Stripping of H^- in low-energy collisions with antiprotons: Classical-trajectory Monte Carlo calculation

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The classical-trajectory Monte Carlo method has been used to determine the cross section for stripping of H^- in collisions with $\bar{p}$. The calculations were done for relative velocities from $0.015\alpha c$ to $1.0\alpha c$. A maximum cross section of about 40 $Å^2$ is found, somewhat smaller than previous estimates.

I. INTRODUCTION

As an extension of the low-energy antiproton ring (LEAR) project at CERN, a scheme of corotating $\bar{p}$ and H^- beams has been proposed.[1] By means of electron cooling, the momentum spread of the particles in the beam needs to be reduced to $\Delta p/p \sim 10^{-4}$ so that it will be possible to produce $p\bar{p}$ atomic systems *in vacuo* by the Auger process.[2] For evaluating the feasibility of such a scheme and determining optimal machine parameters, it is important to study electron detachment of H^-, since this process is the main source of H^- beam loss.

We focus here on beam-beam interactions, i.e., the reaction

$$H^- + \bar{p} \rightarrow H + e^- + \bar{p} \ , \tag{1a}$$

at relative velocities $v_{\rm rel} \lesssim 0.1\alpha c$, corresponding to the operating conditions planned for LEAR. Interest in reaction (1a) and in the similar process,[3]

$$H^- + H^- \rightarrow H^- + H + e^- \ , \tag{1b}$$

stems from the fact that they can limit the usable beam intensity. Experimentally, beams as intense as possible are desirable for $p\bar{p}$ production. On the other hand, the beam tends to destroy itself through reactions (1) if it is too intense (see Ref. 4 for a discussion of the H^- beam lifetime). Several estimates of the cross section for reactions (1) have been given in Ref. 5. In that work stripping probabilities were derived analytically by resorting to a WKB approximation in the framework of an effective single-particle scheme.

In the present work a quite different approach is taken. Based on the successes of the classical-trajectory Monte Carlo (CTMC) method in the studies of ionization in proton[6] and negative-muon[7] collisions with the hydrogen atom, a similar method is applied to the H^- stripping problem. The dynamics of one electron and the antiproton are calculated in the field of a polarizable neutral atomic core. Cross sections for reaction (1) are obtained and compared with the previous estimates.

II. EFFECTIVE POTENTIAL

We describe H^- as a single-electron system interacting with a polarizable atomic core. The effective potential can be written

$$V_{\rm eff} = -V_{\rm core} + V_{\rm pol} \ . \tag{2}$$

The first term, describing the interaction of a point charge with the *frozen core*, is

$$V_{\rm core} = \left[\frac{1}{r} + 1\right] e^{-2r} \ . \tag{3}$$

The second term, which is due to induced polarization of the core, is

$$V_{\rm pol} = -\tfrac{1}{2}\alpha_H \, |\, \mathbf{E}_{\rm eff} \,|^2 \ , \tag{4}$$

where α_H is the polarizability of the hydrogen core, equal to $\frac{9}{2}$ in atomic units,[8] and $\mathbf{E}_{\rm eff}$ is the effective electric field on the core.

At large distances the electric field created by the outer electron is just

$$\mathbf{E} = \hat{r}/r^2 \ . \tag{5}$$

We assume that the effective potential at any distance can still be expressed by Eq. (2) taking

$$\mathbf{E}_{\rm eff}(\mathbf{r}) = \mathbf{E}(\mathbf{r}) \exp(-r_0^2/2r^2) \ , \tag{6}$$

where r_0 is a suitably chosen constant. The exponential factor in Eq. (6) removes the unphysical singularity of the polarization term as $r \rightarrow 0$, and at the same time Eq. (6) reduces to Eq. (5) as $r \rightarrow \infty$. We determine the parameter r_0 by the condition that the potential in Eq. (2) has a single quantum mechanically bound state with the correct binding energy, $-E_0 = 0.754$ eV, the electron affinity of the H atom. By numerical integration of the Schrödinger equation we find $r_0 = 1.596 a_0$. From the corresponding single-particle density[9] we obtain the expectation values $\langle r \rangle = 3.1$ and $\langle r^2 \rangle = 14.1$, which may be compared with the accurate values[10] $\langle r \rangle = 2.7$ and $\langle r^2 \rangle = 11.9$. Another

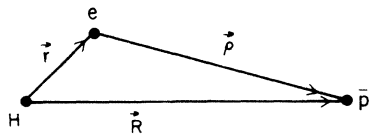

FIG. 1. Coordinates for the effective three-body system H-e^--$\bar{p}$.

reason for the choice of the particular cut-off function used in Eq. (6) is that the resulting potential is very similar to the adiabatic potential (discussed below) at $r \gtrsim 2a_0$ where adiabatic response of the core might be expected.

