

AD-A168 262

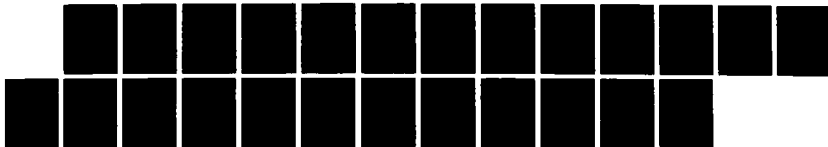
ANTIPROTON-HYDROGEN ATOM ANNIHILATION(U) LAWRENCE
LIVERMORE NATIONAL LAB CA D L MORGAN MAY 86 UCID-20748
AFRPL-TR-86-019 HPR-RPLL59004

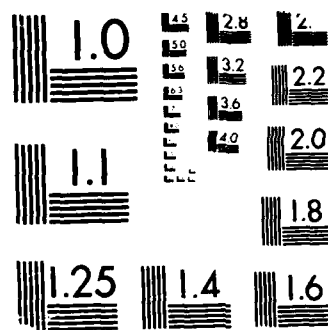
1/1

UNCLASSIFIED

F/G 20/0

ML





MICROCOPY RESOLUTION TEST CHART
 (REF. A) (STANDARDS 1963-A)



AD-A168 262

Final Report
for the period
April 1985 to
December 1985

Antiproton-Hydrogen Atom Annihilation

May 1986

Author:
D. L. Morgan, Jr.

Lawrence Livermore National Lab
P. O. Box 808
Livermore, CA 94550

UCID-20748
MIPR: RPL 59004

Approved for Public Release

Distribution is unlimited. The AFRPL Technical Services Office has reviewed this report, and it is releasable to the National Technical Information Service, where it will be available to the general public, including foreign nationals.

DTIC
ELECTE
JUN 12 1986
S A D

DTIC FILE COPY

prepared for the: **Air Force
Rocket Propulsion
Laboratory**

Air Force Space Technology Center
Space Division, Air Force Systems Command
Edwards Air Force Base,
California 93523-5000

86 6 10 168

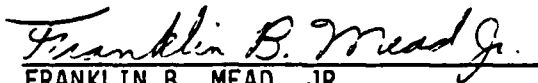
NOTICE

When U.S. Government drawings, specifications, or other data are used for any purpose other than a definitely related government procurement operation, the government thereby incurs no responsibility nor any obligation whatsoever, and the fact that the government may have formulated, furnished, or in any way supplied the said drawings, specifications, or other data, is not to be regarded by implication or otherwise, or conveying any rights or permission to manufacture, use, or sell any patented invention that may in any way be related thereto.

FOREWORD

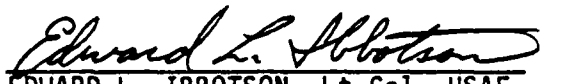
This report was prepared for the Air Force Rocket Propulsion Laboratory (AFRPL) under MIPR RPL-59004 by the Lawrence Livermore National Laboratory (LLNL) under the auspices of the U. S. Department of Energy. The work was performed at the LLNL during the period April 1985 to December 1985. Principal investigator for the LLNL was Mr David L. Morgan, Jr. Project Manager for the AFRPL was Dr Franklin B. Mead, Jr.

This technical report has been reviewed and is approved for publication and distribution in accordance with the distribution statement on the cover and on the DD Form 1473.


