Antiproton - Hydrogen Atom Rearrangement-Annihilation Cross Section*

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UCRL--94652
DE86 016080

ABSTRACT

For antiproton energies of several eV or less, annihilation in matter occurs through atomic rearrangement processes in which the antiproton becomes bound to a nucleus prior to annihilation. Annihilation cross sections via rearrangement at such energies are much higher than for direct antiproton - nucleon annihilation and are therefore of consequence to antiproton annihilation propulsion of space craft and, in general, to the annihilation of antiprotons that have come to rest in matter. Existing calcualtions of the antiproton - hydrogen atom rearrangement cross section are semiclassical and employ the Born-Oppenheimer approximation. They also employ various arguments in regard to the behavior of the system when the Born-Oppenheimer approximation breaks down at small antiproton - proton separations. These arguments indicate that rearrangement is essentially irreversible.

In the present study, a detailed investigation was made of the antiproton - hydrogen atom system when the Born-Oppenheimer approximation breaks down. The results of this study indicate that the previous arguments were approximately correct, but that there is a significant probability for rearrangement reversing prior to annihilation. This probability is estimated to be about 20%. This consequent reduction in annihilation cross section has little or no negative consequences for antiproton annihilation propulsion at the present time. However, because of the approximate nature of this result and because more accurate values will be required in the future, it is important to conduct an accurate, fully quantum-mechanical calculation of antiproton - hydrogen atom rearrangement.

*Work performed for the Air Force Rocket Propulsion Laboratory under the auspices of the U.S. Department of Energy by the Lawrence Livermore National Laboratory under Contract W-7405-Eng-48.

1. INTRODUCTION

The interaction of low-energy antiprotons (< 1 eV) with hydrogen (or other) atoms is important in annihilation propulsion of spacecraft[1] and in experiments involving antiprotons where they come to rest before annihilating. At such low energies, an atomic rearrangement occurs. The electron (e^-) of the hydrogen atom (H) is emitted while the proton (p) of the hydrogen atom and the antiproton ($\bar{p}$) form an excited bound state of protonium (Pn)[2]:

$$\bar{p} + H \rightarrow Pn + e^- . \qquad (1)$$

The $\bar{p}$ and p in Pn inevitably annihilate after undergoing radiative decay to states of lower energy. The energy lost by the $\bar{p}$ by entering a negative-energy, bound state is transferred to the e^-. That energy is slightly in excess of the 13.6 eV binding energy of the e^- in H. The cross section for annihilation through reaction 1 at energies below about 20 eV is much greater than that for annihilation of an antiproton on a bare proton.[3] Hence the interest in this and similar reactions for use in antiproton annihilation propulsion. Similarly high annihilation cross sections result when the H is replaced by another atom or molecule and/or the $\bar{p}$ is replaced by an antihydrogen atom (an antiproton with a positron bound to it, which is emitted along with the electron).[2,3]

1.1 Annihilation Cross Section

Morgan and Hughes determined the cross section for reaction 1 (see Fig. 1) by employing a semiclassical, impact-parameter approximation in which the $\bar{p}$ - H relative motion is assumed to be classical, while the motion of the e^- in H is treated quantum mechanically.[2,3] The e^- motion is determined for the gound state by using the Born-Oppenheimer approximation.[4] Solving for the electron motion gives the electron energy as a function of $\bar{p}$-p separation, R (see Fig. 1). This energy determines the potential energy between the $\bar{p}$ and the H for the $\bar{p}$ - H classical orbits (R not fixed).[2,3]

When the impact parameter, b, of the orbit is greater than a particular value, b_c, which depends on the collision energy ($\lesssim$ 1 eV), the inner turning point (R_{min}) is not much smaller than b_c; the $\bar{p}$ and H stay relatively far

apart and no rearrangement (reaction 1) occurs (see Fig. 1). However, as b becomes less than b_c, R_{min} drops discontinuously from large values to values much smaller than the critical radius, R_c. For $R < R_c$ ($= 0.639\ a_o$[5]) the e- is no longer bound to the p. Morgan and Hughes assumed that once R became less than R_c, rearrangement occurred with near-unity probability; the electron left the region and the $\bar{p}$ became bound to the p since it had lost energy to the escaping electron. Thus the rearrangement and annihilation cross section was $\sigma = \pi b_c^2$ (Fig. 2).