The effective potential for the $H^- + \bar{p}$ system (see Fig. 1 for notation) is then constructed from Eq. (2):

$$V_{\rm tot}^{\bar{p}p}(r,R,\rho) = -V_{\rm core}(\mathbf{r}) - V_{\rm core}(\mathbf{R}) + \frac{1}{\rho} - \tfrac{1}{2}\alpha_H \,|\, \mathbf{E}_{\rm eff}(\mathbf{r}) + \mathbf{E}_{\rm eff}(\mathbf{R}) \,|^2 . \quad (7)$$

The terms in Eq. (7) have an immediate interpretation. The first two terms represent the interaction of the electron and antiproton, respectively, with the frozen atomic core, and the third term is the Coulomb repulsion between e and $\bar{p}$. The last term accounts for the polarization of the H core resulting from the vector sum of the electric fields of the two charged particles e and $\bar{p}$. Equation (7) is exact in the limit of large distances ($r,R \gg 1$), but there is some arbitrariness in using it over all space. Calculations performed with possible variants of the effective potential are also made and compared in Sec. IV with the results obtained using Eq. (7).

III. METHOD OF CALCULATION

The techniques used in the paper are quite similar to those described in Refs. 7 and 11, so we shall only outline the procedure here.

(i) The initial r and p values are selected randomly from uniform distributions in $(0,r_{\rm max})$ and $(0,p_{\rm max})$. These values can be immediately rejected if $E = \frac{1}{2}p^2 + V(r)$ is greater than zero.

(ii) We define a function

$$f(E) = \exp\left[-10^4\left[\frac{E}{E_0} - 1\right]^2\right], \quad (8)$$

which represents a numerical approximation to the on-the-energy-shell microcanonical distribution. The function

$$w(r,p) = 16\pi^2 r^2 p^2 f(E) \quad (9)$$

is evaluated and compared to a random number $\chi \in (0,w_{\rm max})$ where $w_{\rm max}$ is the maximum value of the function w in phase space. If $w(r,p) > \chi$, then r and p are accepted as initial conditions; otherwise the selection process returns to step (i). The values of $r_{\rm max}$ and $p_{\rm max}$ in (i) are chosen large enough that $w(r,p)$ is negligibly small for $r > r_{\rm max}$ or $p > p_{\rm max}$. We found $r_{\rm max} = 3$ and $p_{\rm max} = 4.5$ adequate for H^-. This procedure of selecting the initial conditions of the target avoids the necessity of predetermining the distribution of each variable used in specifying initial conditions.

(iii) The cosine of the angle α between the vectors $\mathbf{r}$ and $\mathbf{p}$ is randomly selected from a uniform distribution in $(-1, 1)$ since $f(E)$ is independent of α.

(iv) The vectors $\mathbf{r}$ and $\mathbf{p}$, until now arbitrarily situated in the yz plane, are rotated by random Euler angles uniformly distributed as $-\pi \le \phi \le \pi$, $-1 \le \cos\theta \le 1$, and $-\pi \le \eta \le \pi$.

(v) The impact parameter b is selected at random from a uniform distribution of $b^2 \in (b_{i-1}^2, b_i^2)$ and b_i is increased until the cross section converges.

(vi) Forces are calculated by numerical differentiation of Eq. (7) using a two-point central-difference formula. This procedure is more efficient than analytic differentiation since the latter involves more expressions to be evaluated. For potentials other than Eq. (7) the differentiation was done analytically.

(vii) The numerical integration of Hamilton's equations of motion for the three-particle system $(H,e,\bar{p})$ is performed using the sixth-order Gear hybrid method.

