Ionization of helium ions by low-energy antiproton collisions

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The cross section for ionization $\bar{p}+\mathrm{He}^{+}\rightarrow\bar{p}+\mathrm{He}^{2+}+e$ at collision energies ranging from threshold to 1 MeV is calculated using a quantum-classical hybrid (i.e., semiclassical) method. Due to the bending effect of $\bar{p}+\mathrm{He}^{+}$ trajectories, the ionization cross section shows a local minimum at the center-of-mass energy of ~150 eV. Also reported is the excitation cross section, which is expected to remain finite at threshold for the same reason as the Gailitis jump appears in excitation of ions by electron impacts.

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I. INTRODUCTION

Recently, it has become possible to carry out a complete quantum mechanical (QM) calculation for ionization in low-energy collisions between antiprotons $\bar{p}$ (or muons μ^{-}) and hydrogen atoms [1,2]. However, such a study still requires time-consuming computation, and cannot be readily made. As another approach appropriate for heavy-particle collisions, we can consider a quantum-classical (QC) hybrid (i.e., semiclassical) approximation, in which electrons are described by using quantum mechanics and heavy particles by classical mechanics. Ordinarily, the QC approximation has been applied for collisions at sufficiently high energies. If the collision energy is low, the dynamics of heavy particles become complicated. However, determining the classical trajectory of heavy-particle motion without any ambiguity is usually difficult in the QC approach. With regard to $\bar{p}+\mathrm{H}$ collisions, fortunately the adiabatic potential of this system was found to be very useful for the evaluation of the heavy-particle motion closely related to the electron emission process [1–3]. Consequently, the QC method could be successfully applied to low-energy ionization [1,2] and additionally even to the $\bar{p}$ capture occurring at energies below the ionization threshold [3].

In the present paper, we calculate the cross section for ionization in collisions between antiprotons and (hydrogenic) helium ions,

$$\bar{p}+\mathrm{He}^{+}\rightarrow\bar{p}+\mathrm{He}^{2+}+e. \tag{1}$$

The chief concern of the present calculation is the low-energy region, i.e., center-of-mass (c.m.) collision energies $E_{\mathrm{c.m.}}$ down to the vicinity of the threshold $I=54.4$ eV. The $\bar{p}$ capture

$$\bar{p}+\mathrm{He}^{+}\rightarrow\bar{p}\mathrm{He}^{2+}+e \tag{2}$$

is an alternative reactive channel when $E_{\mathrm{c.m.}}<I$, and was already investigated in detail by the present author using both the QM and QC methods [4] (hereafter referred to as paper I). Because the antiproton has negative charge, the strong Coulomb attractive field, the range of which is longer than the centrifugal one, works between $\bar{p}$ and He^{+}, and has a big influence on low-energy collisions: The cross section for the $\bar{p}$ capture (2) diverges in the zero-energy limit, and the resonances are very rich in the $\bar{p}+\mathrm{He}^{+}$ collisions. The situation is just the same as exemplified in the $e+$ion system. In paper I, the QC approximation was shown to be very good for the calculation of the nonresonant part of the capture cross section. For a description of the resonance phenomena, the complete QM treatment is necessary, and the QC approximation should normally be of no use. Nevertheless, it was further found in paper I that the QC calculation was still useful for the cross section averaged over resonances. If the energy is above the ionization threshold, no resonance phenomena occur, and hence the QC method becomes directly applicable to the collision problem without any implication. Thus, we can expect that the QC method is quite suitable for the calculation of the ionization (1). The present paper carries out the QC calculation, and investigates the influence of the strong attraction working between $\bar{p}$ and He^{+} on the ionization process (1).

II. CALCULATION

The details of the QC method are reported elsewhere [1–4]. Here, only a brief summary of the numerical method is given. In the present QC method, the relative motion of $\bar{p}$ and He^{+} is assumed to be a classical trajectory determined by using the adiabatic potential for the lowest (1σ) state. As mentioned in the Introduction, the use of the adiabatic potential is of critical importance [1–4]. In what follows, we refer to this QC approximation as QC-A to emphasize this potential choice. For comparison, we also carried out the calculations by introducing two other versions of the QC approximation: (1) the Coulomb potential $-1/R$ (R being the distance between $\bar{p}$ and He^{+}) is used instead of the adiabatic potential (QC-C); and (2) a linear trajectory (i.e., no potential) is assumed for the relative motion (QC-L).