FRANKLIN B. MEAD, JR.
Project Manager

FOR THE DIRECTOR


EDWARD S. HUSTON, Maj, USAF
Chief, Space Propulsion Branch


EDWARD L. IBBOTSON, Lt Col, USAF
Deputy Chief, Liquid Rocket Division

UNCLASSIFIED

SECURITY CLASSIFICATION OF THIS PAGE

REPORT DOCUMENTATION PAGE

1a. REPORT SECURITY CLASSIFICATION UNCLASSIFIED		1b. RESTRICTIVE MARKING ATC 8262			
2a. SECURITY CLASSIFICATION AUTHORITY		3. DISTRIBUTION/AVAILABILITY OF REPORT Approved for Public Release: Distribution is Unlimited			
2b. DECLASSIFICATION/DOWNGRADING SCHEDULE					
4. PERFORMING ORGANIZATION REPORT NUMBER(S) UCID- 20748		5. MONITORING ORGANIZATION REPORT NUMBER(S) AFRPL-TR-86-019			
6a. NAME OF PERFORMING ORGANIZATION Lawrence Livermore National Laboratory	6b. OFFICE SYMBOL (If applicable)	7a. NAME OF MONITORING ORGANIZATION Air Force Rocket Propulsion Laboratory			
6c. ADDRESS (City, State and ZIP Code) P.O. Box 808 Livermore CA 94550		7b. ADDRESS (City, State and ZIP Code) AFRPL/LKC Edwards AFB CA 93523-5000			
8a. NAME OF FUNDING/SPONSORING ORGANIZATION	8b. OFFICE SYMBOL (If applicable)	9. PROCUREMENT INSTRUMENT IDENTIFICATION NUMBER MIPR: RPL 59004			
8c. ADDRESS (City, State and ZIP Code)		10. SOURCE OF FUNDING NOS.			
		PROGRAM ELEMENT NO.	PROJECT NO.	TASK NO.	WORK UNIT NO.
11. TITLE (Include Security Classification) ANTIPROTON-HYDROGEN ATOM ANNIHILATION (U)		62302F	5730	00	IV
12. PERSONAL AUTHOR(S) Morgan, David L., Jr.					
13a. TYPE OF REPORT Final	13b. TIME COVERED FROM 85/04 TO 85/12	14. DATE OF REPORT (Yr., Mo., Day) 86/5		15. PAGE COUNT 23	
16. SUPPLEMENTARY NOTATION					
17. COSATI CODES			18. SUBJECT TERMS (Continue on reverse if necessary and identify by block number)		
FIELD	GROUP	SUB. GR.			
20	08		Proton-antiproton annihilation, low collision energy, rearrangement-annihilation cross section, Born-Oppenheimer approximation, reattachment probability		
19. ABSTRACT (Continue on reverse if necessary and identify by block number)					
→ 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. Existing calculations 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 →					
20. DISTRIBUTION/AVAILABILITY OF ABSTRACT UNCLASSIFIED/UNLIMITED ☒ SAME AS RPT. ☐ DTIC USERS ☐			21. ABSTRACT SECURITY CLASSIFICATION UNCLASSIFIED		
22a. NAME OF RESPONSIBLE INDIVIDUAL FRANK B. MEAD, JR.		22b. TELEPHONE NUMBER (Include Area Code) (805) 277-5440		22c. OFFICE SYMBOL AFRPL/LKC	

UNCLASSIFIED

SECURITY CLASSIFICATION OF THIS PAGE

Section 19:
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.

UNCLASSIFIED

SECURITY CLASSIFICATION OF THIS PAGE

TABLE OF CONTENTS

<u>Section</u>	<u>Page</u>
1. Introduction.....	1
1.1 Annihilation Cross Section.....	1
2. The $\bar{p}$ - H System and Born-Oppenheimer Breakdown.....	6
3. The $\bar{p}$ - H System for $R \leq R_x$	9
3.1 Reattachment Probability.....	13
4. Conclusions and Discussion.....	16
References.....	17

Accession For	
NTIS GRA&I	☒
DTIC TAB	☐
Unannounced	☐
Justification	
By	
Distribution/	
Availability Codes	
Dist	Avail and/or Special
A1	



LIST OF TABLES AND FIGURES

<u>Tables</u>	<u>Page</u>
Table 1. Various energies pertinent to the $\bar{p} - H$ system.....	7
Table 2. Values of the electron mean velocity, u and u' , compared to the antiproton velocity, v	9
 <u>Figures</u>	
Figure 1. Morgan-Hughes description of $\bar{p} - H$ scattering.....	2-3
Figure 2. The $\bar{p} - H$ rearrangement cross section.....	5
Figure 3. $\bar{p} - p$ orbit for $R \leq R_x$	11
Figure 4. Motion of the $\bar{p}$ and p in the center of , , mass frame for $R \leq R_x$	14

1. INTRODUCTION

In antiproton annihilation propulsion of spacecraft, a possible choice for the annihilation process is low-energy antiprotons (kinetic energy ≤ 1 eV) annihilating with the protons of hydrogen atoms.⁽¹⁾ At such energies, an atomic rearrangement occurs in which the electron (e^-) of the hydrogen atom (H) is emitted while the proton (p, positive) of the hydrogen atom and the antiproton ($\bar{p}$, negative) form an excited bound state of protonium (Pn)⁽²⁾:



The p and $\bar{p}$ 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 by solving the Schroedinger equation for the ground state of the e^- in the field of a negative charge (the $\bar{p}$) and a positive charge (the p) that are separated by a fixed distance, R (see Fig. 1). The approximation of holding the p and $\bar{p}$ (or other nuclei) fixed, while determining the electron motion, is known as the fixed-nucleus or Born-Oppenheimer approximation.⁽⁴⁾ Solving for the electron motion gives the electron energy as a function of R. This energy, along with the $\bar{p}$ - p attraction determines the potential energy (or force)

