# Quantum-mechanical study of ionization in slow collisions of antiprotons with hydrogen atoms

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The cross sections for the ionization $\bar{p}+\mathrm{H}\rightarrow\bar{p}+p+e$ at low collision energies are computed with a complete quantum-mechanical method of time-dependent wave-packet propagation, which was applied to the protonium formation ($\rightarrow\bar{p}p+e$) by the present author [Phys. Rev. A **65**, 012706 (2002)]. The ionization process shows very large cross sections even near threshold energy. An impact-parameter semiclassical method, in which the trajectory bending is taken into account by the introduction of the adiabatic potential, is also examined for the calculation of the ionization cross section. The semiclassical results are in good agreement with the quantum-mechanical results.

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A theoretical study by Schultz *et al.* [1], though using a classical trajectory Monte Carlo (CTMC) approach, has shown that the cross section for ionization of hydrogen atoms by antiproton ($\bar{p}$) impacts,

$$\bar{p}+\mathrm{H}\rightarrow\bar{p}+p+e, \tag{1}$$

remains large even when the center-of-mass (c.m.) collision energy ($E$) becomes very near the ionization threshold ($I=13.6$ eV). Such a feature is never observed in the ionization by electron or proton impacts. Since an antiproton is a heavy particle having negative charge, the $\bar{p}$ collisions offer a unique and interesting problem in atomic physics. Recently, a lot of reliable calculations based on impact-parameter semiclassical approach [1–13] were carried out for the ionization (1), and are in good agreement with each other and also with the experimental results measured at $E\geqslant 15$ keV by Knudsen *et al.* [14]. However, all the semiclassical studies except Ref. [6] considered only the high energy region of $E>100$ eV. This is because a linear trajectory was assumed for the relative motion in most of the semiclassical studies (referred to as SC-L). The effect of the trajectory bending would be non-negligible at $E\lesssim 500$ eV [6,10]. Complete quantum-mechanical (QM) study should be inevitable in that case.

This paper, carrying out the QM calculation, reports the cross sections for (1) at energies near $I$. A time-dependent wave-packet propagation technique, which was useful for the study of the protonium formation ($\rightarrow\bar{p}p+e$) at $E<I$ [15,16], is applied to the ionization (1). The calculation of ionization using this QM method was already made for the system of a negative muon ($\mu^-$) and a hydrogen atom [17], i.e.,

$$\mu^-+\mathrm{H}\rightarrow\mu^-+p+e. \tag{2}$$

However, since the $\bar{p}$ mass is about nine times heavier than the $\mu^-$ mass, the QM calculation becomes much more laborious for the $\bar{p}$ impacts.

We also apply the impact-parameter semiclassical method (SC-B) to the low-energy ionization by considering the effect of the trajectory bending with use of the adiabatic potential. The SC-B method was found to work well for the ionization (2) [17] and further for the protonium formation at $E<I$ [16,18].

The details of the QM and SC-B methods are described in Refs. [15,17]. The QM wave-packet has been propagated on grid points of configuration space, represented by Jacobi coordinates corresponding to the $\bar{p}+\mathrm{H}$ arrangement. The grid is constructed from zero points of orthogonal polynomials. The numerical parameters of the present calculations are mostly the same as those of the previous ones [15,17]: the number of grid points for the electron radial and polar coordinates $(r,\theta)$ is $N_r=30$, $N_\theta=3$; the electron magnetic quantum numbers included are $\lambda=-1,0,1$; and the width parameter of the wave-packet is $\delta=0.4$. The center of the wave-packet has been initially set at a relative ($\bar{p}$-H) distance $R=R_0$, and, after sufficiently long time evolution, the transition probabilities have been extracted at some distance $R=R_\mathrm{f}$. The values of $R_0$ and $R_\mathrm{f}$ must be large enough so that the extracted probabilities become independent of them. In the previous QM calculation for $E<I$ [15], $R_0=R_\mathrm{f}=4$ a.u. was sufficient. In the SC-B calculation of the ionization (2), however, $R_\mathrm{f}=12$ a.u. was needed for energies up to 200 eV. Since this large value makes the QM calculation extremely laborious, $R_\mathrm{f}=7$ a.u. has been chosen in the present study. The error due to this choice is estimated to be $\lesssim 2\%$ at $E<40$ eV from the SC-B calculations using $R_\mathrm{f}=7$ a.u. and $R_\mathrm{f}=12$ a.u., as shown in Table I. In the QM calculation, the number of grid points for the $R$ coordinate is $N_R=225$ for the total angular momentum quantum number $L\geqslant 20$ and $N_R=360$ for $L<20$. The value of $R_0=5$ a.u. has been selected.

