# Comparison of single-electron removal processes in collisions of electrons, positrons, protons, and antiprotons with hydrogen and helium

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We present and compare total cross sections for single-electron removal in collisions of electrons, positrons, protons, and antiprotons with atomic hydrogen and helium. These cross sections have been calculated using the classical trajectory Monte Carlo technique in the velocity range of 0.5–7.0 a.u. (6.25–1224 keV/u). The cross sections are compared at equal collision velocities and exhibit differences arising from variations in mass and sign of charge of the projectile. At low and intermediate velocities these differences are large in both the ionization and charge transfer channels. At high velocities the single-ionization cross section for each of these singly charged particles becomes equal. However, the differences in the single-charge-transfer cross sections for positron and proton impact persist to very large velocities. We extend our previous work [Phys. Rev. A **38**, 1866 (1988)] to explain these mass and sign of the charge effects in single-electron removal collisions.

## I. INTRODUCTION

In a recent work[1] we have explained how variations in projectile mass are responsible for the differences in the single-ionization and single-charge-transfer cross sections for the positron and proton impact of helium. In brief, we found that the ionization cross sections differed at small collision velocities due to a simple dynamical effect but converged as velocity was increased. However, while also differing at small velocities, the charge transfer cross sections did not converge at large velocities. We found that at large velocities, positrons remain at least several times more likely to remove an electron from helium by capture than equivelocity protons. This occurs due to the positron's smaller momentum and corresponding greater tendency to easily vector momentum match with an orbital electron, capturing it in the collision.

Here we present an extension of this work by including electron and antiproton projectiles in the comparison of the single-ionization cross sections in helium and by performing the calculations for all four projectiles, electrons, positrons, protons, and antiprotons $(e,\bar{e},p,\bar{p})$, colliding with atomic hydrogen. Inclusion of all four of these singly charged particles in comparisons of the cross sections provides a fundamental test of theory because it allows a single-collision parameter to be varied at a time, thus isolating the effects of varying mass and sign of charge.

For example, $\bar{e}$-$p$ comparisons allow a superior discrimination of the mass effect since the open channels in these collisions are the same. In contrast, $e$-$p$ comparisons involve a change in both mass and sign of the charge, and therefore branching between the open channels must be taken into account. Similarly, $p$-$\bar{p}$ comparisons allow the sign of the charge effect to be determined without simultaneously changing the projectile mass. Simulation of the collision of these singly charged particles $(e,\bar{e},p,\bar{p})$ with atomic hydrogen allows an additional point of comparison with existing experimental measurements and with an independent estimation of the ratio of the positron and proton charge transfer cross sections at large velocities.[2]

The classical trajectory Monte Carlo (CTMC) technique, described in detail by Abrines and Percival,[3] Olson and Salop[4] and others, is a simulation of the ion-atom collision in which a large ensemble of projectile-target configurations is sampled subject to the classical evolution of initial states created to approximate the quantum-mechanical atomic distributions. It is well suited for the study of the mass and sign of the charge effects, since it includes an explicit treatment of the collision dynamics. Furthermore, the CTMC method treats all of the projectiles $(e,\bar{e},p,\bar{p})$ within the same theoretical framework, thus isolating the result from changes in the level or nature of approximation used.

Thus our aim in Sec. II is to explain how the effects of varying projectile mass and sign of the charge give rise to differences in the single-ionization and single-charge-transfer cross sections in $(e,\bar{e},p,\bar{p})$ collisions with atomic hydrogen and helium.

## II. RESULTS AND DISCUSSION

In Figs. 1 and 2 we display the results of our new CTMC calculation of the total cross section for single ionization in collisions of $(e,\bar{e},p,\bar{p})$ with atomic hydrogen and helium, respectively, along with a representative sample of the available experimental measurements of these processes. Similarly, in Figs. 3 and 4 we plot the total cross section for single charge transfer in collisions of $(\bar{e},p)$ with atomic hydrogen and helium found using our CTMC treatment, as well as representative experimental measurements. These cross sections are compared at equal collision velocity to illustrate the mass dependence of the reactions. Also, in the upper portion of each figure we present the ratio of the cross sections referred to that for protons, since in each case it is the proton-impact data that is considered most well established and there-

 