Morgan and Hughes demonstrated the validity of the classical motion by showing that the results were not altered when that motion was treated quantum mechanically with an optical-model potential energy.[2] However, their arguments that rearrangement was permanent for $b < b_c$ were only qualitative. A possibility for reattachment lowers the rearrangement-annihilation cross section. The problem in considering reattachment is that the Born-Oppenheimer approximation breaks down for $R \lesssim R_c$. In lieu of a full quantum-mechanical solution valid for $R \lesssim R_c$, it is difficult to quantitatively demonstrate that the e- is indeed emitted with high probability when R becomes less than R_c. The purpose of the work reported here has been to examine, quantitatively, what goes on during the time when the Born-Oppenheimer approximation breaks down.

2. BORN-OPPENHEIMER BREAKDOWN

The Born-Oppenheimer approximation is valid when the mean velocity (in an rms sense) of the electron relative to the proton is much larger than the velocity of the antiproton relative to the proton, as is true here when R is a few times a_o or greater. However, as R decreases, the mean velocity of the electron decreases as it is pushed farther from the proton (its negative energy approaches zero) while the velocity of the antiproton increases due to its attraction to the H atom (induced dipole attraction for large R). For $R = R_c$ in the Born-Oppenheimer approximation, the energy and velocity of the electron have become zero, so in that approximation the cross-over point of the velocities is at a small value of R but greater than R_c.

The value of R at which crossover occurs (R_x) was found by using two different methods to determine u, the mean velocity of the electron. Both use the Born-Oppenheimer energy of the electron, ε, determined from references 2, 5, and 6. ε is given in Table 1 along with V, the $\bar{p}$ - H potential energy,

$$V = \varepsilon - e^2/R - \varepsilon_o, \tag{2}$$

where e is the unit electric charge, and ε_o is the ground state energy of the electron in H. The virial theorem[7] is assumed to apply to ε, so the kinetic energy of the electron is -1/2 ε and u is therefore $(-\varepsilon/m)^{1/2}$, where m is the electron mass. In the second method a quantity, ε', is used in place of ε, giving u' in place of u. ε' is determined from ε by subtracting an R-dependent portion of the e^- - $\bar{p}$ mean potential energy, since this energy has only a small dynamic effect on the e^- for $R \gtrsim$ a few a_o.[8] ε' is given in Table 1, and u and u' are given in Table 2 where they are compared to the $\bar{p}$ - p relative velocity, v, which is determined for a $\bar{p}$ collision energy of 0.027 eV. It applies for $b < b_c$ and is not significantly dependent upon collision energy for collision energies $\lesssim$ 1 eV.

By plotting the velocities in Table 2, it is found that $R_x = 0.79\ a_o$ when ε is used and $R_x = 0.68\ a_o$ when ε' is used - nearly equal values in spite of the large differences between ε and ε'. Since the Born-Oppenheimer approximation becomes invalid as R decreases through R_x, it will be assumed that it is valid until $R = R_x$. In the following section, the evolution of the $\bar{p}$ - H system is modeled for $R < R_x$.

3. The $\bar{p}$ - H SYSTEM FOR $R \leq R_x$

For $R \leq R_x$ the value of ε (or ε') in Eq. 2 is small enough to be neglected so

$$V = -\frac{e^2}{R} + \frac{e^2}{2a_o}, \tag{3}$$

where $1/2\ e^2/a_o = -\varepsilon_o = 13.6$ eV is the energy the $\bar{p}$ loses to the e^-. Thus, for

$R \leq R_x$ the p will be in a portion of an eliptical orbit relative to the $\bar{p}$ as pictured in Fig. 3. If the electron remains unbound, the $\bar{p}$ will stay in the full orbit (in the classical picture) until radiative decay occurs. Since V is a conlomb potential energy (with an added constant) the characteristics of the $\bar{p}$ motion for $R \leq R_x$ can readily be determined.[8] The $\bar{p}$ stays within R_x for a time, t_x, between 18 and 27 atomic time units, depending on its initial kinetic energy, its impact parameter, and the choice made for R_x. During this time it traverses an angle of 295^0 to 360^0 around the p. As it passes through R_x on the way out it is moving with the same speed but in nearly the opposite direction as it had when on the way in.

