Target Structure Induced Suppression of the Ionization Cross Section for Very Low Energy Antiproton-Hydrogen Collisions

H. Knudsen,[1,*] H. A. Torii,[2] M. Charlton,[3] Y. Enomoto,[2] I. Georgescu,[4] C. A. Hunniford,[5] C. H. Kim,[2] Y. Kanai,[4] H.-P. E. Kristiansen,[1] N. Kuroda,[2] M. D. Lund,[1] R. W. McCullough,[5] K. Tökesi,[6] U. I. Uggerhøj,[1] and Y. Yamazaki[4]

[1]*Department of Physics and Astronomy, University of Aarhus, DK 8000, Denmark*
[2]*Institute of Physics, Komaba, University of Tokyo, 153-8902, Japan*
[3]*Department of Physics, Swansea University, SA2 8PP, United Kingdom*
[4]*Atomic Physics Laboratory, RIKEN, (Saitama) 351-0198, Japan*
[5]*Department of Physics and Astronomy, Queens University Belfast, BT7-1NN, United Kingdom*
[6]*ATOMKI, Debrecen, H-4001, Hungary*

(Received 31 August 2010; published 17 November 2010)

Low energy antiprotons have been used previously to give benchmark data for theories of atomic collisions. Here we present measurements of the cross section for single, nondissociative ionization of molecular hydrogen for impact of antiprotons with kinetic energies in the range 2–11 keV, i.e., in the velocity interval of 0.3–0.65 a.u. We find a cross section which is proportional to the projectile velocity, which is quite unlike the behavior of corresponding atomic cross sections, and which has never previously been observed experimentally.

DOI: 10.1103/PhysRevLett.105.213201 PACS numbers: 34.10.+x, 34.50.Fa

Recently, low energy antiprotons have been used to give benchmark experimental data for the development of atomic collision theory [1,2]. Such projectiles are especially well suited for this purpose since they do not allow electron capture, and hence leave the theorists with an essentially one-center quantum mechanical problem for the description of the target electrons. In contrast to fast collisions, where perturbation theory is a good starting point, at projectile velocities much lower than those of the target electrons, we are dealing with a strong, long-lasting interaction with the projectile, which poses severe challenges for the theoretical models. The data [1,2] which were obtained for a helium target, essentially agree with most of the theoretical results in the case of single ionization in low energy collisions, whereas double ionization theory still leaves much to be desired.

For the simplest neutral molecular target, molecular hydrogen, there exists only one comprehensive calculation for low energy impact in the present velocity region [3]. It is a nonperturbative time-dependent close coupling method applied to fully treat the correlated dynamics of the electrons. Nevertheless, as we shall see below, its results do not agree with those of the present measurements.

Based on the data presented here, we suggest that the molecular target allows a mechanism of dynamic suppression of the single ionization process which has not been supported by experimental data until now [4].

The experimental technique used here to obtain cross sections for slow antiprotons colliding with molecular hydrogen is basically the same as that used in Refs. [1,2]. In short, antiprotons delivered by the CERN AD are slowed down and captured in a Penning trap where they are cooled and radially compressed [5,6]. They are then extracted at an energy of 250 eV through a differentially pumped beam line into a scattering chamber which is raised to a voltage, U. The resulting antiproton kinetic energy is then $eU +$ 250 eV, and very well defined.

In the scattering chamber, the antiprotons collide with deuterium molecules in a jet of density approximately 10^{12} cm^{-3}. The resulting ions are extracted by a 266 V/cm perpendicular electric field and then spatially and temporally focused onto a microchannel plate (MCP) detector while the projectiles proceed onto another MCP detector. From the two detector signals measured in coincidence, we accumulate a time-of-flight (TOF) spectrum of the ions, from which we extract the cross section. For that purpose, the product of the integral target density and the ion detector efficiency was determined by replacing the antiproton beam with a 3 keV pulsed electron beam. For normalization, we used the cross section of 3 keV electrons on H_2 given by Kossmann *et al.* [7]. Since the flight time of the created D_2^+ ions is approximately 0.7 μ sec , excited molecular ions which fragment with a lifetime much shorter than that will not be observed.

In these measurements, as well as in some earlier measurements on atomic and molecular hydrogen, we used the deuterium isotope. This allows a 40% higher target density for the same induced background pressure in the experimental chamber, and it avoids a sometimes significant background peak from H^+ arising from water in the residual gas. However, the theoretical calculations with which we compare below, assume either a target of the light hydrogen isotope, or that the target nucleus/nuclei are very heavy. This introduces no problems, since it is expected that an isotope effect in the hydrogen ionization cross sections is smaller than 1% at the lowest energies

which we are concerned with here, and much less at higher energies [8].