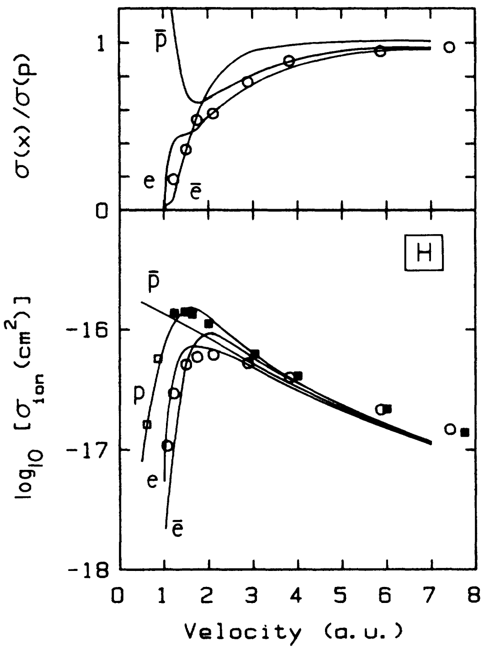


FIG. 1. Total cross section for single ionization of atomic hydrogen by electron, positron, proton, and antiproton impact (lower section): CTMC (solid curves) and experimental measurements for protons [Ref. 13 (open squares) and Ref. 14 (solid squares)], and for electrons [Ref. 15 (open circles)]. The ratio of the electron, positron, and antiproton to proton cross sections (upper section): CTMC (solid curves) and the ratio of the experimental measurements for electrons to interpolated values of the experimental measurements for protons.

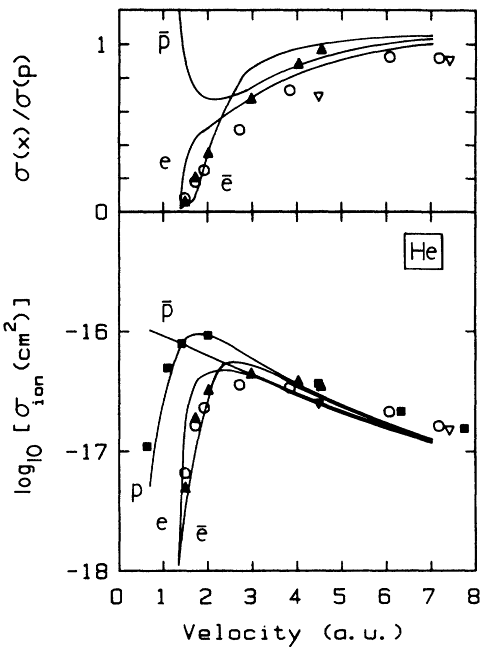


FIG. 2. Total cross section for single ionization of helium by electron, positron, proton, and antiproton impact (lower section): CTMC (solid curves) and experimental data for protons [Ref. 18 (solid squares)], for antiprotons [Ref. 19 (inverted open triangles)], for electrons [Ref. 20 (open circles)], and for positrons [Ref. 9 (solid triangles)]. The ratio of the electron, positron, and antiproton to proton cross sections (upper section): CTMC (solid curves); and the ratio of the experimental measurements for electrons, positrons, and antiprotons to interpolated values of the experimental measurements for protons.

fore serves as a benchmark. We also note the generally good agreement between our CTMC calculations and the experimental results.

These figures indicate at once that there are substantial differences in the cross sections for the various singly charged particles. On closer inspection, we see that for ionization, the cross sections differ largely only at relatively small velocities, and converge to a common value for velocities greater than about 6 a.u. (corresponding to energies above approximately 1 MeV/u). However, the positron and proton charge transfer cross sections do not converge at large velocities, indicating that an effect associated with the varying projectile mass remains important. To try to explain how these differences arise, we begin our discussion by considering the high-velocity behavior of ionization cross sections.

The Bethe-Born approximation dictates that at large collision velocities the single-ionization cross section for electrons, positrons, protons, and antiprotons should be identical. That is, the cross section should be independent of the projectile mass and the sign of its charge for these four particles. As Figs. 1 and 2 show, the ratio of the $e$, $\bar{e}$, and $\bar{p}$ cross sections to that for protons does indeed approach the value 1. Our results indicate, however, that the magnitudes of the cross sections, while converging, are not equal. In fact, we find that the positively charged particles ($\bar{e},p$) have very nearly the same cross section, but have a significantly larger cross section than the negatively charged particles ($e,\bar{p}$).

For example, in collisions with atomic hydrogen at a velocity of 2.84 a.u., corresponding to an energy of 200 keV/u, the positron and proton cross sections are equal to within about 7%, as are the electron and antiproton cross sections, but the positron and proton cross sections are about 20% greater than the electron and antiproton values. As velocity is increased, this sign of the charge effect diminishes in importance. At a velocity of 6.33 a.u. (1 MeV/u), the positron and proton cross sections differ by only about 1% and are about 12% greater than the electron and antiproton cross sections.

