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Atom-Antiatom Interactions*

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Atom-antiatom rearrangement collisions in which the nucleus-antinucleus bound state is formed are important processes in atom-antiatom interactions. We give a general discussion of the atom-antiatom interatomic potential energy V and calculate V for $H-\bar{H}$, $\bar{p}-H$, and $\bar{M}-Ar$ where \bar{M} means antimuonium (μ^-e^+ atom). We apply the semiclassical and optical-potential methods to determine cross sections for rearrangement collisions. At low energies these collisions are the dominant processes leading to particle-antiparticle annihilation.

I. INTRODUCTION

The concept of antimatter and speculation on its existence in the universe is more than seven decades old.¹ Atom-antiatom interactions are of great importance in any matter-antimatter encounter when either the matter or antimatter consists at least in part of atoms or antiatoms that are not wholly ionized. This is the case in the laboratory for the interaction of heavy negative antiparticles produced in accelerator experiments with target matter. It may also be true for the interactions between large amounts of matter and antimatter in the universe.

The existence and consequences of cosmological antimatter have been considered by Alfvén and Klein,² Harrison,³ Omnès,⁴ and others.⁵ Cosmologies have been developed in which the universe contains equal amounts of initially mixed matter and antimatter. After a large degree of annihilation the matter and antimatter separate into different regions but may continue to interact at their boundaries.

In any "big-bang" model or other model of the universe that involves temperatures that were at one time $\gtrsim 10^{13}$ K, particle-antiparticle production in thermal collisions was prevalent in that stage of development. Thus, antimatter existed in copious amounts at one time in the universe according to such models irrespective of whether or not it was in equal amount to the matter. It is then conceivable that the same mechanisms proposed by the

above authors²⁻⁴ or other mechanisms resulted in the separation of at least some of the antimatter from the matter.

It is therefore possible that antimatter does exist now or did exist in sufficient amount and for a sufficient time that there are presently observable consequences of its existence. One such possible consequence is the isotropic cosmic γ -ray background spectrum above 1 MeV. Stecker, Morgan, and Bredekamp⁶ and Stecker and Puget⁷ have considered γ rays that would result from the decay of neutral π mesons produced by annihilation in a thermal hydrogen-antihydrogen mixture. They find that the spectrum of such γ rays coming from red shifts of up to about 200 agrees well with the experimental results. Other possible consequences that have been considered include the possibilities that quasars may consist of annihilating matter and antimatter^{8,9} that the Tunguska "meteor" consisted of antimatter,^{10,11} and that ball lightning may be caused by particles of antimatter.¹²

It has been pointed out by the present authors that atom-antiatom interactions are important in the treatment of matter-antimatter annihilation.¹³ In any matter-antimatter mixture in which the atoms and antiatoms are not wholly ionized, atom-antiatom rearrangement collisions can lead to bound states of the nucleus and antinucleus from which the annihilation can proceed.^{11,13,14} Since the cross sections for such collisions at low energies are considerably higher than the direct particle-antiparticle annihilation cross sections,¹³

atom-antiatom interactions may play a dominant role in such a mixture. It is the purpose of this paper to give a detailed treatment of atom-antiatom interatomic potential energies and rearrangement collisions.

In Sec. II we give a general discussion of the principal features of atom-antiatom interatomic potential energies and compare them to atom-atom interatomic potential energies. In Sec. III we discuss the various aspects of atom-antiatom rearrangement collisions and present two methods with which approximate values of the cross sections may be calculated. In Secs. IV-VII we present our calculations of interatomic potential energies and rearrangement cross sections for certain specific atom-antiatom pairs. The results are compared to the results of others where they exist. Brief reports of this research have been published.^{13,14}

The existence of antimatter in the universe is at present speculative, and it is not at all clear under what physical circumstances cosmological atom-antiatom interactions should be considered. For collision energies above about 100 eV the direct particle-antiparticle annihilation cross sections apply. At lower energies rearrangement collisions are important. If densities are not sufficiently high to lead to breakup, annihilation follows formation of the nucleus-antinucleus bound state, and the annihilation cross sections are then given by the rearrangement cross sections.