(viii) The final-state determination is as depicted in Fig. 1 of Ref. 7 (the factor γ there, used to compare internal energies with the external potential, was set to 0.6).

(ix) Except at the two lowest velocities, enough trajectories were run to reduce the standard deviation of the calculated cross section to about 10%.

IV. RESULTS AND DISCUSSION

Results obtained using the effective potential in Eq. (7) are summarized in Table I. The relative $H^- - \bar{p}$ velocity is denoted by $v_{\rm rel}$, $b_{\rm max}^{\rm ion}$ is the largest impact parameter where H^- *ionization actually occurred,* $b_{\rm max}$ denotes the largest impact parameter sampled, $N_{\rm tot}$ is the total number of trajectories integrated, and $N_{\rm ion}$ is the number of these trajectories that resulted in ionization. Finally, the error bars correspond to one standard deviation.

Qualitatively, one notices small cross sections at the lowest velocities, where dominance of the Coulomb repulsion prevents H^- and $\bar{p}$ from approaching closely enough for ionization to occur. The cross section reaches a maximum of about 40 Å^2 at $v_{\rm rel} \simeq 0.05$ and then slowly decreases with increasing velocity, corresponding to the fact that the shorter interaction times are less effective in disturbing the electron motion.

We now consider the sensitivity of the results to the choice of the potential. Although there is some arbitrariness in the form of the polarization term introduced in Eq. (7), it is important to realize that polarization has to be taken into account. For example, if the polarization term is neglected in the description of H^-, then the potential $V = V_{\rm core}(r)$ has no quantum mechanically bound state. Furthermore, one sees from Table I that the typical distances important for H^- ionization are $R \simeq b_{\rm max}^{\rm ion} \simeq 8a_0$. At these distances, the magnitude of the polarization term in the H-$\bar{p}$ interaction is $|V_{\rm pol}| \simeq \frac{1}{2}\alpha_H R^{-4} \sim 10^{-3}$ a.u., which is much larger than the core term $V_{\rm core} \simeq e^{-2R} \sim 10^{-7}$ a.u. To demonstrate the importance of core polarization in ionizing collisions, we have performed calculations replacing Eq. (7) with a potential $V_{\rm tot}^{fc}$ given by the frozen core (fc) terms only:

TABLE I. CTMC results for $H^- + \bar{p}$ stripping obtained utilizing the vector-polarizable H core.[a]

$E_{c.m.}$ (eV)	$v_{rel}(\alpha c)$	$b^{ion}_{max}(a_0)$[b]	$b_{max}(a_0)$[b]	N_{tot}	N_{ion}	$\sigma_{ion}(10^{-16}$ cm^2)[c]
2.81	0.015	2.22	6.124	75	1	0.4±0.4
5.00	0.02	5.68	9.798	75	18	20.3±4.2
11.25	0.03	7.27	9.798	150	59	33.2±2.8
31.24	0.05	8.09	11.314	200	71	40.0±3.8
125.0	0.1	9.29	11.314	200	67	37.7±3.8
499.9	0.2	9.56	11.314	200	61	34.3±3.7
1999.7	0.4	9.19	11.314	200	60	33.8±3.6
4499.3	0.6	10.62	12.649	500	94	26.5±2.5
12 498.0	1.0	8.02	11.314	400	68	19.1±2.1

[a]Our "standard" potential. See Eq. (7).
[b]b_{max} is the largest impact parameter sampled; b^{ion}_{max} is the largest impact parameter at which ionization actually occurred.
[c]$\sigma_{ion}=(N_{ion}/N_{tot})\pi b^2_{max}$. The error estimate is statistical only (1 standard deviation): $\Delta\sigma_{ion}=\sigma_{ion}[(N_{tot}-N_{ion})/N_{tot}N_{ion}]^{1/2}$.

TABLE II. CTMC results for $H^- + \bar{p}$ stripping obtained utilizing the frozen H core.[a]

$E_{c.m.}$ (eV)	$v_{rel}(\alpha c)$	$b^{ion}_{max}(a_0)$	$b_{max}(a_0)$	N_{tot}	N_{ion}	$\sigma_{ion}(10^{-16}$ cm^2)
125.0	0.1	6.52	9.798	150	37	20.8±3.0
499.9	0.2	6.88	9.798	150	38	21.4±3.0
1999.7	0.4	8.83	11.314	200	37	20.8±3.1
4499.3	0.6	8.29	11.314	400	78	22.0±2.2
12 498.0	1.0	9.93	12.649	500	66	18.6±2.1

[a]See Table I for notation.

