Collisional mechanisms for single and double ionization of He by protons and antiprotons

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Classical trajectory Monte Carlo calculations have been used to elucidate the collision mechanisms responsible for the differences in the single- and double-ionization cross sections of He atoms by protons and antiprotons in the energy range from 250 to 1000 keV. The calculations employed the Bohr helium-atom model which includes the $1/r_{12}$ electron-electron interaction. The unexpected large observed difference [Andersen *et al.*, Phys. Rev. Lett. **57**, 2149 (1986)] in the ratio R of double to single ionization for proton and antiproton collisions is reproduced by the calculations. The calculations indicate that the antiproton double-ionization cross section is larger than that for protons because of two effects. The first effect is that the antiproton can push one electron into the other from larger impact parameters than for protons which must be between the nucleus and the first electron in order to pull it into a trajectory which collides with the second electron. The most important effect, however, is that at small impact parameters the antiproton screens the helium nucleus causing a Coulomb explosion while the proton increases the binding of the two electrons. The calculations also show a component of the difference in the ratio R at low energies ($E \leq 500$ keV) is due to the single-ionization cross sections with protons predicted to have a larger cross section than antiprotons (36% difference at 250 keV).

The investigation of the single- and double-ionization reactions for proton-helium,

$$p^+ + \mathrm{He} \rightarrow p^+ + \mathrm{He}^+ + e^- , \quad (1a)$$

$$p^+ + \mathrm{He} \rightarrow p^+ + \mathrm{He}^{++} + e^- , \quad (1b)$$

and antiproton-helium collisions

$$p^- + \mathrm{He} \rightarrow p^- + \mathrm{He}^+ + e^- , \quad (2a)$$

$$p^- + \mathrm{He} \rightarrow p^- + \mathrm{He}^{++} + e^- , \quad (2b)$$

provides a sensitive probe of the dynamics of ionizing collisions. In the above reactions the only difference is the sign of the charge of the incident projectile. Since first-order theories such as the Born approximation predict that the cross sections are proportional to the *square* of the incident charge q^2 for single ionization and q^4 for double ionization, one is lead to believe that there should be no difference in the cross sections for reactions (1) and (2).

However, measurements conducted at CERN by Andersen *et al.*[1] show a large difference in the ratio of the double- to single-ionization cross sections

$$R = \sigma_{02}/\sigma_{01} \quad (3)$$

for proton and antiproton projectiles. Theoretical confirmation has been provided by Reading and Ford[2] who have developed a large, quantum-mechanical, coupled-states program. These authors point out that it is necessary to include the $1/r_{12}$ electron-electron interaction in calculations in order to reproduce the large difference in the double-ionization cross sections for (1b) and (2b) (see Fig. 1).

In order to more fully understand the collision mechanisms, we have conducted classical calculations that allow us to follow the positions and velocities of the four particles during the collision. The Hamiltonian for the four-

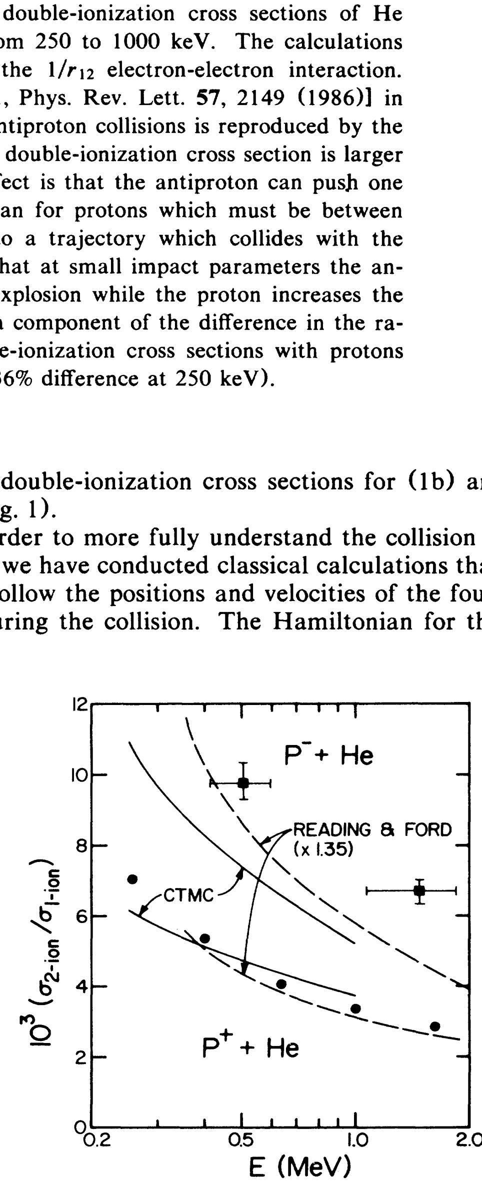

FIG. 1. Ratio of double- to single-ionization cross sections for antiprotons (upper solid and dashed lines and filled square data points) and for protons (lower solid and dashed lines and filled circle data points). The experimental data points are from Andersen *et al.* (Ref. 1) and the dashed lines are the quantum-mechanical calculations of Reading and Ford (Ref. 2) multiplied by a factor of 1.35 to reflect the lack of $l \geq 2$ orbital angular momentum states in the basis set expansion. The solid lines are our classical trajectory Monte Carlo calculations.