This sign of the charge effect may be explained in terms of the differences in the ejected electron spectra for positively and negatively charged projectiles. These differences occur because the positively charged particles create a region of reduced net force on the atomic electron. This region, which is centered about the midpoint between the atomic core and the singly charged positive projectile, has come to be known as the "saddle-point region." Electrons that are ionized due to this effect of force cancellation originate with velocities approximately one-half of that of the projectile velocity and thus have come to be called $v/2$ electrons.[5–7]

In fact, in his calculation of the ratio of the double to

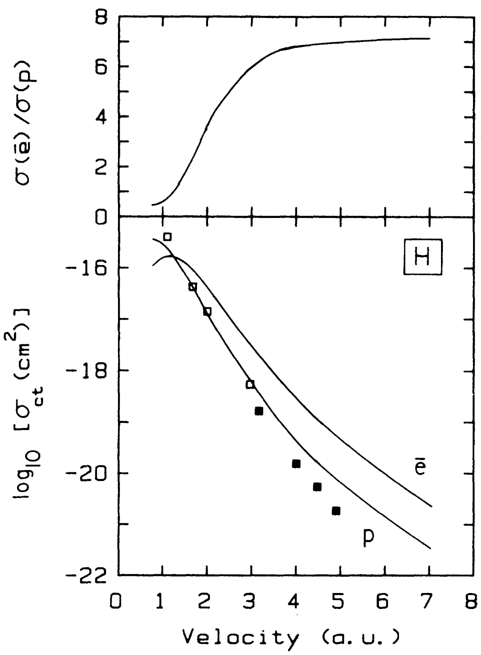


FIG. 3. Total cross section for single charge transfer in collisions of positrons and protons with atomic hydrogen (lower section): CTMC (solid curves) and experimental measurements for protons [Ref. 16 (open squares) and Ref. 17 (solid squares)]. The ratio of the positron and protons cross sections (upper section): CTMC (solid curve).

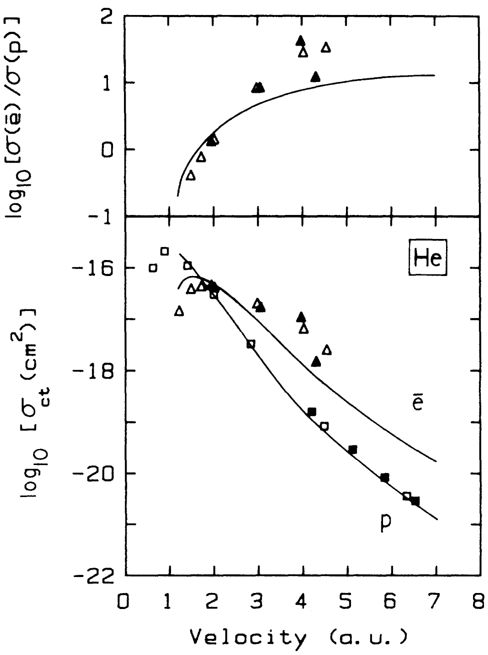


FIG. 4. Total cross section for single charge transfer in collisions of positrons and protons with helium (lower section): CTMC (solid curves) and experimental measurements for protons [Ref. 16 (open squares) and Ref. 21 (solid squares)] and for positrons [Ref. 9 (open triangles) and Ref. 10 (solid triangles)]. The ratio of the positron and proton cross sections (upper section): CTMC (solid curve) and the ratio of the experimental measurements for positrons to interpolated values of the experimental measurements for protons.

single ionization of helium by proton and antiproton impact using the CTMC technique, Olson[6] found that at high velocities the direct-impact ionization partial cross sections for protons and antiprotons are the same. However, the saddle-point ionization partial cross section for ionization is greater for protons. Thus, owing to the positive sign of their charge, positrons and protons may remove electrons by creating a region of reduced binding energy, a mechanism not possible for the negatively charged electrons and antiprotons, which accounts for their greater efficiency in single ionization at relatively large collision velocity.

Thus, at high velocities, the sign of the charge difference explains the relative magnitude of the $(\bar{e},p)$ and $(e,\bar{p})$ ionization cross sections. We also note that within these groupings according to charge sign, the heavier particles, protons, and antiprotons have slightly larger ionization cross sections than do their lighter counterparts. At a velocity of 3.83 a.u. (367 keV/u) the proton-impact ionization cross section in helium is about 3% greater than that for positron impact. Similarly, at this velocity, the antiproton-impact cross section is about 6% greater than that for the electron impact of helium. This projectile mass effect is simply a manifestation of the fact that the lighter particles have a smaller amount of energy in excess of the ionization threshold than do the lighter particles. This effect is, of course, much more important at smaller velocities but still persists to high intermediate velocities.

At low collision velocities, the effects of varying projectile mass and sign of charge, along with the branching between the ionization and charge transfer channels, itself a sign of the charge effect, superimpose to produce a more complicated situation. The mass effect is significant, since at very small velocities, electrons and positrons have very little energy above the ionization threshold. Consequently, it is much more likely that protons or antiprotons, with their much greater energy, will cause ionization. Hence the low-velocity ordering of the ionization cross section magnitudes, $\sigma(p,\bar{p}) > \sigma(e,\bar{e})$, is due primarily to a mass effect.

