Ionization of atomic hydrogen by antiproton impact

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The ionization and excitation cross sections of atomic hydrogen with antiprotons are calculated using the close-coupling method, where the wave function is expanded by atomic states only on protons. The resulting total cross sections are in good convergence and in agreement with other calculations based on the close-coupling method with considerably large basis set. The angular distribution of ionized electrons is calculated by substituting the obtained wave function in the close-coupling method into the integral form of the transition amplitude. Above 100 keV, the angular distributions of ionized electrons are compared for proton- and antiproton impacts.

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I. INTRODUCTION

Experimental research using slow antiprotons ($\bar{p}$) has been studied at the Antiproton Decelerator (AD) of CERN. A user group named *ASACUSA Collaboration* is going to produce an ultraslow $\bar{p}$ beam and use it for atomic collisions or spectroscopies at AD [1]. The cross sections for atomic collisions using a slow $\bar{p}$ projectile will be measured with small uncertainties in the near future.

The collision of $\bar{p}$ with atomic hydrogen is considered important where a heavy negative-charged particle collides with the simplest atomic system. For collision energy below the ionization threshold, the protonium ($\bar{p}p$) formation becomes dominant. In the present work, we consider collision energies above 1 keV where the protonium formation is negligible and the impact-parameter method is valid [2]. Since the electron capture does not occur in the case of $\bar{p}$ impact, which greatly differs from the p impact, the expansion of the wave function in terms of atomic orbitals centered only on protons is likely to work well. While such a calculation was reported by Hall *et al.* [3], we try to develop a similar approach to the one-center close-coupling (CC) calculation with larger basis sets. Here we show the cross sections for the ionization and the excitation in $\bar{p}+\mathrm{H}$ collisions. The present total ionization cross section is compared with other authors' results with comparatively large-scale calculations [3–5,7]. Some partial contributions for the ionization cross section and the differential cross sections (DCS's) are shown with respect to the ejection angle of ionized electrons. An integral form for the transition matrix is adopted to calculate the DCS's using the wave function resulting from the CC calculation. In addition, the angular dependencies of ionized electrons for the $p^{\pm}$-impacts are compared above 100 keV. Atomic units are used unless otherwise stated.

II. THEORY

Let $\mathbf{R}$ denote the position vector of $\bar{p}$ from p. In the impact-parameter method [2], the internuclear motion is classically treated as $\mathbf{R}=\mathbf{b}+\mathbf{v}t$ with impact parameter $\mathbf{b}$, a collision velocity $\mathbf{v}$ that is perpendicular to $\mathbf{b}$, and time t. The electronic motion is described by the solution of the time-dependent Schrödinger equation

$$\left[h(\mathbf{r})+V(\mathbf{r},\mathbf{R}(t))-i\left(\frac{\partial}{\partial t}\right)_{\mathbf{r}}\right]\psi(\mathbf{r},\mathbf{R})=0, \tag{1}$$

where $\mathbf{r}$ is the position vector of the electron from the proton, and h is the Hamiltonian of atomic hydrogen. The interaction between $\bar{p}+\mathrm{H}$ is given by

$$V=-1/R+1/|\mathbf{r}-\mathbf{R}|. \tag{2}$$

The total wave function is expanded as

$$\Psi=\sum_i c_i(b,t)\,\phi_i(\mathbf{r})\exp(-i\epsilon_i t). \tag{3}$$

Here ϕ_i is an atomic wave function with energy ϵ_i, and it can be written as

$$\phi_i\equiv\phi_{nlm}=S_{nl}(r)[(-1)^m Y_{lm}(\hat{\mathbf{r}})+Y_{l,-m}(\hat{\mathbf{r}})]/\sqrt{2(1+\delta_{m,0})}, \tag{4}$$

where Y_{lm} are the spherical harmonics. For the coordinates $\mathbf{r}=(x,y,z)$, the z-x plane is taken on the collision plane involving $\mathbf{b}$ and $\mathbf{v}$ and the z axis is chosen along $\mathbf{v}$. Since the Hamiltonian is symmetric under the reflection $y\rightarrow -y$, and the electronic state is in the ground state before the collision, the angular part of ϕ_i is symmetric under the reflection.

