$\overline{\mathbf{H}}$ and $\overline{\mathbf{H}}^+$ production cross sections for the GBAR experiment

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Abstract. The production and cooling of the \overline{H}^+ ion is the key point of the GBAR experiment (Gravitational Behaviour of Antihydrogen at Rest), which aims at performing the free fall of antihydrogen atoms to measure \bar{g} , the acceleration of antimatter on Earth. \bar{H}^+ ions will be obtained from collisions between a positronium cloud and antiprotons delivered by the AD/ELENA facility at CERN, with intermediate formation of antihydrogen atoms. In order to optimise the experimental production of \overline{H}^+ ions, we computed the total cross sections of the two corresponding reactions, within the same theoretical framework of the Continuum Distorted Wave – Final State (CDW-FS) model. The different contributions of the \overline{H} excited states have been systematically investigated for different states of Ps. The results exhibit an increase of the \overline{H} production toward low kinetic energies, in agreement with experimental data and previous calculations, whereas the largest \overline{H}^+ production is obtained with low energy ground-state antihydrogen atoms. These theoretical predictions suggest that the overall production of \overline{H}^+ could be optimal for 2 keV antiproton impact energy, using positronium atoms prepared in the 2p state.

1. Introduction

The GBAR experiment (Gravitational Behaviour of Antihydrogen at Rest) has been recently approved by the CERN Research Board [1]. It aims at performing the free fall of antihydrogen atoms in order to measure g, the gravitational acceleration of antimatter on Earth, and thus test the Weak Equivalence Principle for antimatter. The main source of uncertainty in this experiment is the initial antihydrogen (\overline{H}) velocity. This is why ultra-cold antihydrogen atoms of a few neV are required. The key idea of the GBAR experiment is to produce \overline{H}^+ ions that can be cooled using techniques developed in cold-atom physics [2]. They will be obtained from a two-step process: (i) creation of antihydrogen from collisions between keV antiprotons (\bar{p}) and a gas of positronium atoms (Ps), (ii) production of \bar{H}^+ from further collisions between these antihydrogen atoms and the positronium cloud. The two reactions are:

$$\bar{p} + Ps(n_{Ps}, l_{Ps}) \longrightarrow \bar{H}(n_H, l_H) + e^-$$
 (1)

$$\overline{H}(n_H, l_H) + Ps(n_{Ps}, l_{Ps}) \longrightarrow \overline{H}^+ + e^-$$
(2)

where the positronium atoms can be optically prepared in any state (n_{Ps}, l_{Ps}) , and \overline{H} can be produced from reaction (1) in any $(n_{\rm H}, l_{\rm H})$ state. Experimentally, the antiproton kinetic energy (delivered by the AD/ELENA at CERN), the positronium excited state and its fraction with respect to the ground state

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can be chosen to increase the number of \overline{H}^+ produced per \overline{p} pulse. The aim of the present theoretical study is to optimise these parameters by computing the total cross sections of reactions (1) and (2).

Although the three-body reaction (1) has been already widely theoretically studied [3,4] this is not the case for the four-body reaction (2) for which only a few theoretical results can be found, often limited to the simplest cases (H(1s) + Ps(n_{Ps} =1,2)) [5]. In the present study, the cross sections of the two reactions have been computed at the same level of approximation within the framework of the Continuum Distorted Wave – Final State model (CDW-FS).

In the following, we give a short description of the CDW-FS model and present our theoretical predictions for both reactions. Atomic units are used unless otherwise specified.

2. Theoretical model

Reactions (1) and (2) are equivalent, according to the principle of microreversibility and using charge conjugation, to the two following reactions:

$$e^+ + H(n_H, l_H) \longrightarrow p + Ps(n_{Ps}, l_{Ps})$$
 (3)

$$e^+ + H^- \longrightarrow H(n_H, l_H) + Ps(n_{Ps}, l_{Ps})$$
 (4)

Cross sections for reactions (1) and (3) (respectively (2) and (4)) are related by a simple kinetic factor [6].

The common theoretical framework chosen here to describe reactions (3) and (4) is called Continuum Distorted Wave – Final State (CDW-FS). It is indeed closely related to CDW methods since special attention is given to the treatment of the boundary conditions, hence the use of Coulomb wave functions to describe exactly the asymptotic states. The presence of a charged target (respectively charged target fragment) in the initial (resp. final) channel requires a particular treatment. Originally introduced to study fast positron/hydrogen-like collisions [7], the CDW-FS model includes distortions in the final channel (*prior* version) related to the Coulomb continuum states of both the positron and the electron in the field of the residual target. The 3-body formulation of the model, well-suited for reaction (3), has been later adapted to 4-body reactions [8], and applied in particular to the case of positronium formation from positron collisions with metastable helium [9], which is very similar to reaction (4). We closely followed the formalism developed in references [7] and [9], where all the details can be found.

In the interest of the GBAR experiment, we want to investigate the low energy regime (down to 1 eV in the centre of mass). We are well-aware that our collisional model is normally only valid for intermediate and high impact energies and that the *post/prior* discrepancy inherent to the CDW approximation increases toward low energies [10]. If the values of the cross sections are certainly not reliable close to the energy thresholds, we can however extract meaningful and valuable information from their relative behaviours since the two reactions are investigated using the same model.