Furthermore, unlike at high velocity where the charge transfer cross sections for positrons and protons are orders of magnitude smaller than the ionization cross section, at small velocities the capture channel is very important. In fact, for low-velocity collisions of positrons and protons with either hydrogen or helium, the charge transfer cross sections are comparable to or larger than the ionization cross sections. This occurs, since at low velocities the collision time is relatively long, and if a positron or proton removes an electron from the target, it has a relatively high probability of capturing it. Also, since the positively charged particles present an attractive potential, the threshold for charge transfer is lower than that for ionization. Therefore at extremely small velocities, charge transfer dominates.

Consequently, the electron removal cross section for positrons and protons is partitioned between ionization and charge transfer. This parititioning accounts for the drastic drop in the positron and proton ionization cross sections at low velocity and their relative magnitudes with respect to the electron and antiproton cross sections. Thus the detailed shape of the ionization cross section in this velocity range is due to the subtle interplay of mass and sign of the charge effects. As collision velocity is increased, the significance of these effects decreases, the cross sections converging to a single value at very large velocities.

Differences in the charge transfer cross sections for positron and proton impact of both atomic hydrogen and helium also exist due to varying projectile mass. As indicated in Figs. 3 and 4, at very low velocities the proton charge transfer cross section is greater than that for equivelocity positrons. This is simply due to the fact that the lighter positrons possess much less energy above the capture threshold than do their heavier counterparts and fewer positrons succeed in removing, and capturing, an electron from the target. As in the case of ionization, this effect diminishes in importance with increasing collision velocity. For example, at a velocity of about 1.5 a.u. the positron and proton capture cross sections become approximately equal.

Unlike the ionization cross sections, however, the charge transfer cross sections do not converge. In fact, the positron charge transfer cross section becomes greater than the proton charge transfer cross section as velocity is increased. This enhancement persists to extremely large velocities, as indicated by the second-order Born and Brinkman-Kramers treatments of positron and proton collisions with helium by Deb, McGuire, and Sil.[8] Furthermore, experimental measurements of the positron charge transfer cross section in helium performed by Fromme *et al.*[9] and Diana *et al.*[10] also indicate this trend.

It should be noted, as may be seen in Fig. 4, that there is some disagreement between theory and experiment as to the magnitude of this enhancement. The experimental measurements of the charge transfer cross section for positron-helium collisions decrease as a function of energy, as about $E^{-1}$ to $E^{-1.5}$, whereas there is a general agreement between theories that the rate of decrease should be between $E^{-3}$ and $E^{-5}$ in the velocity regime of the measurements. Schultz and Olson[1] have proposed a resolution of this disagreement previously. The plausibility of this resolution is considered in greater detail in a forthcoming work,[11] along with the presentation of our new treatment of the collisions of positrons with krypton, a system recently investigated experimentally by Diana *et al.*[12]

Explanation of the enhancement of the positron charge transfer cross section relative to that of equivelocity protons has been found by examining the differential scattering cross sections and from detailed analysis of the individual trajectories which lead to charge transfer using the CTMC method. We note that due to their relatively small mass and momentum, positrons may be scattered to large angles, and may be decelerated by the target. In rare events, positrons may even by accelerated temporarily in the pseudomolecule, which is transiently formed in the collision. In contrast, protons suffer very little deflection or energy loss in charge transfer collisions. Consequently, positrons are much more readily deflected and braked into trajectories which more readily vector momentum match with, and therefore capture, an orbital electron.

Our CTMC calculations for atomic hydrogen indicate that the ratio of positron to proton charge transfer cross sections reaches a value of about 7 for large velocities, in close agreement with the high-velocity limit of the Brinkman-Kramers approximation as given by McGuire *et al.*,[2] who find that the ratio should reach a value of 6.6. In the case of helium, we find that the positron cross section becomes about 13 times as large as the proton cross section for velocities greater than about 6 a.u., also in agreement with the second-order Born and Brinkman-Kramers results of Deb, McGuire, and Sil,[8] who find that for velocities greater than 50 a.u., the ratio should be between 12 and 15.

It should be noted that the experimental determinations of the positron charge transfer cross sections indicate that the ratio might be considerably larger at high velocities, perhaps as large as 50 to 60. Future extension of the measurements to higher velocity, along with further theoretical investigation, may determine conclusively the degree to which the charge transfer cross section for positrons is enhanced relative to that for protons. Nevertheless, our investigations have led to a simple model of the collision dynamics which give rise to the differences in behavior of the single-electron removal processes in atomic hydrogen and helium for electron, positron, proton, and antiproton impact.

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