In Fig. 1 we show our experimental data for the cross section for single, nondissociative ionization of molecular hydrogen by antiproton impact as a function of the projectile velocity measured in atomic units. Also shown are measurements of the same cross section by Hvelplund *et al.* [9] at higher antiproton energies. It is reassuring to note that the two data sets, obtained via quite different experimental techniques, agree well with each other.

We have fitted these data for projectile velocities below 1 a.u. with a straight line, and it can be seen that the data agree well with a linear fit, suggesting that the cross section is proportional to the projectile velocity.

The experimental data are compared with the two-center atomic orbital close coupling calculations by Lühr and Saenz [3]. Their theory is basically on the same level of sophistication as many of the calculations which agree with our measurements of the ionization cross section of helium [1]. Lühr and Saenz calculated the cross section for transfer of energy exceeding the ionization potential, 15.4 eV, and their cross sections therefore include the contribution from dissociative ionization. We show in Fig. 1 the sum of the cross sections for production of H_2^+ and H^+ ions measured by Hvelplund *et al.* [9]. It can be seen that the calculation neither reproduces the magnitude of the experimental data for the hydrogen molecule, nor their velocity dependence.

We also compare our measurements with results for the atomic hydrogen target. Here we do not have experimental data for collisions with projectile energies below 30 keV (1.1 a.u. in velocity) [10], but there exist a number of theoretical calculations which should be reliable in this case of a very simple target. We choose to plot the so-called "one-center atomic orbital close coupling calculation" results of Igarashi *et. al.* [11] as well as the calculation by Lühr and Saenz [12] (which applies the same model as the calculation of Lühr and Saenz [3] discussed above) in Fig. 1 as representative of the cross section for atomic hydrogen. Also shown is a low-velocity calculation by Cohen [4], who applied a classical trajectory Monte Carlo approach based on the restraints by Kirschbaum and Wilets [13]. It is gratifying to see the agreement of these theories for the simple atomic hydrogen target. (The corresponding result by Cohen for molecular hydrogen is surprisingly large. For example, he gives the total ionization cross section at a projectile velocity of 0.1 a.u. to be 2.5 $Å^2$) The calculation by Cohen includes the capture of the projectile by the target nucleus, which explains the onset of a steep rise at the lowest velocities.