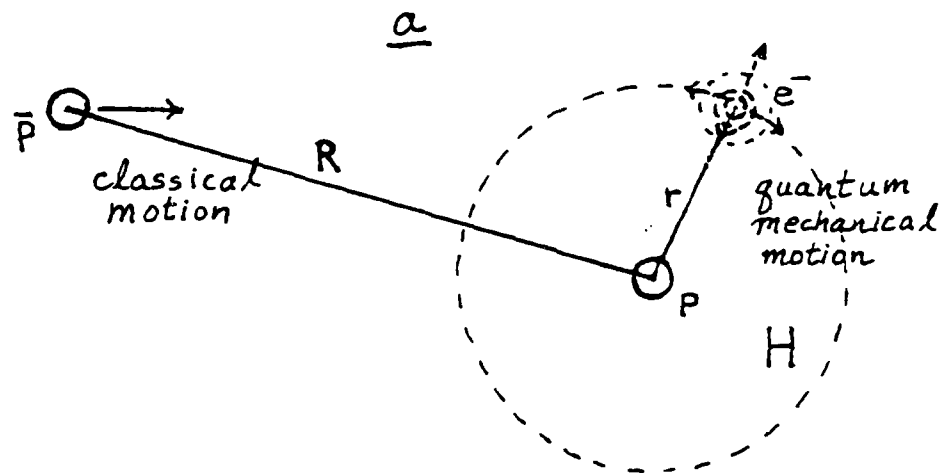


Fig. 1. Morgan-Hughes description of $\bar{p}$ - H scattering (not to scale).

- a: R 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, b , of the $\bar{p}$ is $> b_c$ (b_c depends on the $\bar{p}$ initial kinetic energy) then $R_{\min} \gg R_c$.
- c: When $b < b_c$ then $R_{\min} \ll R_c$ 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.

Parts b and c are on the following page.

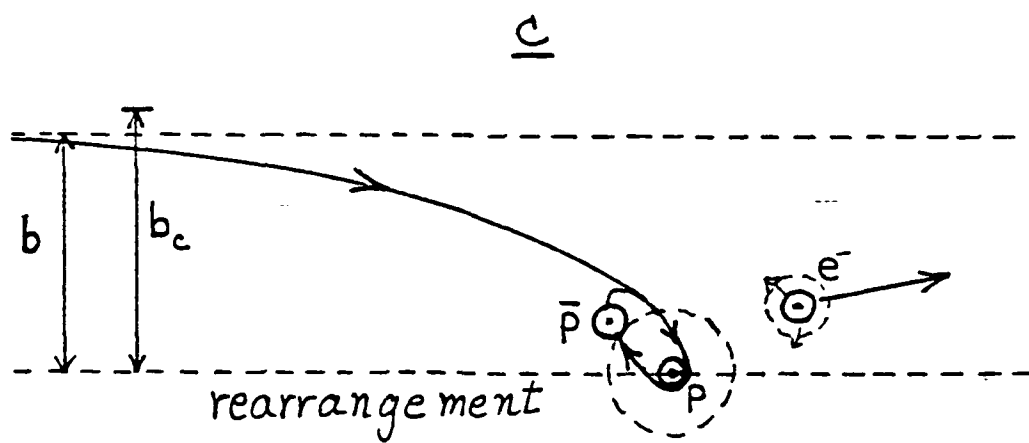
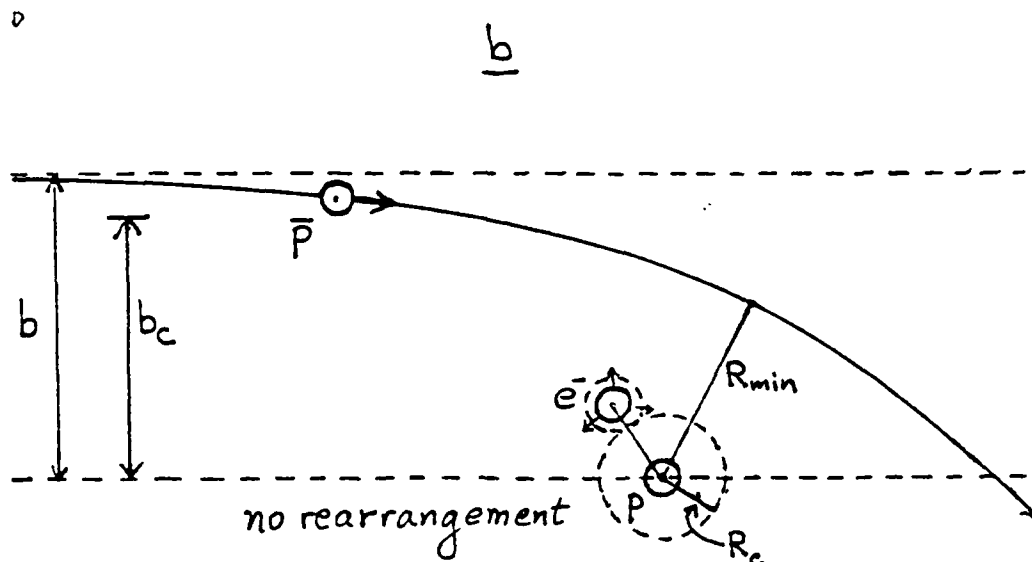