The radial function S_{nl} is expanded using the Sturmian functions as

$$S_{nl}(r)=r^l\exp(-\alpha r)\sum_k a_{kn}^{(l)}L_k^{2l+2}(2\alpha r), \tag{5}$$

where L_k^{2l+2} are the associated Laguerre polynomials and α is an arbitrary constant. The coefficients $a_{kn}^{(l)}$ are determined by the variational calculation for the Hamiltonian of atomic hydrogen. The Sturmian functions for orbital angular momentum l contain contributions from all bound and continuum states with the same angular momentum. They are orthogonal and free from overcompleteness, which are often encountered when using Slater orbitals. In addition, the convergence of expansions can be studied in a systematic manner with an increasing number of basis functions [8].

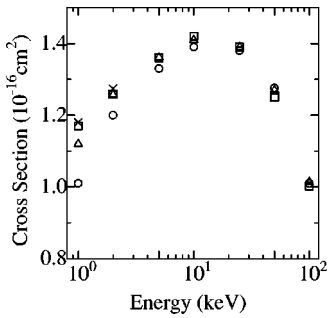

FIG. 1. Convergence behavior in the present calculations for the total ionization cross section. 263 states for $l=0-5$ (○), 477 states for $l=0-8$ (△), 699 states for $l=0-8$ (□), and 478 states for $l=0-12$, $m=0-2$ (×).

By substituting Eq. (3) into the Schrödinger equation (1), we have coupled equations with respect to the expansion coefficients.

$$i\frac{d}{dt}c_i=\sum_j \exp[i(\epsilon_i-\epsilon_j)t]\langle\phi_i|V|\phi_j\rangle c_j, \tag{6}$$

where

$$\langle\phi_i|V|\phi_j\rangle=\int d\mathbf{r}\ \phi^* V\phi_j. \tag{7}$$

The above-coupled equations are solved with the initial condition $c_i(\mathbf{b},-\infty)=\delta_{i,1s}$. The cross section into state $i\equiv(n,l,m)$ is given by

$$\sigma_{nlm}=2\pi\int db\, bP_{nlm}(\mathbf{b}), \tag{8}$$

where $P_{nlm}(b)=|c_{nlm}(b,+\infty)|^2$ is the transition probability into state i at impact parameter b. The total cross sections for ionization and excitation are calculated by

$$\sigma_{\rm ion}=\sum_{nlm}{}' \sigma_{nlm} \tag{9}$$

and

$$\sigma_{\rm exc}=\sum_{nlm}{}'' \sigma_{nlm}, \tag{10}$$

respectively. In the above equations, Σ'_{nlm} means the sum over states with $\epsilon_{nlm}\geqslant 0$ and Σ''_{nlm} the sum over states with $\epsilon_{nlm}<0$, excluding the initial state.

Though the total ionization cross sections are obtained as a sum of excitation cross sections in the states with positive energies in the CC calculation, the DCS's cannot be obtained with respect to the momentum $\mathbf{k}$ for ionized electrons, namely $d\sigma/d\mathbf{k}$. To overcome this, we use the integral form for the transition amplitude

$$T_{\mathbf{k}}(\mathbf{b})=-i\int_{-\infty}^{+\infty}dt\langle\exp(-i\epsilon_{\mathbf{k}}t)\phi_{\mathbf{k}}|V|\psi\rangle, \tag{11}$$

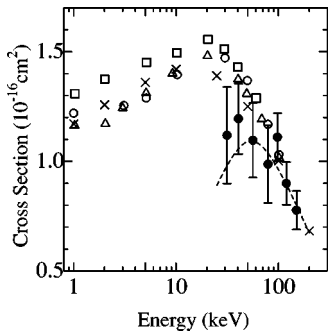

FIG. 2. Total ionization cross section in $\bar{p}$+H. calculations: Present (×), Hall *et al.* [3] (○), Schiwietz *et al.* [4] (△), Wells *et al.* [5] (□), and CDW-EIS model [7] (− − −). Measurement: Knudsen *et al.* [9] (●).