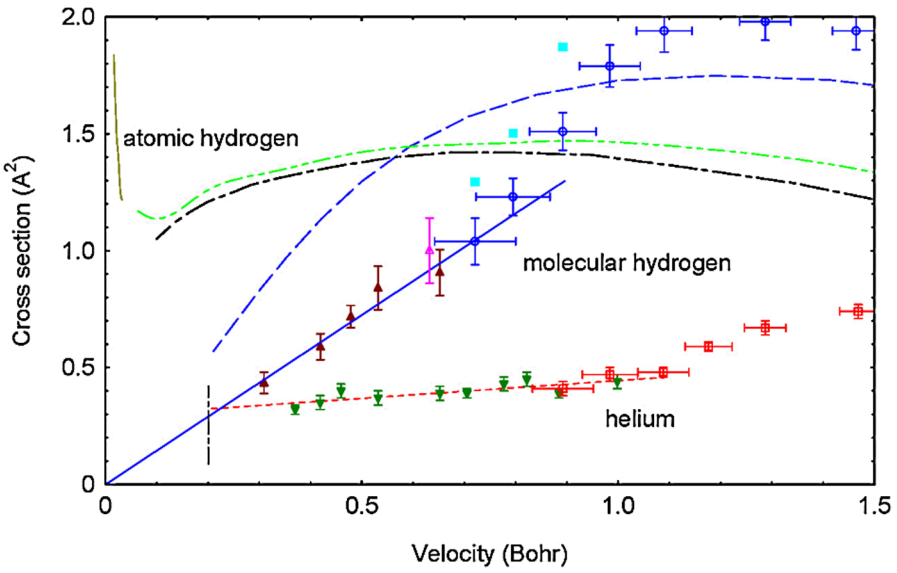

FIG. 1 (color online). Experimental data and theoretical calculations of the cross section for single ionization by antiproton impact on atomic hydrogen, molecular hydrogen and helium as a function of the projectile laboratory velocity. For atomic hydrogen, we show as dashed-dotted black curves calculations by Lühr and Saenz [12] and by Igarashi *et al.* (green dash-dot-dot) [11]. Also shown as a brown solid curve is the low-velocity calculation of the total cross section for ionization by Cohen [4]. In the case of the molecular hydrogen target, we show the experimental data of the present work (▲ run in 2010, △ run in 2009) as well as previous data obtained by our group, (○), published in Hvelplund *et al.* [9]. The straight, solid line is a linear fit to these data below a velocity of 1 a.u. The data points marked ■ indicate the sum of the cross sections for nondissociative and dissociative ionization of molecular hydrogen by Hvelplund *et al.* [9]. The long-dashed dark blue curve shows a calculation of this cross section by Lühr and Saenz [3]. The vertical line indicates the projectile energy above which more than 90% of the D_2^+ ions created and more than 90% of the projectiles deflected in the collisions are collected by our apparatus. For the helium target, we show experimental data by Hvelplund *et al.* (□) [9] and by Knudsen *et al.* (▼) [1]. The short-dashed, nearly horizontal line is a straight-line fit to these data below 1 a.u. to guide the eye.

Figure 1 also presents our experimental data for the single ionization of helium by antiproton impact as published in Knudsen *et al.* [1] and Hvelplund *et al.* [9]. The short-dashed straight line has been fitted to these data for projectile velocities below 1 a.u.

As can be seen, the projectile velocity dependences of the cross sections for the two atoms are rather similar, being almost independent of the projectile velocity for velocities in the range 0.2–1 a.u., with a slightly decreasing tendency towards lower velocities. This is dramatically different from the velocity-proportional dependency of the molecular target cross section in this velocity range, and calls for an explanation.

Since we are concerned with a regime of low projectile velocities (compared with the velocities of the target electrons), we may seek guidance from the adiabatic model of ionization by Fermi and Teller [14]. For a very slow antiproton approaching atomic hydrogen, the electron wave function will expand dramatically, and at the so-called critical distance $R_c = 0.639a_0$ the electron will not be bound by the proton-antiproton dipole (a_0 is the Bohr radius). Therefore in this model the ionization cross section will be independent of projectile velocity, and equal to $\pi R_c^2 = 0.35$ Å^2. For the helium target, there is no such critical distance, since even at zero distance between the nucleus and the antiproton, there is a state bound with 0.77 eV, namely, that corresponding to the H^- ion. Adiabatic ionization of helium is therefore excluded, and in this model the cross section should be vanishing at zero projectile velocity. The case of molecular hydrogen was treated by Wightmann [15], who assumed the internuclear distance of the molecule to be fixed, and let an antiproton move around inside the molecule, finding the electronic binding energy as function of the antiproton position. He found a volume with an approximate cross section of a_0^2 where the binding energy was "less than 0.135 eV if not zero."

The above discussion of adiabatic ionization is not as relevant as might be expected at first sight. This is due to the effect of collisional broadening, as also discussed by Wightmann [15] and later by, e.g., Schiwietz *et al.* [16]. Let us regard a collision of an antiproton with velocity 0.2 a.u. with a target of extension, e.g., equal to $2a_0$. From Heisenberg's uncertainty relation we get a resulting energy uncertainty of 2.8 eV. This means that for our three targets, irrespective of the existence of adiabatic ionization, there should be an ionization cross section in our velocity regime which is governed by collisional broadening of a state which at zero projectile velocity is characterized by having no, or a very small binding energy. The projectile velocity dependencies of all these cross sections should therefore be similar within this "adiabatic, collision broadened" model, given by πr_{eff}^2, where r_{eff} is the antiproton-target nucleus distance where the collision broadened state allows release of the electron.

Since there is actually a large difference between the projectile velocity dependency of the cross section for the molecule, and for the two atomic targets, we would like to suggest that the reason stems from the molecular structure as follows: During the approach of the projectile to one of the protons, the proximity of a "second" positive nucleus allows a dynamic effect, where the electron wave function temporarily shifts away from the antiproton-proton dipole. The slower the antiproton, the more time the electron cloud has to adjust, and hence the smaller the cross section for ionization.

Based on these considerations, we would like to suggest an amendment to the above model, namely, the inclusion of the probability for release to take place while it is energetically possible: P_{release}. We then get

$$\sigma^+ = \pi r_{\mathrm{eff}}^2 P_{\mathrm{release}}.$$

We suggest that P_{release} for atomic targets is numerically large (≈ 1), and slowly varying with the projectile velocity, while for the molecular target it is much smaller and inversely proportional to the collision time, which means proportional to the projectile velocity [17].