Fig. 1 continued. Parts b and c.

between the $\bar{p}$ and the H, which is used in calculating the relevant features of the $\bar{p}$ - H classical orbits (R not fixed).^(2,3)

The classical orbits have an interesting property for antiproton kinetic energies less than about 1 eV. When the impact parameter, b , is greater than a particular value, b_c , which depends on the collision energy, the inner turning point (point of closest approach, designated $R_{\min}$) 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 be much smaller than the critical radius, R_c . R_c is the value of R less than which the e^- is no longer bound to the p in H because of the strong repulsive force of the $\bar{p}$. Wightman⁽⁵⁾ determined the value of R_c to be $0.639a_0$ where $a_0 = 5.29 \times 10^{-9}$ cm is the first Bohr radius of hydrogen. (Wightman's calculation was for negative muon - hydrogen which is equivalent to $\bar{p}$ - H in the Born-Oppenheimer approximation). Following Wightman, 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 $\sigma = \pi b_c^2$. This cross section is shown in Fig. 2.

Morgan and Hughes demonstrated the validity of using classical orbits for the $\bar{p}$ - H 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 with high probability the e^- left the scattering region permanently for $b < b_c$ and did not, in fact, reattach itself to the proton with a significant probability were only qualitative. If there is a possibility for reattachment, then the rearrangement-annihilation cross section is lower than their value. The problem in considering reattachment is that the Born-Oppenheimer approximation breaks down for $R \lesssim R_c$. Thus, in lieu of a full quantum-mechanical solution of the problem, with essentially no approximations, 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.

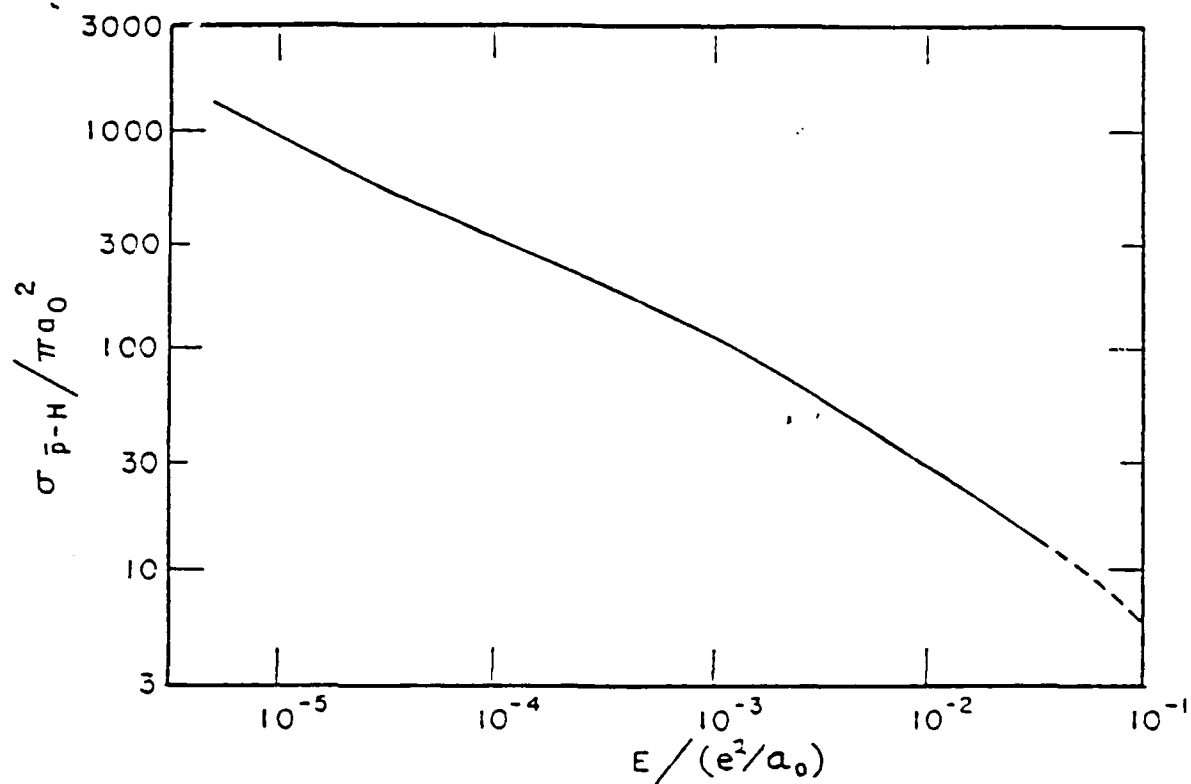


Fig. 2. The $\bar{p}$ - H rearrangement cross section as a function of the $\bar{p}$ - H kinetic energy in the center of mass frame as calculated by Morgan and Hughes. (2)

