. Thus, the experiments on the electron impact excitation of hydrogen molecules are the fourth type of the atomic experiments that proved the existence of the SFHA (the three previous types of

atomic experiments proving the existence of the SFHA being listed in the Introduction of the present paper).

The rough estimates provided in the present paper are intended to get the message across and to motivate further experimental and theoretical works on this subject.

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Appendix A. On Using the Term "Flavor"

Both the regular and singular solutions to the Dirac equation outside the proton correspond to the same energy. As this means the additional degeneracy, then according to the fundamental theorem of quantum mechanics, there should be an additional conserved quantity. In other words, the situation is that hydrogen atoms have *two flavors*, differing by the eigenvalue of this additional, new conserved quantity: hydrogen atoms have *flavor symmetry* [16].

It is called so by analogy with quarks that have flavors: for example, there are up and down quarks. For representing this particular flavor symmetry, there was assigned an operator of the additional conserved quantity: the isotopic spin I—the operator having two eigenvalues for its z-projection: $I_z = 1/2$ assigned to the up quark and $I_z = -1/2$ assigned to the down quark.

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