Figure 1 shows the adiabatic potential as a function of the relative distance R. The adiabatic potential approximates closely to the pure Coulomb potential $-1/R$ at large distances, and makes the transition to $-2/R$ as $R\rightarrow 0$. Because the adiabatic potential is much more attractive than the Coulomb potential $-1/R$ at $R<1$ a.u., the assumption of a simple Coulomb trajectory for the relative motion would be unrealistic for the calculation of the low-energy collisions. If the probabilities of nonadiabatic transition were large, the adiabatic potential might be of no use. Fortunately, paper I shows that these probabilities are small in the $\bar{p}+\mathrm{He}^{+}$ system. (It should be mentioned nevertheless that the adiabatic po-

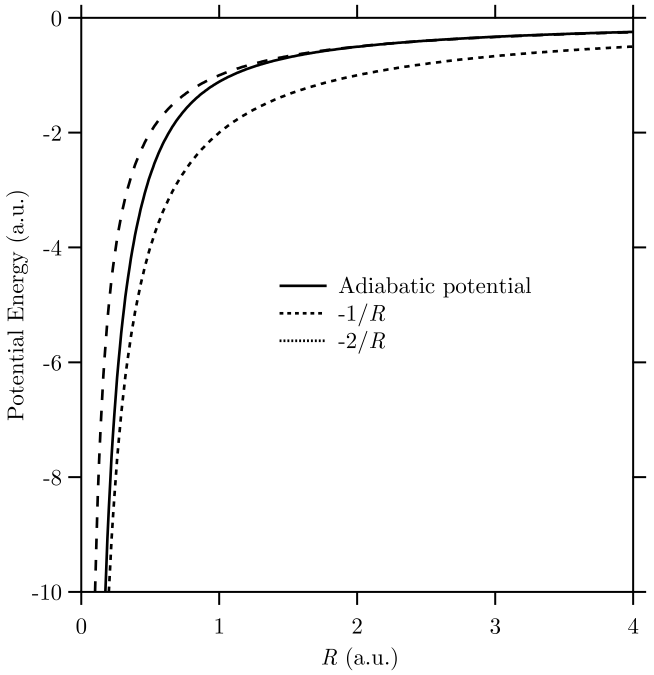

FIG. 1. Adiabatic potential curve of the $\bar{p}+He^+$ system for the lowest (1σ) state as a function of the relative distance R. For comparison, the Coulomb potentials $-1/R$ and $-2/R$ are also plotted.

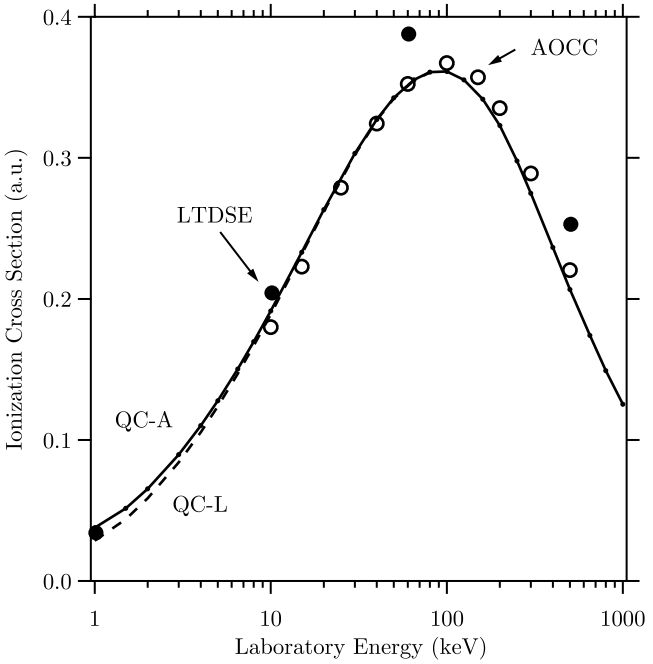

FIG. 2. Ionization cross sections in the high-energy region as a function of the laboratory incident energy E_{lab}, obtained by using the QC-A (adiabatic potential) and QC-L (no potential) methods. Also shown are the results of Wherman *et al.* [19] using the atomic orbital close-coupling (AOCC) method, and the results of Schultz *et al.* [22] using the lattice time-dependent Schrödinger equation (LTDSE) method.

tential is still useful even if the nonadiabatic transition probabilities are close to unity [1–3].)