where $\phi_{\mathbf{k}}$ is the Coulomb wave function normalized as

$$\langle\phi_{\mathbf{k}}|\phi_{\mathbf{k}'}\rangle=\delta(\mathbf{k}-\mathbf{k}'). \tag{12}$$

ψ is the total wave function that is approximated by the wave function in Eq. (3). This is hereafter referred to as the integration method. The differential cross section for the ionized electron momentum is given by

$$\frac{d\sigma}{d\mathbf{k}}=\int d\mathbf{b}|T_{\mathbf{k}}(\mathbf{b})|^2. \tag{13}$$

III. RESULTS

A. Cross sections for the ionization and the excitation

We set the exponent $\alpha=0.6$ in Eq. (5). Four different basis sets are used in the present study: (a) 263 states for $l=0-5$, (b) 477 states for $l=0-8$, (c) 699 states for $l=0-8$, and (d) 478 states for $l=0-12$, $m=0-2$. For the partial wave l, the typical number of Sturmian functions is $15-l$ for the basis (a) and (b) and $21-l$ for basis (c) and (d). The atomic energies of the hydrogen atoms are better than 11 digits for the $n=1-3$ manifolds. Some of the states with negative energies represent the Rydberg states; those with positive energies represent the continuum. All azimuthal components allowed for the orbital angular momentum are coupled in the basis (a), (b), and (c). The contribution from high m is strongly suppressed for slow collisions, which will be shown in Sec. III B. Though azimuthal components are restricted up to $m=2$ in the basis (d), it is actually the largest basis for low energies.

The present ionization cross sections are shown in Fig. 1. The cross sections in the bases (a), (b), and (c) are in good agreement above 25 keV. With decreasing energy, the basis (a) deviates from other cross sections. The results of the bases (b) and (c) agree well above 2 keV. The basis (d) is more reliable below 2 keV. The results of the bases (c) and (d) are in good agreement at 1 keV. Thus the basis (c) shows good convergence above 1 keV.

The present ionization cross section in the basis (c) is compared with other calculations and the data measured by Knudsen *et al.* [9] in Fig. 2. The present cross sections are tabulated in Table I. Hall *et al.* included 273 states for $l=0-5$ in their one-center CC calculation [3]. Schiwietz *et al.*

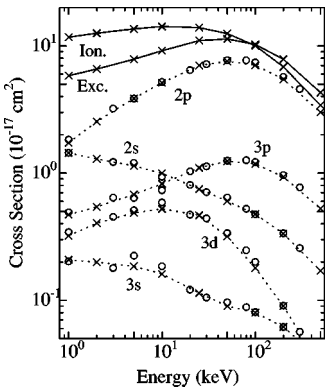

FIG. 3. The excitation cross sections into $n=2$ and 3 manifolds, and total cross sections for the ionization and the excitation. Present ($\times$); Hall *et al.* [3] ($\circ$).

[4] also carried out one-center CC calculation using 350 states [3]. The results of present work, Hall *et al.*, and Schiwietz *et al.*, which are calculated using the one-center CC method, are all in good agreement. On the other hand, Wells *et al.* solved the Schrödinger equation directly on the three-dimensional lattice [5]. The cross section of Wells *et al.* is about 10% larger than that of one-center CC calculations, which is consistent with their estimation. Discussion on the accuracy of the lattice calculations are found in Refs. [5] and [6]. The CDW-EIS calculation [7], which is a high-energy approximation, is valid only above 100 keV. The data measured by Knudsen *et al.* [9], which have large error bars for lower collision energies, differ considerably from the results of CC calculations. The new measurements of cross sections in $\bar{p}+\mathrm{H}$ are being awaited.

Figure 3 displays the excitation cross sections into $n=2$ and 3 sublevels, the total ionization cross section, and the total excitation cross section. The excitation cross sections also show good convergence among the present four basis sets. They agree well with the excitation cross sections of Hall *et al.* [3]. As for the total cross sections for excitation and ionization, they are comparable around 100 keV, and the ionization is dominant for low energy, owing to the charge cancellation of target protons by the close collision of $\bar{p}$.

TABLE I. The present cross sections are given in 10^{-16} cm^2 for the ionization of $\bar{p}$ impact and for the electron removal of p impact, which are calculated by the CC method or by the integration method.