In this paper we take atom-antiatom interactions to mean interactions between the members of any pair consisting of a neutral or ionized atom and a neutral or ionized antiatom, exclusive of the case in which both atom and antiatom are wholly ionized. We consider only Coulomb interactions; all radiative effects and all relativistic effects, such as magnetic interactions and retardation, are unimportant for the results obtained here. Likewise, the effects of annihilation on the atom-antiatom interatomic potential energies and rearrangement cross sections are negligible.

II. ATOM-ANTIATOM INTERATOMIC POTENTIAL ENERGIES

The atom-antiatom interatomic potential energy V is the difference between the total energy of the atom-antiatom pair calculated with the nuclei held fixed at an internuclear distance R and the energy for the nuclei fixed at $R = \infty$. Knowledge of this potential energy is necessary for calculating the rearrangement cross sections by the methods given in Sec. III.

In considering V for an atom-antiatom pair and in comparing it to V for the corresponding atom-atom pair it is useful to employ the Rayleigh-Schrödinger perturbation expansion¹⁵ for V in which the Coulomb potential energy between the particles

of the atom and the particles of the antiatom is taken to be the perturbation potential energy v . The Hamiltonian of the system therefore has the form

$$H = H_0 + v, \quad (2.1)$$

where H_0 is the unperturbed part of the Hamiltonian with the nuclei held fixed. If the charge of the nucleus is Ze , the charge of the antinucleus is $-\bar{Z}e$, the number of electrons is N , and the number of positrons is \bar{N} , then

$$H_0 = -\frac{1}{2} \sum_{i=1}^N \nabla_i^2 - \sum_{i=1}^N \frac{Z}{r_i} + \sum_{i=1}^{N-1} \sum_{j=i+1}^N \frac{1}{|\vec{r}_i - \vec{r}_j|} - \frac{1}{2} \sum_{\bar{i}=1}^{\bar{N}} \nabla_{\bar{i}}^2 - \sum_{\bar{i}=1}^{\bar{N}} \frac{\bar{Z}}{\bar{r}_{\bar{i}}} + \sum_{\bar{i}=1}^{\bar{N}-1} \sum_{\bar{j}=\bar{i}+1}^{\bar{N}} \frac{1}{|\vec{r}_{\bar{i}} - \vec{r}_{\bar{j}}|} \quad (2.2)$$

and

$$v = -\frac{Z\bar{Z}}{R} + \sum_{i=1}^N \frac{\bar{Z}}{|\vec{R} + \vec{r}_i|} + \sum_{\bar{i}=1}^{\bar{N}} \frac{Z}{|-\vec{R} + \vec{r}_{\bar{i}}|} - \sum_{i=1}^N \sum_{\bar{i}=1}^{\bar{N}} \frac{1}{|\vec{R} + \vec{r}_i - \vec{r}_{\bar{i}}|}, \quad (2.3)$$

where subscripts i and \bar{i} denote the i th electron and \bar{i} th positron, the \vec{r}_i are the vector distances from the nucleus to the electrons, the $\vec{r}_{\bar{i}}$ are the vector distances from the antinucleus to the positrons, and \vec{R} is the vector distance from the antinucleus to the nucleus. Atomic units are used in Eqs. (2.2), (2.3), and throughout the paper (except that the Bohr radius a_0 is included when distances are stated).

The unperturbed energies and normalized eigenstates of the system are denoted by E_k and ψ_k . These quantities are solutions of the unperturbed Schrödinger equation

$$(H_0 - E_k)\psi_k = 0. \quad (2.4)$$

In order for the ψ_k to be solutions to Eq. (2.4) they must be the product of unperturbed wave functions of the atom and antiatom or the normalized sum of such products, each having the same E_k . Such products cannot involve exchange in the electron and positron positions because of the different signs of the electron and positron charges.