In the present study, we consider only the event of electron emission, and cannot distinguish between the two channels of protonium formation and ionization [17]. However, the probability of electron emission becomes identical to the ionization probability if $E\gg I$. Because of the large mass difference between $\bar{p}$ and $e$, we can expect that the probability of protonium formation decreases rapidly at energies exceeding $I$ [19].

Figure 1 shows the time evolution of the wave-packet for the relative radial motion $R$ in the QM calculation for $L=30$. Plotted are three cases of the initial wave-packets having the central collision energies $E_0=10$ eV ($<I$), 15 eV

 

TABLE I. Cross sections (in a.u.) for the electron emission, $\bar{p}+\mathrm{H}\rightarrow\bar{p}+p+e$ and $\rightarrow\bar{p}p+e$, calculated by the QM and SC-B ($R_f=7$ and 12 a.u.) methods. The present values can be practically regarded as the ionization cross sections when $E\geqslant 20$ eV. (See text.)

| c.m. energy (eV) | QM | SC-B $R_f=7$ a.u. | SC-B $R_f=12$ a.u. |
|---|---|---|---|
| 16 | 5.96 | 6.06 | |
| 18 | 5.72 | 5.82 | |
| 20 | 5.54 | 5.64 | 5.57 |
| 22 | 5.39 | 5.48 | |
| 24 | 5.21 | 5.36 | |
| 26 | 5.13 | 5.26 | |
| 28 | 5.07 | 5.17 | |
| 30 | 5.00 | 5.09 | 5.01 |
| 32 | 4.94 | 5.03 | |
| 34 | 4.91 | 4.97 | |
| 36 | | 4.93 | |
| 38 | | 4.88 | |
| 40 | | 4.85 | 4.75 |

($\simeq I$), and 20 eV ($>I$). The major part of the final wave-packet stays in the finite region of $R\lesssim 6$ a.u. (i.e., $\bar{p}p+e$) when $E_0=10$ eV, and seems to propagate far away (i.e., $\bar{p}+p+e$) when $E_0=20$ eV. In these three cases, the principal reaction products become quite different, though we can find that the electron emission probabilities are nearly the same ($\simeq 0.9$). In the QM calculation of the cross section, the initial wave packets have been prepared for $E_0=20$ and 30 eV, and can cover the energy range of $16\leqslant E\leqslant 34$ eV.

Figure 2 shows the electron emission or ionization cross sections obtained by the present QM, SC-B, and SC-L calculations, by the previous SC-B calculation [6], and by the CTMC calculation of Schultz *et al.* [1]. The protonium formation cross sections obtained by the QM [15] and CTMC [1] calculations are also included for the purpose of reference.

The present QM cross section increases as $E\rightarrow I$, and seems to smoothly connect to the QM protonium-formation cross section. This feature of the electron emission was found also in the CTMC calculations [1,20]. However, the CTMC ionization cross section sharply drops to zero at $E\lesssim 16$ eV, where protonium formation becomes eventually a dominant reaction channel as $E\rightarrow I$. From the CTMC calculation, we infer that the present electron-emission cross sections at $E=16$ and 18 eV may have small but non-negligible contribution from protonium formation. If the QM calculation were carried out for the initial wave-packet having $E_0\sim I$ (e.g., $E_0=15$ eV in Fig. 1), the two channels would become equally important. To extract the pure ionization cross section in the QM calculation, we must make frame transformation into Jacobi coordinates corresponding to the $\bar{p}p+\mathrm{e}$ arrangement and further perform wave-packet propagation [15]. It requires more computational time, and remains in future work.

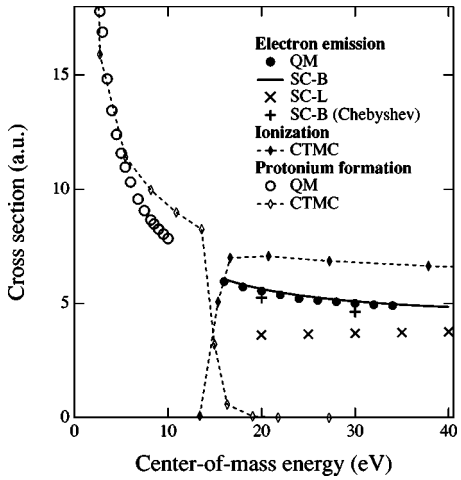


FIG. 2. Cross sections for electron emission, ionization, and protonium formation as a function of the center-of-mass collision energy $E$. *Electron emission* ($E>I$): QM of the present study (●), SC-B(—) and SC-L (×) of the present study, SC-B of Sakimoto using a Chebyshev grid [6] (+). *Ionization* ($E>I$): CTMC of Schultz *et al.* [1] (♦). *Protonium formation* ($E<I$): QM of Sakimoto [15] (○), CTMC of Schultz *et al.* 1 (◇).