body system is

$$H=\frac{p_a^2}{2m_a}+\frac{p_b^2}{2m_b}+\frac{p_c^2}{2m_c}+\frac{p_d^2}{2m_d}+\frac{z_a z_b}{r_{ab}}+\frac{z_a z_c}{r_{ac}}+\frac{z_a z_d}{r_{ad}}+\frac{z_b z_c}{r_{bc}}+\frac{z_b z_d}{r_{bd}}+\frac{z_c z_d}{r_{cd}}\ , \quad (4)$$

where the subscripts a, b, c, and d refer to the incident ion, target nucleus, and the two electrons, respectively. The z_i are the respective charges of the four particles. A set of 24-coupled first-order differential equations is solved for the x-y-z positions and momenta of each particle,

$$\dot{Q}_i=\frac{\partial H}{\partial p_i},\ \dot{P}_i=-\frac{\partial H}{\partial q_i}\ . \quad (5)$$

The Bohr model for the He atom was used and consists of both electrons in a circular orbit 180° out of phase with one another and explicitly includes the $1/r_{12}$ electron-electron interaction term. This model has been demonstrated[3] to yield qualitative agreement with experiment for single- and double-ionization collisions, and was the first to correctly predict the He double-ionization cross section for 1-MeV protons.[4]

The classical trajectory Monte Carlo (CTMC) results for the ratio of the double- to single-ionization cross sections for reactions (1) and (2) are shown in Fig. 1. We observe an enhancement of the ratio for antiproton collisions relative to proton collisions. However, as with the quantum-mechanical results of Reading and Ford,[2] our calculations are in qualitative agreement with experiment but fail to give as large an enhancement as is observed.

To understand the reasons for the different ratio R for protons and antiprotons, it is illustrative to plot the ratios of the single-ionization cross sections and the double-ionization cross sections for the two projectiles. Figure 2 shows our results along with data points from Andersen *et al.*[1] along with their revised data.[5] Indeed, at high energies, as discussed by Reading and Ford, the enhanced ratio R for antiprotons is exclusively due to the larger cross section for double ionization by antiprotons relative to protons. However, we find there is another component to the ratio which should be investigated at lower energies. This is that the single-ionization cross section for protons is calculated to be larger than that for antiprotons and the difference amounts to 36% at 250 keV (see Table I). This prediction is in contrast to first-order theories that imply the single-ionization cross section simply scales as q^2. Furthermore, CTMC calculations which do not include the $1/r_{12}$ interaction also see this effect. Hence, this difference is not due to a complicated four-body collision mechanism. We should note that even at 250 keV the charge-transfer cross section is negligibly small compared to the single-ionization cross section.

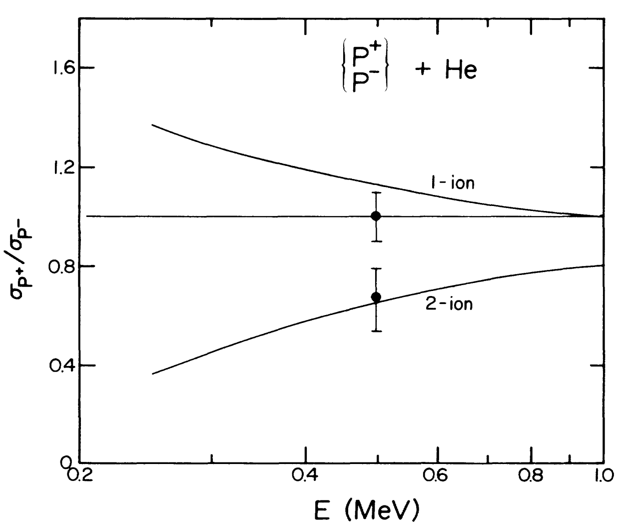

FIG. 2. The ratio of proton-to-antiproton single-ionization cross sections; the upper line is from our CTMC calculations and the data point is from Andersen *et al.* (Ref. 5). The lower line obtained from CTMC calculations and the lower data point (Ref. 1) are the ratio of the double-ionization cross sections for protons vs antiprotons colliding with helium.

An advantage of the CTMC method is that it is possible to follow the positions and momenta of the particles during the collision process. In fact, we have made video displays of the relevant trajectories in order to understand the collision mechanisms. For the double ionization process, we see the importance of four-body collisions in both proton and antiproton collisions. For large impact parameter collisions ($b \gtrsim 0.5a_0$), which contribute $\sim$30% to the total double-ionization cross section, the double-ionization events occur via scattering of one electron by the projectile in a curved trajectory around the helium nucleus to where the electron interacts with the second electron via the $1/r_{12}$ interaction, resulting in both electrons being ionized.