2. THE $\bar{p}$ - H SYSTEM AND BORN-OPPENHEIMER BREAKDOWN

The Born-Oppenheimer approximation is valid when the mean velocity of the electron relative to the proton is much larger than the velocity of the antiproton relative to the proton. Such is true at the kinetic energies of interest when R is a few times a_0 or greater, principally because the antiproton mass (same as the proton mass) is about 1836 times the electron mass. However, as R decreases, the mean velocity of the electron decreases as it is pushed farther from the proton and its energy approaches zero from a negative value while the velocity of the antiproton increases due to its attraction to the H atom. For $R = R_0$ in the Born-Oppenheimer approximation, the energy and velocity of the electron have dropped to zero, so the cross-over point of the velocities is at a small value of R but greater than R_0 .

Before considering what happens when the Born-Oppenheimer approximation breaks down, it is necessary to determine the value of R , in that approximation, at which the cross-over point of the velocities occurs. That value of R , designated R_x , was found by using two different methods to determine u , the mean velocity of the electron. Both make use of the Born-Oppenheimer energy of the electron, ϵ , which is given in Ref. 2, (add $a_0/R - 1/2$ to V in Table VI of that reference to obtain ϵ in atomic units), where for values of R less than $5 a_0$, ϵ is taken from work by Wightman⁽⁵⁾ and Bates.⁽⁶⁾ ϵ is given in Table 1 along with V , the $\bar{p}$ - H potential energy. ϵ and V are related by

$$V = \epsilon - e^2/R - \epsilon_0 \quad , \quad (2)$$

where $e = 4.80 \times 10^{-10} \text{ cm}^{3/2} \text{ g}^{1/2} \text{ s}^{-1}$ is the unit electric charge, and $\epsilon_0 = -1/2 e^2/a_0$ is the ground state energy of the electron in H. In the first method, the virial theorem⁽⁷⁾ is assumed to apply to ϵ , so the kinetic energy of the electron is $-1/2 \epsilon$ and u is therefore $(-\epsilon/m)^{1/2}$, where $m = 9.11 \times 10^{-28} \text{ g}$ is the electron mass.

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

$\bar{p}$ - p separation, $R[a_0]$	$\bar{p}$ - H potential energy, $V[e^2/a_0]$	e^- energy, $\epsilon[e^2/a_0]$	adjusted e^- energy, $\epsilon'[e^2/a_0]$
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 $\epsilon' = \text{const.} \times (R/a_0 - 0.639)^v$, $v \approx 2$

A problem with determining u in the first method involves the fact that ϵ has a substantial contribution from the potential energy between the $\bar{p}$ and the quantum mechanically distributed e^- . For values of R equal to a few a_0 (and greater) this is mainly a static contribution; it has only a small effect on the dynamics of the electron motion. Hence the second method for determining u , in which part of the $\bar{p} - e^-$ potential energy is subtracted from ϵ (making it more negative) before applying the virial theorem. The fraction of this potential energy to subtract is uncertain, but the fraction is about unity when R is large and less than unity for $R = 1$ or $2 a_0$ where the $\bar{p}$ affects the dynamics of the electron motion. For the fraction, $1 - e^{-R/a}$ is chosen where R is in units of a_0 and a is the mean radius of the e^- distribution (also in units of a_0). Thus,

$$\epsilon' = \epsilon - (1 - e^{-R/a}) \left(\frac{1}{R} - \left(\frac{3}{2a} + \frac{1}{R} \right) e^{-3R/a} \right), \quad (3)$$

where the first quantity in parenthesis is the fraction, and the second quantity in parenthesis (with an inner parenthetic expression) is the mean $\bar{p} - e^-$ potential energy. In Eq. 3, R is in units of a_0 and ϵ and ϵ' are in units of e^2/a_0 . The $\bar{p} - e^-$ mean potential energy was determined by assuming that the e^- distribution is approximately hydrogenic, i.e. it has the form $\text{const.} \times e^{-3R/a}$ (wave function = $\text{const.} \times e^{-3R/(2a)}$). Under the same assumption, $a = (-9/(8\epsilon'))^{1/2}$. When this equation for a is substituted into Eq. 3, that equation can be solved iteratively for ϵ' as a function of R . The resultant values of ϵ' are given in Table 1.