The treatment of the H^{\circ} ion can be performed at different levels of approximation. H^{\circ} is a weakly bound system (ionisation potential: 0.76 eV) which only exists in its ground state and exhibits strong electronic correlation effects. A large variety of wave functions is available in the literature. At present, the most accurate is proposed by Le Sech [11]. For the sake of computational simplicity, we used the uncorrelated Chandrasekhar wave function [12], which includes radial correlations (but not angular).

3. Results

We systematically computed the cross sections of reactions (3) and (4) for Ps(1s) to Ps(3d) and H(1s) to H(4f). The contribution of the higher hydrogen excited states ($n_H > 4$) can be estimated using the well-known n^{-3} rule. We have checked that this correction is usually small. All cross sections are given as a function of the initial antiproton kinetic energy in the laboratory frame, where the positronium atom is supposed to be at rest.

3.1. Reaction (1)

In Figure 1, we have chosen to present in detail our theoretical predictions for the case of Ps(1s). For the sake of clarity, for a given quantum number n_H , the cross sections have been summed over the l_H states. Due to the energy threshold values for $n_H \ge 2$ and to the very low cross sections for $n_H = 1$, almost no \overline{H} are expected to be produced below 5 keV. Above thresholds, the production of higher excited states of \overline{H} is favored (the same behaviour is found for the other states of Ps). This agrees with other calculations [3]. We also compared our cross sections summed over the \overline{H} states with the experimental results (inclusive measurements) of Merrison *et al.* [13], where hydrogen atoms were formed by impact of protons on a positronium target. Although our theoretical predictions slightly overestimates the \overline{H} production, the agreement with the experimental data is rather good, thus validating the use of the CDW-FS model for evaluating the cross sections of the 3-body reaction (1).





Figure 1. Cross sections for reaction (1) with Ps(1s) and \overline{H} labelled by n_H (see text) as a function of the antiproton impact energy. Available experimental data are represented by black dots with error bars [13].

Figure 2. \overline{H} production cross sections (summed over n_H from 1 to 4) as a function of the antiproton impact energy, for Ps(1s) to Ps(3d).

In Figure 2, we compare the total cross sections summed over all the computed \overline{H} states, for Ps(1s) to Ps(3d). Except for Ps(1s), the production of \overline{H} is maximal in the range 2-4 keV, Ps(2s), Ps(2p) and Ps(3p) exhibiting the highest cross sections.

3.2. Reaction (2)

The most accurate value of the H⁻ ground-state energy is -0.5277 a.u. [14]. This happens to be almost equal to the sum of the binding energies of hydrogen in its ground state (-0.5 a.u.) and of the positronium atom in a state $n_{Ps} = 3$ (-0.02778 a.u.). Therefore, in that peculiar case, we can expect the \overline{H}^+ formation to be highly efficient (nearly resonant) almost at zero impact kinetic energy. Indeed, as can be seen on Figure 3, a sharp increase of the cross section at zero impact energy is observed for Ps(3d) (also for Ps(3p), not shown on the figure). However, it is worth noticing that reaction (2) with Ps(2p) in the entrance channel is once again dominant. This might be attributed to the high polarisability of the 2p orbital. Another very important observation is that the contribution of the excited states of \overline{H} to the production of \overline{H}^+ is always negligible, except in the case of Ps(1s). For ground state \overline{H} , Ps(2s) and Ps(3s), not shown on Figure 3, are just below Ps(1s).



Figure 3. Cross sections for reaction (2) as a function of the antiproton impact energy. Only results for Ps(1s), Ps(2p) and Ps(3d) are presented. Solid curves represent antihydrogen ground-state in the entrance channel, while the dashed curves correspond to the contribution of all other \overline{H} excited states. The arrows indicate the threshold energies.

4. Conclusion

Excitation of positronium atoms can indeed lead to a higher rate of \overline{H}^+ production for GBAR. Despite the dramatic increase of the cross section close to the threshold of reaction (2) with Ps(3d), this might not be the best option since below 1 keV antiproton impact energy, very few antihydrogen atoms will be produced through reaction (1). Our calculations rather suggest that Ps(2p) would be the most attractive solution and the optimal antiproton impact energy around 2 keV. However, Ps(2p) (and also Ps(3p)) is a short-lived state requiring to set-up a sophisticated laser system: these experimental constraints may lead to favour Ps(3d) over the p-states. Nonetheless, one should not forget that in reality, most of the positronium atoms will remain in their ground state (as they are produced).

The present study also highlights the need to de-excite the \overline{H} produced through the first reaction. It leads also to important experimental constraints. Therefore, in order to accurately handle the evolution of the different Ps and \overline{H} populations over time, a simulation of the interaction region is deeply needed. Moreover, work on the influence of the angular correlations in H⁻ is also currently underway.

Once again, it must be emphasised that our collisional model (CDW-FS) might not yield quite reliable results at very low impact energy (near threshold) where more sophisticated calculations (e.g. coupled channel models) are needed. Nevertheless it can provide valuable information on the relative behaviour of the cross sections relevant for the design of the GBAR experiment.

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