However, a question naturally arises as to why the antiproton projectile produces a much larger double-ionization cross section than that for the proton? One factor we observe is that the antiproton preferentially scatters the first electron inward via its repulsive interaction toward the second electron from larger impact parameters than the proton projectile. In contrast, the proton must have a trajectory between one electron and the helium nucleus in order to attract this electron into a trajectory that will collide with the second electron. Moreover, for small-impact-parameter collisions which make a major contribution to the cross sections, the larger probability for double ionization by antiprotons relative to protons ap-

TABLE I. Calculated ratio of the single-ionization cross sections for protons versus antiprotons colliding with helium. The statistical errors are at the single-standard-deviation level.

E (keV)	$\sigma_{p^+}/\sigma_{p^-}$
250	1.36 ± 0.07
500	1.13 ± 0.05
	(expt. 1.0 ± 0.1)[a]
750	1.05 ± 0.05
1000	1.01 ± 0.05

[a]From revised cross-section measurements of Andersen *et al.* (Ref. 5).

TABLE II. Calculated partial cross sections (in units of 10^{-18} cm^2) for single ionization assigned to the three regions of closest proximity to the target nucleus, midpoint between the nuclei and the projectile nucleus. The statistical errors from the CTMC calculations are also given.

E (keV)	System	Target	Midpoint	Projectile
250	$p^+ + He$	29.5 ± 1.2	26.7 ± 1.2	2.0 ± 0.3
	$p^- + He$	29.0 ± 1.2	13.6 ± 0.8	0.2 ± 0.1
500	$p^+ + He$	22.1 ± 0.8	7.7 ± 0.5	0.1 ± 0.1
	$p^- + He$	21.4 ± 0.8	5.2 ± 0.4	. . .
750	$p^+ + He$	16.7 ± 0.6	3.2 ± 0.2	. . .
	$p^- + He$	16.5 ± 0.6	2.5 ± 0.2	. . .
1000	$p^+ + He$	13.1 ± 0.5	1.8 ± 0.2	. . .
	$p^- + He$	13.1 ± 0.5	1.6 ± 0.2	. . .

pears to be due to the transient destabilization of the helium atom when the antiproton screens the nucleus, producing an effective nuclear charge of $+1$. The proton, however, increases the transient binding with the helium nuclear charge increasing from $+2$ to $+3$. The screening and antiscreening effect becomes increasingly important as the velocity is lowered and the time of the collision increases (see Fig. 2). Thus, dynamical four-body effects greatly influence the double-ionization reaction. A theoretical model based on a static representation of the helium atom will be unable to explain the experimental observations. To verify the latter statement, we have conducted three-body CTMC calculations and have used the independent electron model[6] to estimate the cross sections. Even though we observed differences in the single-ionization cross sections for protons and antiprotons (see the following two paragraphs), the ratio R for the double- to single-ionization cross sections was identical within statistical errors for the two projectiles.

An interesting prediction is made concerning the ratio of the proton to antiproton single-ionization cross sections. The theoretical calculations indicate the proton will be much more efficient than an antiproton in removing a single electron from a helium atom (see Fig. 2 and Table I). At low energies, 250 keV, the enhancement for protons is predicted to be $\sim 36\%$. An experimental data point at 500 keV is inconclusive in confirming the trend.[5]

Analysis of the positions of the ionized electrons after the collision show that the enhancement for protons is not due to charge transfer to the continuim. We find the target-centered ionization (i.e., direct-impact ionization) is similar within statistical uncertainties for both projectiles (Table II). However, the midpoint, or "saddle-point," electrons flux is considerably enhanced for the proton case. The saddle-point electrons are ionized electrons that are born at $\sim v/2$ in the saddle-point region near the distance of closest approach of a positively charged projectile to the target nucleus. Differential cross-section measurements confirm that the classical calculations are able to reproduce the shape and magnitude of the angular and energy dependence of the ejected electrons spectra for proton-helium collisions.[7]

In conclusion, classical calculations have been utilized to help understand the collision dynamics of proton and antiproton collisions on helium. The calculations indicate that a dynamical theoretical model, which includes all the four-body interactions, must be used to explain the enhanced double-ionization cross section for antiprotons relative to that for protons. A major component of the larger double-ionization cross section for antiprotons relative to protons is found to be due to the screening of the helium nucleus by antiprotons in small-impact-parameter collisions. Furthermore, the CTMC calculations lead to the prediction that the single-ionization cross section for protons will be significantly larger than that for antiprotons at the lower energies. The effect is due to the enhanced presence of saddle-point electrons in the proton versus the antiproton spectra. Experimental measurements of the single-ionization cross sections at energies of ~ 250 keV are encouraged.

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