The time-dependent Schrödinger equation for the electron motion was directly solved on a grid of points in the configuration space [1–4]. The discrete-variable-representation (DVR) technique [5–7] was employed for the direct solution. The present set of the numbers of grid points is exactly the same as used in the QC calculation of paper I, and gives a relative error of the calculated transition probability less than 1%. The DVR method was critically examined first in the chemical reaction problem [5,6,8–10], and has been accepted in a variety of fields [1–4,7,11–17]. The mathematical foundation was summarized by Calogero [18]. In the DVR, the property of orthogonal polynomials is fully utilized. The interaction matrix involves only diagonal elements, which are values of the interaction at grid points, and the nondiagonal matrix, coming from the kinetic energy operators (thus taking a sparse and typically banded structure), can be evaluated in an algebraic form. Owing to this simplicity, the DVR is very efficient for accurate numerical calculations.

In the low-energy calculation of paper I, the boundary of the relative distance could be set to a small value $R_0=2$ a.u., where, using the adiabatic states, the initial condition was given and the final transition probabilities were calculated. However, a larger boundary is needed for the collisions occurring at higher energies: we chose $R_0=6$ a.u. for $E_{c.m.}<1$ keV, and $R_0=40$ a.u. for $E_{c.m.}\geq 1$ keV in the present calculation.

III. RESULTS AND DISCUSSION

Several types of solution for QC approximation have been applied to the ionization process (1) in the high-energy region of $E_{c.m.}\gtrsim 1$ keV [19–25]. To make a comparison with previous results, first we calculated the ionization cross sections in the high-energy region, and show the results in Fig. 2 as a function of the laboratory incident energy $E_{lab}=[(m_{\bar{p}}+m_{He^+})/m_{He^+}]E_{c.m.}$, with $m_{\bar{p}}$ being the $\bar{p}$ mass and m_{He^+} the He^+ mass. Also included in the figure are the results obtained by Wehrman *et al.* [19] using the atomic orbital close-coupling (AOCC) solution and by Schultz *et al.* [22] using the lattice time-dependent Schrödinger equation (LTDSE) solution. (The results of the other groups [23–25] are not so much different from these two.) The discrepancy among the present and previous results are within 10% except for the LTDSE calculation at $E_{lab}=500$ keV. The present calculation agrees better with the AOCC one. The agreement with the previous results guarantees the accuracy of the present computation for high energies as well as for low energies.

The use of the adiabatic potential might be rather inappropriate in the high-energy collisions. However, the effect of trajectory bending due to the attractive potential in itself becomes negligible as the energy increases. In fact, we can see that the QC-A results are only slightly different from the QC-L ones. As a consequence, the adiabatic potential is always usable in the collision calculation regardless of the energy. Figure 2 seems to suggest that the cross section is getting smaller with decreasing E_{lab} from ~100 keV. However, as seen in Fig. 3, this is true only if the trajectory bending effect is negligible.

Figure 3 shows the behavior of the ionization cross sections in the low-energy region of $I<E_{c.m.}<800$ eV, obtained

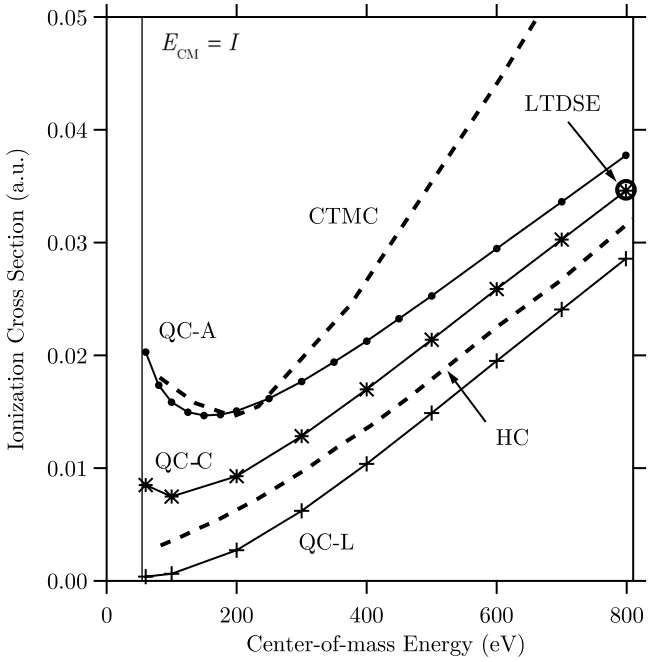

FIG. 3. Ionization cross sections in the low-energy region as a function of the center-of-mass collision energy $E_{c.m.}$, obtained by using the QC-A (adiabatic potential), QC-C (Coulomb potential), and QC-L (no potential) methods. Also shown are the results of Schultz *et al.* [21,22] using the LTDSE, hidden crossing (HC), and classical trajectory Monte Carlo (CTMC) methods.