For $R \leq R_x$ the e^- motion is aproximated as that of an evolving Gaussian wave packet. It is assumed that the evolution is unaffected by the $\bar{p}$ and p because of the large spread of the e^- distribution compared to R for $R \leq R_x$. Thus, the wave function for the e^- is

$$\psi_{e^-} = \pi^{-3/4}(\beta + it/\beta)^{-3/2} \, e^{-\frac{r^2}{2(\beta^2+it)}} \quad , \qquad (4)$$

where t is the time following the first instance that $R = R_x$, β is a constant, and all quantities are in atomic units. The kinetic energy of the electron in this description is $3/(4\beta^2)$. This energy may be equated to the kinetic energy that the electron has at $t = 0$ ($R = R_x$) (when the Born-Oppenheimer approximation breaks down). Using the virial theorem, this latter energy is $-\epsilon/2$ or $-\epsilon'/2$ at $R = R_x$. (For $R = R_x$, $\epsilon = -0.00166$ and $\epsilon' = -0.00211$). Thus

$$\beta = (-3/(2\epsilon))^{1/2} \text{ or } (-3/(2\epsilon'))^{1/2}, \qquad (5)$$

giving $\beta = 30.1\ a_0$ for ϵ and $\beta = 26.7\ a_0$ for ϵ'. Hence the earlier statements that the e^- distribution is spread over distances much greater than R_x.

3.1 *Reattachment Probability*

The reattachment probability, P, is calculated in the sudden approximation:

$$P = \left| \int \psi_1^* \psi_2 \, d\tau \right|^2, \tag{6}$$

where ψ_1 is the normalized e^- wave function when $R = R_x$ the first time and ψ_2 applies when $R = R_x$ the second time (see Fig. 4). R_x is chosen because it is the nominal value of R where the e^- motion becomes uncoupled from the $\bar{p}$ - p motion as the $\bar{p}$ moves inward and the point where coupling can be reestablished as the $\bar{p}$ moves outward. In addition, R_x is close to R_c where, in the Born-Oppenheimer approximation, the e^- switches between bound and unbound states.

When the values of β along with $t = 0$ and t_x are placed in Eq. 4, it is seen that there is essentially no increase in size or other change in form in ψ_{e^-} due to time evolution from $t = 0$ to $t = t_x$. Since the size of ψ_{e^-} (the mean radius is $2\pi^{-1/2}(\beta^2 + t_x^2/\beta^2)^{1/2}$) is much greater than the changes in position (which are not larger than R_x), changes in position will also not result in significantly dissimilar wave functions going into Eq. 4. Thus the only significant difference between ψ_1 and ψ_2, and thence the only reason P differs from one, comes from the change in the velocity of the proton on which the wave functions are centered. Therefore one may take

$$\psi_1 = \pi^{-3/4} \beta^{-3/2} e^{-\frac{r^2}{2\beta^2}}$$

$$\psi_2 = \pi^{-3/4} \beta^{-3/2} e^{-\frac{r^2}{2\beta^2} + ikz}$$

where k is the electron wave number corresponding the approximate reversal in velocity of the proton and z is the component of position in the direction of the velocity change. Eq. 4 then gives

$$P = e^{-\left(\frac{\beta^2 v^2}{2} x\right)} = 0.22$$

where v_x is the $\bar{p}$-p relative velocity for $R = R_x$. The value of P is essentially independent of whether ε or ε' is used to determine ψ and v_x.

At face value, a value for the reattachment probability of about 20% means that the Morgan-Hughes results for the $\bar{p}$ - H rearrangement-annihilation cross section[2,3] should all be reduced by about 20%. However, the accuracies of two approximations that went into this value are unclear. The first approximation is the assumption that the Born-Oppenheimer approximation is valid and accurate for all values of R greater than R_x, the point where the electron mean velocity is equal to the antiproton velocity, and that the electron motion is wholly uncoupled from the $\bar{p}$ and p for $R < R_x$. The second approximation is the assumption that the electron wave function is a gaussian wave packet for $R < R_x$. In reality, the transition from Born-Oppenheimer motion of the electron to uncoupled motion occurs gradually over a range of values of R, and the form of the wave function for $R < R_x$ is more complicated than the gaussian form assumed.

4. CONCLUSIONS AND DISCUSSION

A investigation has been made of antiproton - hydrogen atom scattering for small values of the antiproton, hydrogen atom separation where the Born-Oppenheimer approximation is invalid. The calculations yield an estimate of 20% for a reduction in the rearrangement cross section calculated by Morgan and Hughes[2,3] that leads to antiproton annihilation with the proton of the hydrogen atom at antiproton energies of several eV or less.