The values of ϵ' for $R \geq 2 a_0$, where the $\bar{p}$ is outside of the e^- distribution, appear to represent the dynamic motion of the e^- more reliably than the values of ϵ since they are closer to the value of $-1/2$ which both ϵ and ϵ' have for $R = \infty$. For smaller R than $2 a_0$ it is surprising that ϵ' is so much greater in magnitude than ϵ . Thus it is likely that a better value of ϵ' probably lies between ϵ and the present value. As will be seen below, this uncertainty in ϵ' has only a small effect on R_x because of the strong dependence of u on R .

Applying the virial theorem to both ϵ and ϵ' yields the values for the mean electron velocity, $u = (-2\epsilon/m)^{1/2}$, or the same with ϵ' in place of ϵ , where m is the mass of the electron, that are given in Table 2. Also given in Table 2 is the velocity of the antiproton relative to the proton. This latter quantity is determined for an antiproton collision energy of $0.001 e^2/a_0 = 0.027 \text{ eV}$. It applies for all impact parameters that are less than b_c . The results are essentially unaltered near $R = R_x$ if lower or higher collision energies are used as long as the energy is $\leq 1 \text{ eV}$. (At higher energies the method used by Morgan and Hughes^(2,3) to determine the cross section may not apply because the discontinuity of $R_{\min}$ becomes considerably less pronounced or disappears).

By plotting the velocities in Table 2, it is found that $R_x = 0.79 a_0$ when ϵ is used and $R_x = 0.68 a_0$ 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 $R < R_x$.

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

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

For $R \leq R_x$ the value of ϵ in Eq. 2 for the $\bar{p} - H$ potential energy V is small enough to be neglected, so for $R \leq R_x$

$$V = -\frac{e^2}{R} + \frac{e^2}{2a_0}, \quad (4)$$

where ϵ_0 has been replaced by its value, $-1/2 e^2/a_0$. Because ϵ (or ϵ') is so small, the mean radius of the electron distribution is much greater than R_x . Thus, V is more properly termed the $\bar{p} - p$ effective potential for $R \leq R_x$. It is equal (c.f. Eq. 4) to the $\bar{p} - p$ potential energy, $-e^2/R$ plus the energy, $1/2 e^2/a_0$, that has been transferred from the antiproton to the electron. This energy, equal to 13.6 eV, is the negative of ϵ_0 . The initial kinetic energy of the antiproton (≤ 1 eV) is less than the energy transferred, hence the fact that the $\bar{p}$ will become bound to the p (in a negative energy state) unless the e^- rejoins the p and transfers the absorbed energy back to the $\bar{p}$. Due to the simple form of Eq. 4 and because it involves the inverse of R , analytic formulae for the orbital motion of the $\bar{p}$ relative to the p can be determined for $R < R_x$. In addition approximate means exist for following the motion of the e^- during this time period.

The analytic formulae for the motion of the $\bar{p}$ are the standard formulae for an attractive $1/R$ potential ($1/R^2$ force) but with an energy of $1/2 e^2/a_0$ subtracted from the initial $\bar{p}$ kinetic energy. These formulae give

$$t_x = \frac{(2M)^{1/2}}{1-2K_0} ((1-2K_0)^{-1/2} (\frac{\pi}{2} - \sin^{-1} (\frac{1 - R_x(1-2K_0)}{(1-2b^2K_0(1-2K_0))^{1/2}})) - (-R_x^2(1-2K_0) + 2R_x - 2b^2K_0)^{1/2}) \quad (5)$$

and

$$\theta_x = \pi + 2 \sin^{-1} \left(\frac{R_x - 2b^2K_0}{R_x(1-2b^2(1-2K_0))^{1/2}} \right) \quad (6)$$

for the time that R is $\leq R_x$ and for the angle (centered on the p) through which the $\bar{p}$ moves, while $R \leq R_x$, in its orbit around the p . In Eqs. 5 and 6, K_0 is the initial collision kinetic energy of the $\bar{p}$ (≤ 1 eV) in the laboratory frame, i.e., the p has no initial kinetic energy. (In the center of mass frame the initial kinetic energy is $K_0/2$). In Eqs. 5 and 6, $M = 1836$ is the $\bar{p}$ ($=p$) mass in units of m (the electron mass), R_x is in units of a_0 , K_0 is in units of e^2/a_0 , t_x is in units of $m^{1/2} a_0^{3/2} e^{-1}$ (atomic time units), and θ_x is in radians. Figure 3 depicts the geometry of the $\bar{p} - p$ motion for $R \leq R_x$. For $K_0 = 0$ to 1 eV and $b = 0$ to b_0 values of t_x range from 23 to 27 atomic units for $R_x = 0.79 a_0$ and from 18 to 22 atomic units for $R_x = 0.68 a_0$, with the maximum values of t_x being for the maximum values of K_0 and b , and the minima of t_x being for $K_0 = 0$ and $b = 0$. For the same ranges of K_0 and b , θ_x varies from 303° to 360° for $R_x = 0.79 a_0$ and from 296° to 360° for $R_x = 0.68 a_0$, with the maximum values of θ_x (360° , which means back to the same point after a full circuit) coming from $b = 0$ (any K_0 in the range) and the minima of θ_x from the maximum values of K_0 and b .