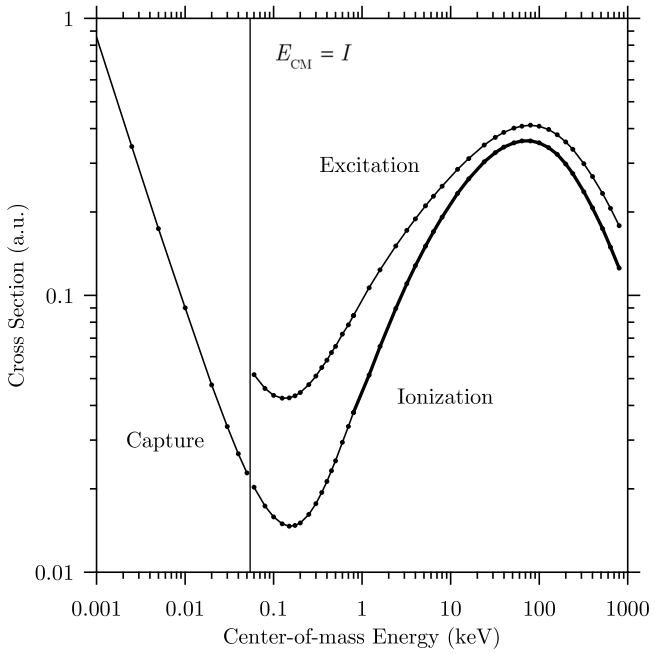

FIG. 4. Cross sections for $\bar{p}$ capture [4], ionization, and total excitation as a function of the center-of-mass collision energy $E_{c.m.}$, obtained by using the QC-A method.

by using the QC-A, QC-C, and QC-L methods. As the energy decreases, we find more significant differences among the three results: especially at $E_{c.m.} \sim I$, the QC-L cross section becomes negligibly small while the QC-A and QC-C results remain large. In the calculation for the $\bar{p}$ (or μ^-)+H system [1,2], it was found that not only the QC-A but also the QC-L methods gave large ionization cross sections near threshold. We can see that the trajectory bending effect is of substantial importance in the case of $\bar{p}+He^+$. A further noteworthy point in Fig. 3 is that the QC-A cross section takes a local minimum at $E_{c.m.} \simeq 150$ eV, which is much higher than the ionization threshold I. Although the QC-C result has a local minimum as well, the upturn behavior is not so obvious. As could also be expected in Fig. 1, only the pure Coulomb potential $-1/R$ cannot sufficiently explain the major part of the trajectory bending effect at low energies. In the $\bar{p}$+H collisions, the minimum and upturn behavior can be observed only vaguely: the ionization cross section is nearly constant ($\sim$5 a.u.) over a wide range of energies below $\sim$10 keV [21,26].

For comparison, the results calculated by Schultz *et al.* [21,22] using the LTDSE, the hidden crossing (HS), and the classical trajectory Monte Carlo (CTMC) methods are also shown in Fig. 3. In the LTDSE and HC calculations, the pure Coulomb potential $-1/R$ was employed for the determination of the relative motion. The LTDSE result at $E_{c.m.} \simeq 800$ eV is very close to the QC-C one. Unfortunately, the LTDSE calculation was not carried out at the lower energies. The HC cross section, monotonically decreasing with decreasing $E_{c.m.}$, shows no local minimum. Of these three calculations done by Schultz *et al.*, the CTMC method takes account of the $\bar{p}+He^+$ attraction which can be much stronger than the pure Coulomb potential $-1/R$. Accordingly, the CTMC calculation can produce a clear upturn behavior at low energies. (The local minimum locates at $E_{c.m.} \sim 200$ eV, higher than that of the QC-A calculation.) Although the CTMC cross sections are all very close to the QC-A results at $E_{c.m.} < 300$ eV, the agreement should be considered to be accidental. It should be remembered that the CTMC method gives cross sections too large at high energies, where the classical treatment is expected to be more satisfactory.

Figure 4 shows the $\bar{p}$ capture and ionization cross sections obtained by the QC-A calculation in the range of $E_{c.m.}$ from 1 eV to 1 MeV. The ionization cross section is slightly bumpy around $E_{c.m.}=1$ keV. This is due to the different boundary distances R_0 chosen in the present calculations below and above the energy $E_{c.m.}=1$ keV. The capture cross section is taken from paper I. At $E_{c.m.} \lesssim 10$ eV, the capture cross section is proportional to $1/E_{c.m.}$ in a very good approximation, because the transition probabilities become almost independent of $E_{c.m.}$ [4]. However, such behavior can no longer be expected at $E_{c.m.} \gg 10$ eV. In the $\bar{p}+He^+$ system, the resonance effect was very important for the capture process [4]. The capture cross section shown in Fig. 4 is the nonresonant one obtained by the elimination of the resonance contribution.