Such a reduction is of limited negative consequence at the present time to considering antiproton annihilation as a means of spacecraft propulsion. It means, for instance, that the density of hydrogen atoms (or other forms of matter for which similar reductions would probably occur) in the annihilation region would have to be increased by only 20% over previous estimates[1] to achieve the same annihilation efficiency. However, because of the approximate

nature of the present calculations and because precise values of the annihilation cross section will be required in the future, it is important to recalculate the antiproton - hydrogen atom rearrangement cross section with an accurate, fully-quantum mechanical method.

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3. D.L. Morgan, Jr. and V.W. Hughes, Atomic Processes Involved in Matter-Antimatter Annihilation, Phys. Rev. D 2, 1389 (1970). (Notes: results for $\bar{p}$ - H are equivalent to p - $\bar{H}$; the bare $\bar{p}$ + p annihilation cross section is less than tht for $e^+ + e^-$).

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7. The virial theorem for an r^{-1}, coulomb potential energy is employed, c.f., H. Goldstein, Classical Mechanics (Addison-Wesley, Reading, Mass., 1957), p. 71. The virial theorem for an r^{-2} potential (ibid.) might also be used, but the results will be about the same; the differences would be less than the differences that result from using ε vs. ε'.

8. D.L. Morgan, Jr., Antiproton - Hydrogen Atom Annihilation, AFRPL TR-86-019, Air Force Rocket Propulsion Laboratory, Edwards Air Force Base, California 93523-5000, May 1986.

Table 1. Various energies pertinent to the $\bar{p}$ - H system. ε and V are taken from References 2, 5, and 6. $a_0 = 5.29 \times 10^{-9}$ cm, $e^2/a_0 = 27.2$ eV.

$\bar{p}$ - p separation, $R[a_0]$	$\bar{p}$ - H potential energy, $V[e^2/a_0]$	e^- energy, $\varepsilon[e^2/a_0]$	adjusted e^- energy, $\varepsilon'[e^2/a_0]$
0.1	-9.500	0	0
0.2	-4.500	0	0
0.4	-2.000	0	0
0.639	-1.565	0	0
0.7	-0.929	-0.00038*	0.0043*
1.0	-0.510	-0.010	-0.183
2.0	-0.087	-0.087	-0.412
4.0	-0.0091	-0.2591	-0.4909
7.0	-0.00136	-0.3580	-0.500013
10.0	-0.000310	-0.400310	-0.500183
20.0	-0.0000141	-0.4500141	-0.5000140

*interpolated using ε or ε' = const. x $(R/a_0 - 0.639)^{\upsilon}$, $\upsilon \approx 2$

Table 2. Values of the electron mean velocity, u and u', compared to the antiproton velocity, v. u and u' are obtained by applying the virial theorem to the electron energy ε and the adjusted electron energy ε', and v is for an initial collision energy of 0.027 eV. Units for the velocities are $e(a_0 m)^{-1/2}$ (atomic velocity units).

$R[a_0]$	u	u'	v
0.1	0	0	0.2012
0.2	0	0	0.1385
0.4	0	0	0.0924
0.639	0	0	0.0674
0.7	0.028	0.092	0.0630
1.0	0.142	0.605	0.0467
2.0	0.417	0.907	0.0194
4.0	0.720	0.991	0.0066
7.0	0.847	1.000	0.0032
10.0	0.895	1.000	0.0024
20.0	0.949	1.000	0.0021

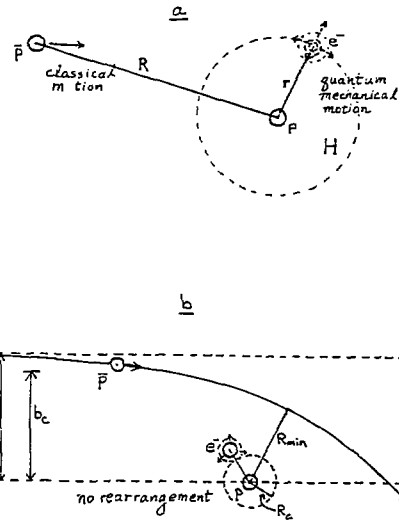
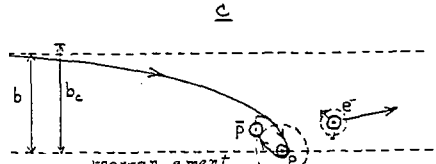


Fig. 1. Morgan-Hughes description of $\bar{p}$ - H scattering (not to scale).

a: p is held fixed while the e^- motion is determined quantum mechanically. This provides the potential energy between the $\bar{p}$ and the H atom to determine the classical orbits of the $\bar{p}$.

b: When the impact parameter, of the $\bar{p}$ is > b_c (b_c depends on the $\bar{p}$ initial kinetic energy) then $R_{min} >> R_c$.

c: When $b < b_c$ then $R_{min} << R_c$ and rearrangement occurs with the e^- emitted and the $\bar{p}$ becoming bound to the p. The annihilation of $\bar{p}$ and p then follows.