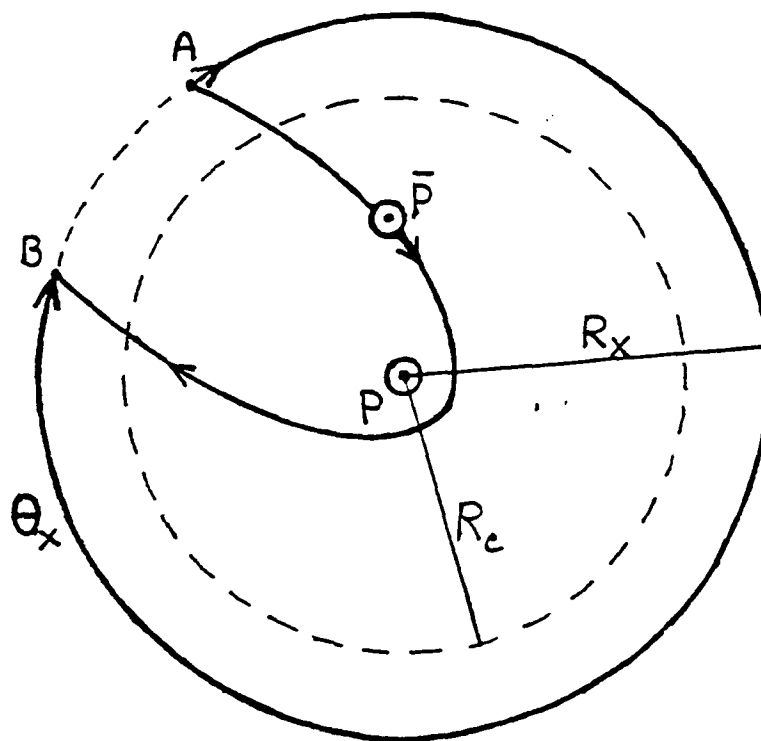


Fig. 3. $\bar{p} - p$ orbit for $R \leq R_x$ (not to scale).

The e^- motion is approximated as that of an evolving Gaussian wave packet, during the time that $R \leq R_x$, while the $\bar{p} - p$ configuration is changing as described above. 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

$$\psi_{e^-} = \pi^{-3/4} (\beta + it/\beta)^{-3/2} e^{-\frac{r^2}{2(\beta^2 + it)}} \quad (7)$$

where t is the time following the first instance that $R = R_x$, β is a constant, all quantities are in atomic units, and $i = (-1)^{1/2}$. Equation 7 is the solution to the time-dependent Schroedinger equation

$$i \frac{\partial}{\partial t} \psi = -\frac{1}{2} \left(\frac{\partial^2}{\partial r^2} + \frac{2}{r} \frac{\partial}{\partial r} \right) \psi \quad (8)$$

The electron probability distribution (referred to above as just the electron distribution) is the square of absolute value of the wave function,

$$|\psi_{e^-}|^2 = \pi^{-3/2} (\beta^2 + t^2/\beta^2)^{-3/2} e^{-\frac{r^2}{\beta^2 + t^2/\beta^2}} \quad (9)$$

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

$$\beta = (-3/(2\epsilon))^{1/2} \text{ or } (-3/(2\epsilon'))^{1/2} \quad (10)$$

and substituting the values of ϵ and ϵ' gives $\beta = 30.1 a_0$ 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 likelihood that the e^- will reattach itself to the p once R again becomes greater than R_x is related to the similarity between two forms of ψ_{e^-} . The first form is ψ_{e^-} at $t = t_x$, when the Born-Oppenheimer approximation can be re-established and the e^- motion can again become coupled to the $\bar{p} - p$ motion, and the second is the ψ_{e^-} that the electron would have if it were to become reattached to the p . From the viewpoint in the center of mass frame of the $\bar{p}$ and p , the former ψ_{e^-} will be taken as given by Eq. 7 for $t = t_x$, located and moving according to the overall velocity it had at $t = 0$, while the latter will be a ψ_{e^-} as given by Eq. 7 at $t = 0$ (last time of attachment) but with the position and velocity of the p at $t = t_x$. The changes in position and velocity may be seen in Fig. 4 where the $\bar{p} - p$ motion for $R \leq R_x$ is shown in the center of mass frame. In the above "position" means the point in space to which $r = 0$ in Eqs. 7 and 9 refers, while "overall velocity" refers to the velocity of that point in the center of mass frame. The meaning of "similarity" will be semiquantitative for size and position changes of ψ_{e^-} , but will be given a precise definition when the effects of velocity-change are considered.