The question is now whether this suppression of single, nondissociative ionization of the hydrogen molecule pointed out above is followed by an increase of the probability for other collision channels. The following product channels are possible at not too low impact velocities:

$$D_2 \rightarrow D_2^+ + e, \qquad D + D^+ + e, \qquad D^+ + D^+ + 2e,$$
$$D^- + D^+.$$

In particular the last process, formation of D^-, might be expected to be enhanced, due to the fact that our model

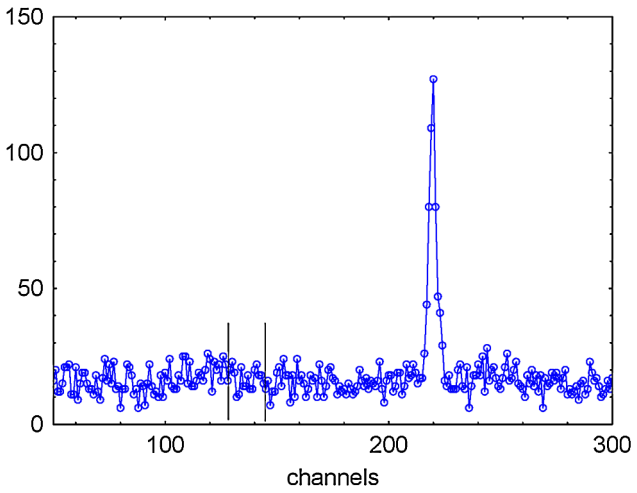

FIG. 2 (color online). An example of a TOF spectrum as observed in these measurements. It was obtained for an impact energy of 10.6 keV. The peak is D_2^+ ions. The two vertical lines indicate the TOF interval where D^+ ions are expected. One channel is 2.44 nsec. Zero TOF is in channel −70.

introduced above involves an intermediate state much like D^-.

Here it should be noted that the last three processes all involve the formation of a free D^+, and therefore should be present in our TOF spectra. Figure 2 shows our measured TOF spectrum for 10.6 keV antiproton impact.

We know the TOF of D^+ and are therefore able to identify the position of such a peak in the TOF spectra. Two questions arise: To which extent does our apparatus accept all D^+ created and what is the width of the D^+ peak? This is hard to estimate with high accuracy, since it involves calculations of the scattering angle of the projectile, the recoil angle and energy and the electronic energy released to the molecular fragments—in collisions where we can apply neither static scattering potentials nor the Franck-Condon principle. However, making simple assumptions on the scattering process and assuming that the energies released in fragmentation are smaller than or like those known for fast ion impact [18], we estimate that for the projectile impact velocities with which we are concerned here, the large majority of any D^+ created should fall in the TOF spectra within the interval indicated in Fig. 2. This even includes D^+ created in a Coulomb explosion (channel 3 above). We can now calculate upper limits (2 st.dev.) of the total cross section for production of D^+ in our collisions and obtain the following results:

E [keV]	$\sigma(D_2{}^+)$[Å^2]	$u.l.\sigma(D^+)$[Å^2] (2st. dev.)
2.40	0.43 ± 0.05	0.10
4.40	0.59 ± 0.06	0.07
5.74	0.72 ± 0.05	0.10
7.07	0.84 ± 0.09	0.12
10.6	0.91 ± 0.10	0.10

A comparison between the second and the third columns shows that there is no ''compensation'' for the suppression of the $D_2{}^+$ production in the other reaction channels, and we can conclude that we observe a general suppression of total ionization in these collisions with the molecular hydrogen target. This mechanism might be at work for antiproton collisions with many (especially nonpolar) molecules. It may also suppress excitation channels. This is in contrast to the case of positive ion collisions, where dissociative channels dominate at these low projectile velocities primarily via dissociative electron capture.

Clearly, the data presented here call for theoretical work to be undertaken.

We would like to thank our collaborators in the CERN ASACUSA Collaboration and the staff at the CERN AD for much help and support. Also thanks are due Poul Aggerholm for his tireless practical help. This work was supported by the Danish Natural Science Research Council, the U.K. Engineering and Physical Sciences Research Council, the Grant-in-Aid for Specially Promoted Research (19002004), MEXT, Japan, and the Hungarian Scientific Research Fund OTKA No. K72172.

*hk@phys.au.dk

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