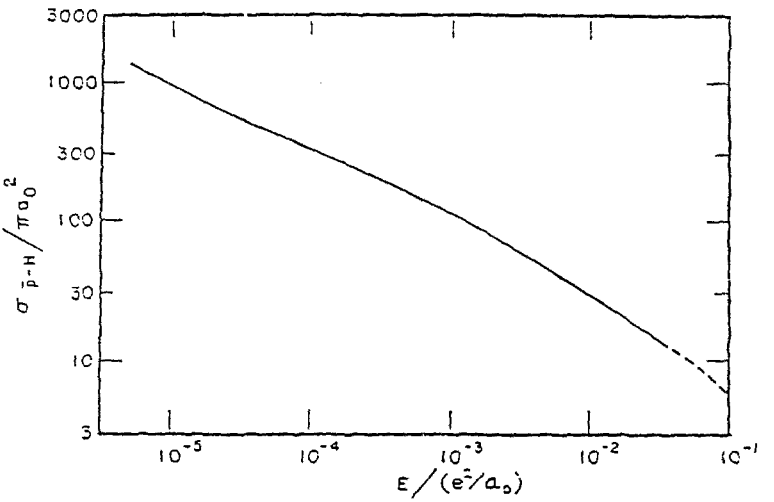


Fig. 2. The $\bar{p}$ - H rearrangement cross section as a function of the $\bar{p}$ - H kinetic energy in the center of mass frame as calculated by Morgan and Hughes.[2]

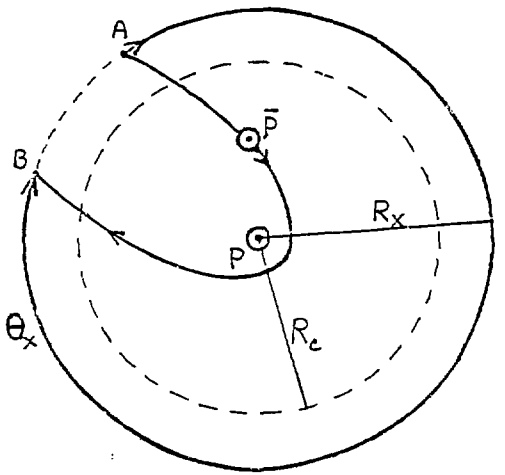


Fig. 3. $\bar{p}$ - p orbit for $R \leq R_x$ (not to scale).

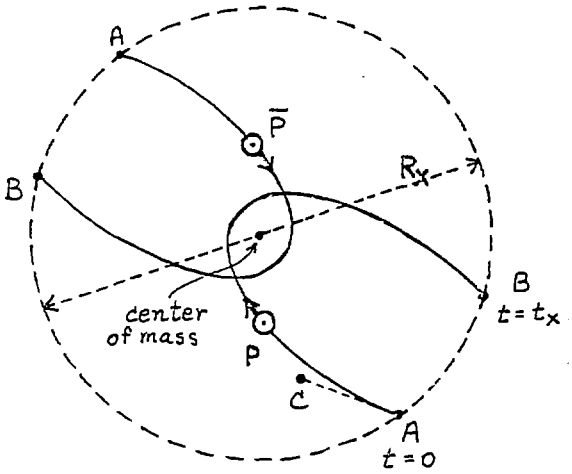


Fig. 4. Motion of the $\bar{p}$ and p in the center of mass frame for $R \leq R_x$ (not to scale). At $t = 0$, when the e^- motion becomes uncoupled from the $\bar{p}$ motion, the e^- wave function, ψ_{e^-} is centered at point A and has an overall velocity equal to the p velocity at $t = 0$. When the p has reached point B (R again $= R_x$) the center of ψ_{e^-} has moved to point C. The reattachment e^- wave function has a form equivalent to that at point A, but it has become slightly larger, is centered at point B, and has an overall velocity equal to the $\bar{p}$ velocity at that point.