As also found for the ionization (2) [17], Fig. 2 shows that the present SC-B results agree well with the QM results. The present study confirms again the usefulness of the SC-B method adopting the adiabatic potential. In a previous SC-B study [6], the grid of the electron radial coordinate $r$ was constructed from the zero points of Chebyshev polynomials (Chebyshev grid), and thereby the electron was artificially confined in a box with a finite size. This causes some problem as the collision energy becomes low. For this reason, the previous SC-B result [6] is slightly smaller than the present results. Subsequent studies [15,17,18] introduced a Laguerre grid [7], which were found effective in the calculation of low-energy collisions.

The SC-L result is always decreasing as $E\rightarrow I$. The linear-trajectory assumption in the semiclassical method is evi-

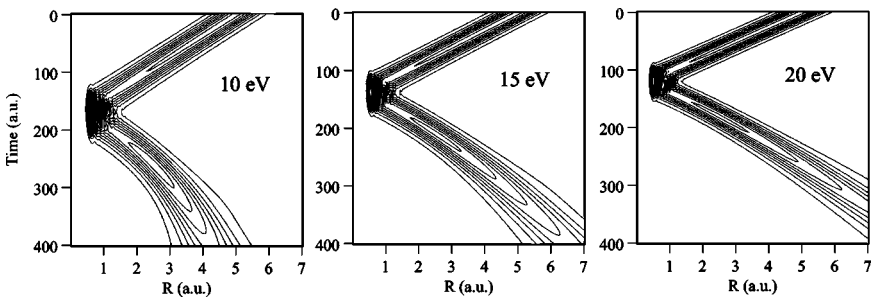


FIG. 1. Time evolution of the QM probability densities integrated over all the coordinates other than the relative radial distance $R$ for the total angular momentum quantum number $L=30$. The central collision energies of the initial wave packets are $E_0=10$, 15, and 20 eV.

dently inappropriate in the low-energy region. Also at intermediate energies $50 < E < 500$ eV, the trajectory bending is still important [6,10] though the QM calculation is practically impossible. There, the SC-B method with use of the adiabatic potential is sufficiently promising for giving reliable cross sections for the ionization process.

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[1] D. R. Schultz *et al.*, Phys. Rev. Lett. **76**, 2882 (1996).
[2] J. C. Wells *et al.*, Phys. Rev. A **54**, 593 (1996).
[3] G. Schiwietz *et al.*, J. Phys. B **29**, 307 (1996).
[4] K. A. Hall, J. F. Reading, and A. L. Ford, J. Phys. B **29**, 6123 (1996).
[5] A. Igarashi, S. Nakazaki, and A. Ohsaki, Phys. Rev. A **61**, 062712 (2000).
[6] K. Sakimoto, J. Phys. B **33**, 3149 (2000).
[7] K. Sakimoto, J. Phys. B **33**, 5165 (2000).
[8] B. Pons, Phys. Rev. Lett. **84**, 4569 (2000).
[9] B. Pons, Phys. Rev. A **63**, 012704 (2001).
[10] X. Tong *et al.*, Phys. Rev. A **64**, 022711 (2001).
[11] N. Toshima, Phys. Rev. A **64**, 024701 (2001).
[12] J. Azuma *et al.*, Phys. Rev. A **64**, 062704 (2001).
[13] S. Sahoo, S. C. Mukherjee, and H. R. J. Walters, J. Phys. B **37**, 3227 (2004).
[14] H. Knudsen *et al.*, Phys. Rev. Lett. **74**, 4627 (1995).
[15] K. Sakimoto, Phys. Rev. A **65**, 012706 (2002).
[16] K. Sakimoto, Phys. Scr., T **T110**, 271 (2004).
[17] K. Sakimoto, J. Phys. B **35**, 997 (2002).
[18] K. Sakimoto, Phys. Rev. A **66**, 032506 (2002).
[19] J. S. Cohen, Phys. Rev. A **36**, 2024 (1987).
[20] J. S. Cohen, Phys. Rev. A **56**, 3583 (1997).