When the values of β along with $t = 0$ and t_x are placed in Eq. 7, 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 $2\pi^{-1/2}(\beta^2 + t^2/\beta^2)^{1/2}$) is much greater than the changes in position (which are not larger than R_x), changes in position will not result in significantly dissimilar wave functions. Thus, the only possible significant lack of similarity between the wave functions to be compared is that which can come from the difference in velocity of their centers. The difference in velocity of the centers of the e^- wave functions is the difference between the velocities of the proton in the center of mass system at $t = 0$ and $t = t_x$. Because θ_x is about 360° (change in direction about 180°) the change in velocity of the proton in the center of mass system is about twice its velocity at $R = R_x$ ($t = 0$). This velocity is one-half the $\bar{p} - p$ (or $\bar{p} - H$) relative velocity, so the change in velocity of the center of the electron wave function is equal to v at $R = R_x$. Thus, the velocity difference is equal, in atomic units, to 0.058 (using ϵ) or 0.065 (using ϵ').

Because of the small effects of change in form and position of e^- , it may be taken to be

$$\psi_{e^-} = \pi^{-3/4} \beta^{-3/2} e^{-\frac{r^2}{2\beta^2}} \quad (11)$$

when $t = t_x$ and at the same time the reattached ψ_{e^-} may be described by

$$\psi_{e^-} = \pi^{-3/4} \beta^{-3/2} e^{-\frac{r^2}{2\beta^2} + ikz}, \quad (12)$$

where the multiplicative factor, e^{ikz} , is due to the change in velocity. The quantity k is the wave number for this change and is equal to v in atomic units (since the mass of the e^- is unity in atomic units) while z is the cartesian coordinate in the direction of the velocity change (the results below are not affected by the choice of direction for the z -axis).

The similarity between the two forms of ψ_{e^-} given by Eqs. 11 and 12 will now be defined specifically as the square of the absolute value of the overlap integral of these two forms for ψ_{e^-} . This quantity, in the "sudden" approximation, is the probability that the e^- will reattach to the p as R passes through R_x on the way out. The sudden approximation is accurate when a system encounters a change in its potential energy that occurs during a time interval that is much shorter than the time required for that system to change significantly. Such conditions are met fairly well here. The result of the integration gives

$$P = e^{-\frac{\beta^2 v^2}{2}} \quad (13)$$

for the probability of reattachment. Using the values of β and v already given, $P = 0.22$ when either ϵ or ϵ' is used to obtain β and v .

At face value, a value for P 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 detailed 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.⁽⁸⁾

REFERENCES

1. D.L. Morgan, Jr., Concepts for the Design of an Antimatter Annihilation Rocket, Journal of the British Interplanetary Society 35, 405 (1982).
2. D.L. Morgan, Jr. and V.W. Hughes, Atom-Antiatom Interactions, Phys. Rev. A 7, 1811 (1973).
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 $p - H$ are equivalent to $\bar{p} - H$; the bare $\bar{p} + p$ annihilation cross section is less than that for $e^+ + e^-$).
4. M. Born and R. Oppenheimer, Ann. Phys. (Leipz.) Ser. 4, 84, 457 (1927); J.L. Hirschfelder, C.F. Curtiss, and R.B. Bird, Molecular Theory of Gases and Liquids (Wiley, New York, 1954), pp. 922-930; N.F. Mott and H.S.W. Massey, The Theory of Atomic Collisions (Clarendon, Oxford, England, 1965), p. 428; W. Kolos, Adv. Quantum Chem. 5, 99 (1970).
5. A.S. Wightman, Phys. Rev. 77, 521 (1950); E.M. Purcell and G.B. Field, Astrophys. J. 124, 542 (1956).
6. D.R. Bates, private communication to R. Drachman.
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. During this study, I made two attempts in that direction. The first involved a pre-existing computer code that treated the $\bar{p} - H$ motion classically, and solved the time-dependent Schroedinger Equation for the motion of the electron of H. Solution of the electron motion, however, assumed that the Born-Oppenheimer approximation applied to angular motion of the electron for all values of R, thus the code had to be altered significantly to remove this restriction. The second attempt involved a new computer method that I had developed for other purposes to solve the Schroedinger Equation for a bound three-body system. Use of this method required generalization to unbound (scattering) systems. In both cases, after some work, I decided that the effort required would exceed the allocation which I had requested and received for this study.

END

DATE

FILMED

DTIC

July 88