DOUBLE AND SINGLE IONIZATION OF He AND H₂ BY SLOW PROTONS AND ANTIPROTONS

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ABSTRACT

Double and single ionization of He and H₂ by proton (p) and antiproton (p̅) impact in the energy region below 50 keV was studied theoretically by using the semiclassical molecular picture. As the energy decreased, the ratio of the double- to the single-ionization cross section increased for p̅ impact and decreased for p impact for both He and H₂. These trends are consistent with recent measurements for He. Ionization mechanisms differ distinctly for p impact and p̅ impact. For p impact, the dominant mechanism for double ionization at the lower energies is sequential ladder climbing by the two electrons through various excited channels and finally into the continuum. For p̅ impact, in contrast, the approaching negative charge distorts both the He and H₂ electron clouds toward the other side of the nucleus and decreases the electron binding energies. These effects enhance electron-electron interactions, increasing double ionization. For the H₂, an effect of molecular orientation is an additional complication in determining the dynamics.

INTRODUCTION

The recent upgrade in the LEAR facility at CERN has led to experiments by Hvelplund et al. [1] on double- and single-ionization cross sections, σ++ and σ⁺, of He for p̅ impact in a low-energy regime, down to 10 keV. The ratio \( \frac{\sigma_{\gamma}}{\sigma_{\gamma'}} \) for proton impact decreased sharply with the energy decreased, while \( \frac{\sigma_{\gamma}}{\sigma_{\gamma'}} \) increased nearly monotonically. At 20 keV, \( \frac{\sigma_{\gamma}}{\sigma_{\gamma'}} \) was larger than \( \frac{\sigma_{\gamma'}}{\sigma_{\gamma}} \) by an order of magnitude.

In intermediate- to low-energy collisions, where the relative speed of the two heavy particles is comparable to or less than the orbital speed of an atomic electron, we need to consider what may collectively be called molecular effects. Because the projectile enters and leaves the interaction region slowly, the target electrons almost have time to adjust their motion to the instantaneous position of the projectile. Hence, knowledge of the adiabatic electronic states of the collision system at each instant is required for our analysis. Possible causes of the differences in magnitude of σ⁺ and σ++ for p̅ impact versus p impact at low to intermediate energies are the following: (i) the Coulomb deflection effect, (ii) the Fermi-Teller effect [2-4], and (iii) the charge polarization effect [5].
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The influence of these effects on the ratios $R_{\sigma}(\bar{p})$ and $R_{\sigma}(p)$ is not immediately evident and deserves investigation. Another point of interest is confirmation of the crucial role of electron correlation in low-energy collisions, in which slow electrons are emitted and interact with the residual ion.

We report the results of our investigation [6], based on a semiclassical molecular-state expansion method, of double and single ionization for $p$ and $\bar{p}$ impact. Both straight-line and Coulomb trajectories for heavy-particle motions were used to examine trajectory effects.

**THEORETICAL MODEL**

Our theoretical treatment has been described previously [7]. Briefly, discrete molecular electronic states were determined by the configuration-interaction (CI) method with the use of Slater-type orbitals as basis functions for the $H_2$. Continuum electronic states for singly ionized states were obtained in the fixed-nuclei static-exchange (Hartree-Fock) approximation to elastic electron scattering from the neutral molecule ($pHe^+$) or the molecular ion ($pHe^+$) [8]. Continuum electronic states for doubly ionized states were constructed by using the perturbation method in which $1/r_{12}$ is the perturbation; the terms up to the first order in the wave function were retained. Therefore, the unperturbed basis functions were continuum, one-electron, diatomic-molecule orbitals. The adiabatic wave packet approach taken spanned the electronic continuum locally [9]. A discretized sampling procedure, based on the Gauss quadrature, was used to select continuum states for the molecular expansion method [8]. All wave functions were properly orthogonalized by the Schmidt procedure. Expanding the total wave function in terms of products of molecular orbitals and electron translation factors and substituting it into the time-dependent Schrödinger equation yielded a set of first-order coupled equations for the expansion coefficients [7]. The coupled equations were solved numerically to extract scattering amplitudes. The square of the scattering amplitude for each process gave the transition probability.

The molecular states included in the calculation were the following: (i) For $\bar{p}$ impact, we used the initial channel, $p + He(1^1S)$; excitation channels $p + He(1sn\ell$ with $n = 2, 3$); single-ionization channels (35 discretized states) $p + He^+(1s) + e$; and double-ionization channels (5-10 discretized states at each singly ionized state $p + He^{2+} + 2e$. (ii) For $p$ impact, we included the initial channel, $p + He(1^1S$; excitation channels $p + He(1sn\ell$, $n = 2, 3$); charge transfer channels $H(1s) + He^+(1s)$ and $H(n=2) + He^+(1s)$; and the same single- and double-ionization channels. The total number of states included in the present calculation was 150-250 for $\bar{p}$ and $p$. As an exploratory test, we determined discrete molecular electronic states for the $pH_2$ by using the multireference single- and double-excitation CI method [10] with Gaussian-type orbitals. In this approach, we mapped three-dimensional adiabatic surfaces for the $\bar{p} + H_2$ system.

**RESULTS**

Figure 1 displays our present results for $R_{\sigma}$ along with measurements for $\bar{p}$ impact by Hvelplund et al. [1] and for $p$ impact by Shah et al. [11]. The qualitative agreement between the two sets of results is good. The agreement of the present double- and single-ionization cross sections for $\bar{p}$ impact with the
FIG. 1. Ratio of double ionization to single ionization due to $\bar{p}$ and $p$ impact. Theoretical results are from the present work. The experimental results are taken from Ref. 1 for $\bar{p}$ impact and from Ref. 11 for $p$ impact.

Measured results of Hvelplund et al. [1] is reasonable (within 45% at energies 20 and 50 keV), while the consistency between results for $p$ impact is somewhat unclear, because Shah et al. [11] did not measure double ionization directly. However, the trend of the increase and decrease in the ratios for $\bar{p}$ and $p$ impact, respectively, is unambiguous.

For $p$ impact, after the first electron is ejected, the second electron moves in the field created by two positively charged particles. This situation leads to a drastic decrease (with decreasing energy) in the double-ionization cross section compared to the single-ionization cross section and hence in the ratio. For $\bar{p}$ impact, as energy decreases, the increase of the effective interaction time of electron-electron coupling leads to increase of double ionization and hence, the ratio.

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REFERENCES


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