Since v is zero at $R = \infty$, the total energy \mathcal{E} at $R = \infty$ is equal to E_p when the system is in the state p , and therefore the interatomic potential energy is given by

$$V_p(R) = \mathcal{E}(R) - E_p. \quad (2.5)$$

The matrix element of v between the two unperturbed eigenstates is

$$A_{kl} = \int \psi_k^* v \psi_l d\tau, \quad (2.6)$$

where k and l each denote the collection of quantum numbers that characterize the unperturbed state

of the system. The perturbation expansion of the interatomic potential energy between the atom and antiatom for the system in a state p is then

$$V_p = \mathcal{E}_1 + \mathcal{E}_2 + \mathcal{E}_3 + \dots, \quad (2.7)$$

with

$$\mathcal{E}_1 = A_{pp}, \quad \mathcal{E}_2 = \sum_{k \neq p} \frac{A_{pk} A_{kp}}{E_p - E_k}, \quad (2.8)$$

$$\mathcal{E}_3 = \sum_{\substack{k \neq p \\ l \neq p}} \frac{A_{pk} A_{kl} A_{lp}}{(E_p - E_k)(E_p - E_l)} - A_{pp} \sum_{k \neq p} \frac{A_{pk} A_{kp}}{(E_p - E_k)^2},$$

where the \mathcal{E}_n denote the contributions to V_p which are of order n in v and where the summations are understood to be integrations when E_k and E_l are in the continuum.

In Eqs. (2.7) and (2.8) the term \mathcal{E}_1 is the electrostatic potential energy between the unperturbed atom and antiatom. For large values of R this term is the sum of the potential energies between the static multipoles of the atom and antiatom. The effect in V_p of distortions in the wave function caused by v appear in the higher \mathcal{E}_n . These distortions involve correlation in the electron and positron positions and/or induced multipoles.

The interatomic potential energy of the corresponding atom-atom pair (the pair formed by replacing the antiatom with its charge-conjugate analog) is given by the preceding equations with two important changes.

First, the unperturbed wave function of the atom-atom pair must satisfy the Pauli principle with respect to exchange of electrons between the two atoms. This is accomplished by requiring that the unperturbed wave function be one of a set of specific linear combinations of products (with equal eigenenergies) of the individual atom wave functions, that involve exchange of electrons between the atoms. By virtue of the atom-atom sign of charge symmetry, such a wave function is a solution to the Schrödinger equation (2.4). The result of this is that each \mathcal{E}_n [Eqs. (2.8)] and consequently V_p [Eq. (2.7)] is the sum of two parts. The first part of $\mathcal{E}_n(V_p)$ is equal to the value that would have resulted if no exchange were present (as in the atom-antiatom case). The terms making up the second part are the result of exchange and are usually denoted "exchange forces." The exchange forces are roughly proportional to the degree of overlap of the electron wave functions of the two atoms and therefore are negligible for large values of R . Such exchange forces are the predominate feature of atom-atom interatomic potential energies for intermediate values of R (roughly $1a_0 \lesssim R \lesssim 6a_0$) when at least one atom is neutral, but they are entirely absent in atom-antiatom interatomic potential energies.

Second, v for the corresponding atom-atom pair

is just the negative of v for the atom-antiatom pair. Thus, each \mathcal{E}_n for an atom-antiatom pair will be equal in magnitude to the nonexchange part of the \mathcal{E}_n for the corresponding atom-atom pair and will have the same sign for n even and the opposite sign for n odd. For long-range values of R (roughly $R \gtrsim 10a_0$), where exchange forces may be neglected, the perturbation expansion for V of an atom-antiatom pair is therefore readily obtainable from the perturbation expansion for V of the corresponding atom-atom pair.

For more specific consideration of the interatomic potential energy for an atom-antiatom pair we delineate three cases, in each of which the atoms and antiatoms are in states of zero total angular momentum and hence possess no static multipoles beyond monopole. In case (i) both atom and antiatom are neutral, in case (ii) one is neutral and the other is ionized, and in case (iii) both are ionized. The important features of V for these cases for small, intermediate, and long-range values of R are as follows.

For an atom-antiatom pair, V is given by

$$V = -Z\bar{Z}/R \text{ as } R \rightarrow 0. \quad (2.9)$$

This dominant term is part of \mathcal{E}_1 [Eqs. (2.3) and (2.5)–(2.8)] and is opposite in sign to the similar term in the corresponding atom-atom pair.