In the QC calculation, we have no way of distinguishing between the ionization (1) and the capture (2) channels at $E_{c.m.} > I$ [1,2]. The present ionization cross section is actually the total electron emission cross section summed over the two channels, and hence smoothly connects to the capture cross section at the ionization threshold. It is very interesting to investigate the competing behavior of the capture and ionization processes at energies above the ionization threshold.

A complete QM treatment is inevitable for this purpose, and remains in future work. However, the cross section for rearrangement reactions like (2) rapidly drops to zero with increasing energy beyond the breakup threshold if the captured and ejected particles have huge mass difference. The capture process (2) is essentially negligible above the ionization threshold except probably in the case of $E-I<$ a few eV [21]. It is hence certain that the local minimum and upturn behavior remain in existence indeed in the ionization process (1).

In collisions between protons and helium ions ($p+\mathrm{He}^+$), the ionization cross section has a maximum at $E_{\mathrm{c.m.}} \sim 150$ keV [27], and becomes negligibly small when $E_{\mathrm{c.m.}} < 30$ keV [28]. In this case, of more importance is the charge transfer process, which has the maximum (~ 0.9 a.u.) of the cross section at $E_{\mathrm{c.m.}} \sim 40$ keV, and then becomes negligible at $E_{\mathrm{c.m.}} \lesssim 1$ keV [28]. No notable reactive channels are to be found for $p+\mathrm{He}^+$ at $E_{\mathrm{c.m.}} \lesssim 1$ keV. In contrast, the $\bar{p}+\mathrm{He}^+$ system, having strong attraction, shows reactivity at low energies. Because the electron has negative charge (and furthermore very light mass), we can expect that the $e+\mathrm{He}^+$ system is active at low energies as well. In fact, the ionization is significant throughout at energies ranging from threshold to 10 keV [29]. The ionization cross section in $e+\mathrm{He}^+$ takes a maximum at an energy (~ 200 eV) comparatively close to threshold, and accordingly the local minimum and upturn behavior cannot be observed [29,30]. In the $e+\mathrm{He}^+$ system, the process corresponding to the capture (2) is not a reactive channel distinguishable from the elastic (or inelastic) one, and is rather considered as the electron exchange effect originating from the Pauli principle.

In Fig. 4, we further show the total excitation cross section summed over all the final excited bound states. The total excitation cross section is always larger than the ionization cross section. This contrasts with the situation in the low-energy $\bar{p}+\mathrm{H}$ collisions that the ionization is the dominant inelastic channel [31]. The excitation cross section in $\bar{p}+\mathrm{He}^+$ also seems to be getting larger as the energy decreases. In the QC-A calculation, we find that the excitation cross section is nonvanishing even at threshold though not shown in the figure. This might be considered to be unphysical because the QC approximation could never take account of the threshold effect. However, a nonzero value of the excitation cross section at threshold can be justified by the Coulomb peculiarity that its range is longer than the centrifugal one [32]. The same situation arises in $e+$ion scattering, and the stepwise discontinuity of the excitation cross section at threshold is known as the Gailitis jump [33,34]. A further study of the threshold behavior is interesting for the excitation of ions by $\bar{p}$ impact. In contrast to the case of $\bar{p}+\mathrm{He}^+$, the excitation cross section in $e+\mathrm{He}^+$ shows a monotonic decrease throughout at energies beyond the ionization threshold [30,35,36], exactly due to the very light mass of the incident electron.

IV. SUMMARY

The long-range strong attraction working between $\bar{p}$ and He^+ causes a significant effect on the low-energy collisions. Consequently, the ionization cross section remains large even near threshold, and shows a distinctive (minimum and upturn) behavior. For the quantitative evaluation of this effect, the assumption of merely a pure Coulomb attraction is insufficient. Knowledge of $e+$ion scattering is helpful to a certain degree for the understanding of the $\bar{p}+\mathrm{He}^+$ collision dynamics. However, we should rather say that the collision features in $\bar{p}+\mathrm{He}^+$ are quite dissimilar from those in the $e+$ion collision because of the very large mass difference between $\bar{p}$ and e. Low-energy $\bar{p}+$ion collisions offer a new and intriguing topic in atomic physics.

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