TABLE III. Adiabatic potential for a hydrogen atom perturbed by a point negative charge.[a]

$R(a_0)$	ϵ_b (a.u.)	$R(a_0)$	ϵ_b (a.u.)
0.65	$0.423\,361\,46\times10^{-28}$	2.40	0.133 133 415
0.70	$0.435\,830\,69\times10^{-10}$	2.50	0.143 582 491
0.80	$0.364\,670\,82\times10^{-5}$	2.60	0.153 656 482
0.90	$0.148\,748\,15\times10^{-3}$	2.70	0.163 348 210
1.00	$0.102\,466\,70\times10^{-2}$	2.80	0.172 657 447
1.10	$0.339\,670\,21\times10^{-2}$	2.90	0.181 589 014
1.20	$0.771\,014\,11\times10^{-2}$	3.00	0.190 151 316
1.30	$0.140\,012\,99\times10^{-1}$	3.50	0.227 850 157
1.40	$0.220\,371\,11\times10^{-1}$	4.00	0.258 293 782
1.50	$0.314\,672\,88\times10^{-1}$	4.50	0.283 095 228
1.60	$0.419\,240\,10\times10^{-1}$	5.00	0.303 548 343
1.70	$0.530\,728\,41\times10^{-1}$	5.50	0.320 631 695
1.80	$0.646\,324\,08\times10^{-1}$	6.00	0.335 075 034
1.90	$0.763\,772\,86\times10^{-1}$	6.50	0.347 423 847
2.00	$0.881\,331\,21\times10^{-1}$	7.00	0.358 089 580
2.10	$0.997\,689\,36\times10^{-1}$	7.50	0.367 386 204
2.20	0.111 189 073	8.00	0.375 556 298
2.30	0.122 325 867	∞	0.500 000 000

[a]From Ref. 12. ϵ_b is the electronic binding energy; $V_a=0.5-\epsilon_b-R^{-1}$.

$$V_{\rm tot}^{fc}(r,R,\rho) = -V_{\rm core}(r) - V_{\rm core}(R) + \frac{1}{\rho} \ . \tag{10}$$

The results, presented in Table II, show values of the cross section that are systematically and significantly smaller than obtained in our calculations including polarization. Comparison with Table I shows that polarization effects are enhanced at the smaller velocities, as expected.

In order to examine the sensitivity of the cross section to the treatment of the potential, we consider a few other alternatives to Eq. (7). A simple change is made by linear superposition of the $\bar{p}$ and e polarization terms rather than the vector sum. The corresponds to an effective potential given by

$$V_{\rm tot}^{lsp}(r,R,\rho) = -V_{\rm core}(r) - V_{\rm core}(R) + \frac{1}{\rho} - \tfrac{1}{2}\alpha_H[E_{\rm eff}^2(r) + E_{\rm eff}^2(R)] \ . \tag{11}$$

Another possibility is to use the adiabatic potential, which is well defined theoretically, for interaction of the hydrogen atom with a point negative charge. The exact adiabatic (Born-Oppenheimer) potential has been calculated by Baird[12] at $R \leq 8a_0$ with the results given in Table III, which we fit by a cubic spline. At larger distances the adiabatic potential can be evaluated using the asymptotic series expansion of Dalgarno and Lewis[13] for $p+H$ (with the signs of odd-order terms reversed). The truncated expansion that is adequate at $R > 8$ is given by

$$V_a \sim -\tfrac{9}{4}R^{-4} - \tfrac{15}{2}R^{-6} + \tfrac{213}{4}R^{-7} - \tfrac{7755}{64}R^{-8} + \tfrac{1773}{2}R^{-9} - \tfrac{2835}{8}R^{-10} \ . \tag{12}$$