In case (i), V at long range is nearly equal to V for the corresponding atom-atom pair where it is dominated by the negative long-range R^{-6} mutually induced dipole-dipole correlation energy that comes from \mathcal{E}_2 . The negative R^{-8} and R^{-10} higher induced multipole terms of \mathcal{E}_2 may also be important. Taken together we therefore have for this case at long range,

$$V = -C_6/R^6 - C_8/R^8 - C_{10}/R^{10} - \dots, \quad (2.10)$$

where the C 's are the same as those in the corresponding atom-atom pair and have been tabulated¹⁶ or may be obtained from approximate formulas.^{16,17} The terms of \mathcal{E}_2 "cut off" within the range of intermediate values of R (i.e., they become less strongly dependent on R and approach constants as $R \rightarrow 0$), and \mathcal{E}_2 remains negative. Within the intermediate range, \mathcal{E}_1 , which is an exponentially decreasing function of R (since it depends on overlap), becomes important. Its sign is positive for $R \gtrsim 2a_0$. Owing to the difference in sign of \mathcal{E}_1 and \mathcal{E}_2 and to the effect of higher \mathcal{E}_n , no prediction about the sign of the potential throughout this range can be given.

In case (ii), V is again nearly equal to that of the corresponding atom-atom pair at long range where it is dominated by the negative monopole-induced-dipole energy of \mathcal{E}_2 . This energy is given by¹⁸

$$V = -Z_i \alpha / 2R^4, \quad (2.11)$$

where Z_i is the absolute value of the charge on the ionized member of the pair and α is the polarizability¹⁹ of the neutral member, which is the same for an antiatom and the corresponding atom. Equation (2.11) and the higher induced multipole and correlation energies of \mathcal{E}_2 cut off in the intermediate range of R where \mathcal{E}_1 , which is again an exponentially decreasing function of R , becomes important. In this case, however, \mathcal{E}_1 and V for the members of this case are probably negative for all values of R .

In case (iii), the dominant term of V is the Coulomb attraction of the net charges of the ion and antiion which comes from \mathcal{E}_1 . For large R this gives

$$V = -Z'\bar{Z}'/R, \quad (2.12)$$

where Z' and $-\bar{Z}'$ are the net respective charges of the ion and anti-ion. For small R this term is given by Eq. (2.9). The V of Eqs. (2.12) and (2.9) differ because of screening by the electrons and positrons. The transition from one form of V to the other will occur for values of $R \lesssim a_0$. At these values of R other parts of \mathcal{E}_1 as well, as the other \mathcal{E}_n , will be important to V . However, for all values of R it is probable that V is negative. For $R > a_0$, V is roughly the negative of V for the corresponding atom-atom pair.

III. ATOM-ANTIATOM REARRANGMENT COLLISIONS

In this section we present a qualitative discussion of atom-antiatom low-energy rearrangement collisions based on the Born-Oppenheimer approximation. The concept of a critical radius for the collision is introduced and two approximate methods for calculating the cross sections for rearrangement collisions are presented.

In any atom-antiatom collision the possibility exists that the particles will undergo a rearrangement in which the nucleus and antinucleus become bound and some or all of the electrons and positrons are emitted. Because of the large available binding energy of the nucleus-antinucleus system, there is always a rearranged state with a total energy equal to that of the initial state. Therefore, there is no lower-energy threshold for atom-antiatom rearrangement. However, when the collision energy, which resides principally in the nucleus and antinucleus, exceeds the change in binding energy of the electrons and positrons during rearrangement, kinetic energy must be carried away by the emitted electrons and positrons. It is unlikely that any more than a small fraction of the collision energy can be transferred to the kinetic energy of the emitted electrons and positrons. The probability of rearrangement is therefore very low at collision energies in excess of the total binding energy of the electrons and posi-

trons.

At collision energies below the lesser of the excitation energies of the atom and antiatom the only inelastic process allowed is that in which the nucleus and antinucleus become bound. We will take "low energy" to mean such energies, and we will give principal consideration here to atom-antiatom collisions at low energy. Steigman²⁰ and Omidvar²¹ have discussed higher-energy collisions.

For low collision energies the velocities of the bound electrons within the atom and bound positrons within the antiatom are much greater than the atom-antiatom relative velocity prior to and during most of the rearrangement. Under this circumstance, according to the Born-Oppenheimer approximation,²² the wave function and energy of the electrons and positrons are very accurately described by the solution to the Schrödinger equation obtained by holding the nucleus and antinucleus fixed, which gives the interatomic potential energy V (Sec. II). The atom as a whole and the antiatom as a whole move under the influence of V . In treating an atom-antiatom collision we will first give consideration to the wave function and energy of the electrons and positrons in the Born-Oppenheimer approximation. In this approximation we take the initial state to be the state in which all electrons and positrons are bound in the ground state in the field of the fixed nucleus and antinucleus. We take the rearranged state to be a state in which one or more of the electrons and positrons (which may be in the form of one or more ground-state positronium atoms) are at infinity with zero kinetic energy and the remaining electrons and positrons are in the ground state in the field of the fixed nucleus and antinucleus. We do not consider excited levels of either state. In cases in which sufficiently low-lying excited levels exist it is expected that the resultant state mixing will not usually have a substantial effect on our results.