	$\bar{p}$ impact		p impact	
Energy (keV)	CC	Integration	CC	Integration
1	1.17			
2	1.26			
5	1.37	1.80		
10	1.40			
25	1.39	1.50		
50	1.25	1.32	2.70	3.16
100	1.00	1.00	1.44	1.49
200	0.68	0.67	0.78	0.78
500	0.34	0.34	0.35	0.35

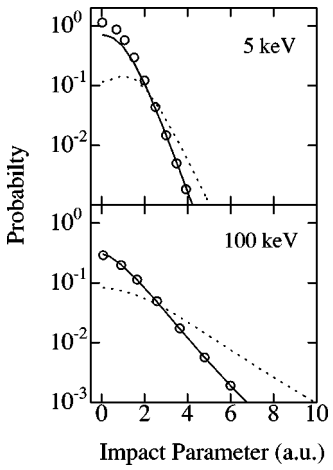

FIG. 4. Impact-parameter dependencies of transition probabilities at 5 and 100 keV for the ionization and the excitation. Total ionization by the CC method (——). Total excitation by the CC method ($\cdots$). Total ionization by the integration method in Eq. (11) ($\circ$).

B. Partial dependencies in the ionization cross sections

The impact-parameter dependencies for the excitation and ionization for energies at 5 and 100 keV are shown in Fig. 4, respectively. We can notice from the figure that the probabilities for the excitation have a longer tail than those for the ionization. The ionization probabilities are dominant at small impact parameters.

Figure 5 shows the fractions of partial waves l and the azimuthal components m for the ionization cross sections at 1 keV and 100 keV. There is a good convergence with l at 100 keV. On the other hand, l convergence is not so good for 1 keV; however, the contributions obtained by assigning high values of m decrease rapidly. Therefore the states of having higher values of l with smaller values of m need to be considered for slow collision. It means that the electronic cloud spreads considerably along the incident direction and its distortion in the perpendicular direction is relatively small. The negligibility of high m is useful in reducing the amount of calculation at low energy, since the computation for slow collision is time consuming owing to the oscillation of $\exp(i\Delta\epsilon t)=\exp(i\Delta\epsilon/v\hat{\mathbf{v}}\cdot\mathbf{R})$ in Eq. (6).

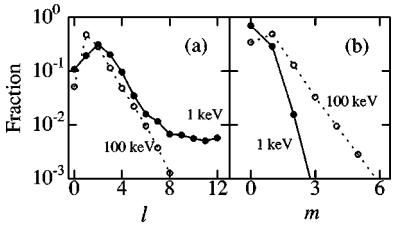

FIG. 5. The fraction of partial contributions in the ionization cross section σ_{ion} at 1 and 100 keV. (a) The fraction for each partial wave l, $\sigma_l/\sigma_{\mathrm{ion}}\cdot\sigma_l=\Sigma'_{nm}\sigma_{nlm}$. (b) The fraction for each azimuthal component, $\sigma_m/\sigma_{\mathrm{ion}}\cdot\ \sigma_m=\Sigma_{nl}{}'\sigma_{nlm}$.

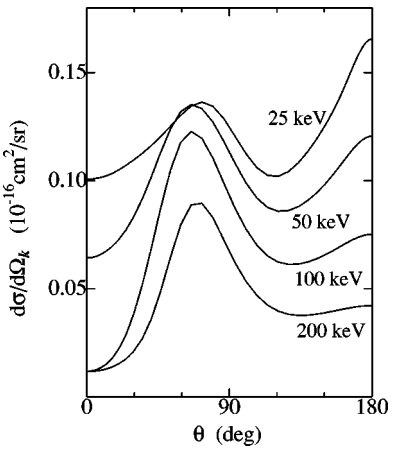

FIG. 6. The differential ionization cross sections $d\sigma/d\Omega_k$ for 25–200 keV in $\bar{p}+\mathrm{H}$ collisions.

C. DCS with respect to the electron ejection angle

We calculated the ionization cross section for $\bar{p}+\mathrm{H}$ using the integration method in Eq. (11) for several collision energies between 5 and 500 keV. The total wave function is approximated using the CC calculation in the basis (c). The Coulomb wave function is expanded in terms of partial waves up to $l=8$.