As can be seen in Fig. 2, this potential is close to the polarized-core potential at $R \gtrsim 2a_0$. However, at small distances the completely adiabatic potential clearly overestimates the attraction. One consequence of this excess attraction is that an electron is quantum mechanically bound in this potential by 1.82 eV, more than twice the true binding energy. An *ad hoc* fix of this defect can be made by modifying the short-range part of the potential. We achieved the correct binding energy by defining a "modified-adiabatic" potential that is more repulsive than the adiabatic potential at small R. This modified potential has the form

$$V_{\rm ma} = 0.875 - 0.344\,582R + 0.056\,508R^2 - \frac{1}{R} \quad \text{for } R < 2 \ , \tag{13}$$

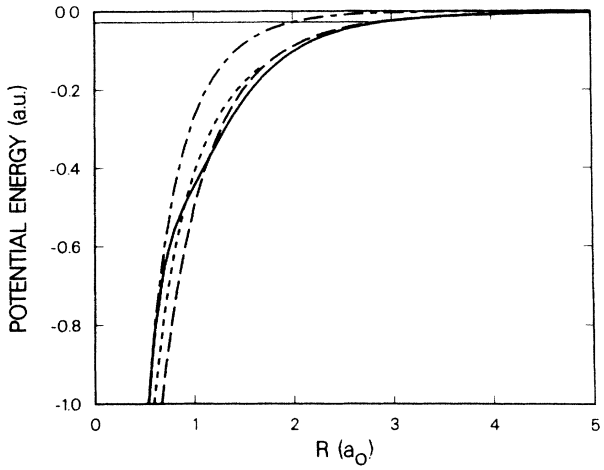

FIG. 2. Comparison of one-electron potentials: polarized core (——), frozen core (— — —), adiabatic (— —), and modified adiabatic (— — — —). The horizontal line segment indicates the energy of the bound state in the polarized-core and modified-adiabatic potentials.

and at $R = 2$ the potential and its derivative continuously become identical to the purely adiabatic potential.

For comparison with the calculations utilizing a polarizable core, cross sections for collision velocity 0.1 were also calculated using the total potentials

$$V_{\rm tot}^{a}(r,R,\rho) = -V_a(r) - V_a(R) + \frac{1}{\rho} \tag{14}$$

and

$$V_{\rm tot}^{ma}(r,R,\rho) = -V_{ma}(r) - V_{ma}(R) + \frac{1}{\rho} \ . \tag{15}$$

The results are given in Table IV. One notices that the second, third, and fifth lines correspond to potentials that (a) yield the quantum mechanically correct binding energy *and* (b) describe correctly the H^--$\bar{p}$ interaction at large distances. These three potentials yield results for the cross section that are consistent within statistical errors. On the other hand, the first and fourth lines, corresponding to potentials that do not satisfy conditions (a) and/or (b), show rather smaller results.[14] In conclusion, confidence in the results of Table I is gained from the stability of the cross sections as the potential is varied without violating physically relevant conditions.

TABLE IV. CTMC results for $H^- + \bar{p}$ stripping at $v = 0.1$, obtained using different treatments of the H core.

Type[a]	$b_{\rm max}^{\rm ion}(a_0)$	$b_{\rm max}(a_0)$	$N_{\rm tot}$	$N_{\rm ion}$	$\sigma_{\rm ion}(10^{-16}\ {\rm cm}^2)$
Frozen core (10)	6.52	9.798	150	37	20.8±3.0
Vector polarization (7)	9.29	11.314	200	67	37.7±3.8
Linear superposition of polarization (11)	9.42	11.314	200	71	40.0±3.8
Adiabatic (14)	6.16	9.798	150	42	23.6±3.1
Modified adiabatic (15)	8.44	11.314	200	66	37.2±3.7

[a]The equation number of the potential is given in parentheses.

In comparison with Ref. 5 the present results are similar in shape but are about a factor of 4 smaller than the "best estimate" of that work (other estimates were even larger). Part of this difference may be due to the microcanonical distribution, which does not allow the target electron to be initially at large nonclassical distances from the nucleus; however, this effect is not expected to be too serious at the low collision velocities considered since the charge density is significantly perturbed even in collisions at impact parameters much larger than the initial size of the target. Our sensitivity studies suggest that the uncertainty due to the arbitrariness in our choice of the polarized-core potential is considerably less than a factor of 2. Hence we believe that the true stripping cross section actually is somewhat smaller than found in previous calculations.

ACKNOWLEDGMENT

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