If the wave function with the CC calculation is sufficiently exact, the two calculations, namely the CC and the integration method, should give the same ionization cross sections. The ionization cross sections that were calculated using the two methods are tabulated in Table I. The two methods revealed a reasonable agreement above 25 keV; however, disagreement is comparably large at 5 keV. The impact-parameter dependence calculated with the integration method is also included in Fig. 4. The probability for 5 keV is larger than 1 at small impact parameter. On the other hand, the CC calculation, in which the unitarity is automatically satisfied, is in good convergence, and its impact-parameter dependence would be reliable even at 5 keV. However, the use of such a wave function in the integration method may lead to too large of a cross section for low energy, which is often the case with perturbation methods. Thus the integration method requires higher accuracy for slow collision.

The DCS's with respect to the electron ejection angles, are shown in Fig. 6 for the collision energies between 25 and 200 keV. The backward ejections are prominent for lower energies. The DCS's in the forward direction are small for 100 and 200 keV, where the collision velocity is faster than the orbital velocity of atomic hydrogen.

The electron removal cross section in $p+\mathrm{H}$ are also included in Table I to verify the validity of the present integration method for the p impacts. Since the charge-transfer channels are neglected in the present CC calculation, the wave function is not accurate for energies where the electron capture is tolerable in the removal cross section. The contribution of the electron capture is about 10% in the electron removal at 100 keV [10].

Figure 7 shows the comparison of the DCS of $d\sigma/d\theta$ for $p^{\pm}$ impacts for collision energies 100, 200, and 500 keV,

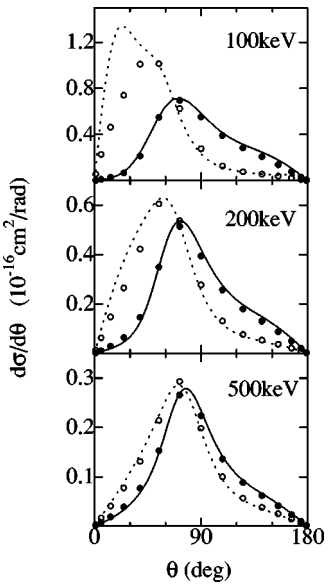

FIG. 7. The comparison of differential cross sections $d\sigma/d\theta$ for $p^{\pm}+\mathrm{H}$ collisions for energies 100 keV, 200, and 500 keV, respectively. θ is the electron ejection angle. $\bar{p}$ impact: present integration method (——); CDW-EIS model (○). p-impact: present integration method (· · ·); CDW-EIS model (●).

respectively. Here θ denotes the electron ejection angle. The DCS of the CDW-EIS model calculated in the present work is also included for comparison [11]. the cross sections for $p^{\pm}$ impacts become similar with increasing energy, as expected. The agreement of DCS's between the present integration method and the CDW-EIS model is surprising for $\bar{p}$ impact, because the CDW-EIS model is a simple distorted-wave method. As for the p impact, the DCS's of the integration method, which include the electron capture, are slightly larger for small angles than those of the CDW-EIS model at 100 and 200 keV. The peaks of $d\sigma/d\theta$ for the p impacts are located at smaller angles than those of the $\bar{p}$ impacts. The difference in the DCS for the ejection angle is simply explained by the postcollision interaction, namely, the interaction after the projectile passes through the target proton. The electrons are pulled in the forward direction for the p impact and pushed back in the opposite direction for the $\bar{p}$ impact.

IV. SUMMARY

The cross sections for $\bar{p}+\mathrm{H}$ collisions are calculated using the one-center CC method with pseudostates above 1 keV. The total cross sections for excitation and ionization have shown good convergence in terms of results. The integral form for the transition matrix is used to calculate the differential cross sections with respect to the ionized electron momentum. The total ionization cross sections of the integration method are too large at low energies due to the unitarity violation at small impact parameter. It gives reasonable cross sections above 25 keV for the $\bar{p}$ impact and above 100 keV for the p impact. Owing to the postcollision interaction, the electron tends to be ionized in the incident direction for the p impact and emitted in larger angles for the $\bar{p}$ impact.

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