In the initial state, for a sufficiently small value of the nucleus-antinucleus distance R , the proximity of the oppositely charged nucleus and antinucleus will reduce the effective charge by which the electrons and positrons are bound, to the extent that at least one electron or positron will become unbound. This value of R is called the critical radius R_c which in most cases will have a value on the order of a_0 . If the exact total-energy curves for the initial state and rearranged state are plotted as functions of R they will join at $R = R_c$.²³ For $R > R_c$ the energy curve of the rearranged state will lie above that of the initial state by an amount equal to the binding energy of the emitted particles (minus the binding energy of positronium, if an electron and positron have been emitted as positronium). For $R < R_c$ the curves will be identical since they describe the same state. The splitting

of one state into two as R increases through R_c occurs because the number of bound states available to the electrons and positrons increases as R increases. In an actual case in which the curves are obtained by an accurate approximate calculation, they will cross or join in the vicinity of R_c . In some cases in which there are either no electrons or no positrons it is possible in principle for all of the electrons or positrons to remain bound for all values of R . In such cases no R_c exists, and we will not consider them further.

In all but the simplest cases that involve only one electron or one positron, more than one R_c will exist. For instance, in the interaction of a neutral helium atom with a singly ionized antihelium atom, there will be one R_c for the unbinding of one electron, a second for the unbinding of one electron and a positronium atom, and a third for the unbinding of the two electrons and the positron as free particles.

The preceding description of the wave function and energy of the electrons and positrons is made under the assumption that the Born-Oppenheimer approximation is valid for all values of R . This approximation is, however, invalid for $R \simeq R_c$ when applied to the motion of the electrons or positrons that become unbound at $R = R_c$. As R approaches R_c from above, the mean velocity of these electrons or positrons approaches zero in the Born-Oppenheimer approximation. Hence, when R approaches R_c there will be a point when their velocities become roughly equal to the atom-antiatom relative velocity. At this point the Born-Oppenheimer approximation breaks down and a direct coupling develops between the motion of the nuclei and the motion of the electrons and positrons that are to become unbound. This coupling will lead to a transferral of kinetic energy to the electrons or positrons of an amount that is roughly equal to the kinetic energy of the nuclear motion times the ratio of the electron or positron mass to the nuclear mass. This transferred kinetic energy is also roughly equal to the portion of the kinetic energy of the atom-antiatom motion that is associated with the electrons or positrons. For $R \simeq R_c$ the Born-Oppenheimer approximation is valid for the motion of any electrons or positrons that remain bound.

The motion of the atom as a whole and antiatom as a whole in the Born-Oppenheimer approximation can be taken with good approximation as the classical orbit in the interatomic potential energy. This approximation is valid in the initial stage of the collision for $R > R_c$. For a sufficiently small impact parameter, R will become less than R_c and a small fraction of the atom-antiatom kinetic energy is transferred to the electrons or positrons that become unbound. However, the effect on the atom-antiatom motion is negligible. After R has

passed through its minimum value it will approach R_c from below, and the system will with high probability remain on the rearranged potential-energy curve.

The high probability for rearrangement occurring when R has been less than R_c can be made plausible in the following way. The correlation in motion between the unbound electrons or positrons and the nucleus and antinucleus is destroyed by the breakdown in the Born-Oppenheimer approximation when $R \simeq R_c$. In addition, the energy transferred to the electrons or positrons is such that their wave function extends throughout a volume of space which is large compared to that occupied by the nucleus and antinucleus. Hence once R has become less than R_c it is highly probable that the final state is one in which rearrangement has occurred.

A semiclassical method can be used to calculate the cross section for rearrangement.²³ The quantum-mechanical atom-antiatom interatomic potential energy is determined in the fixed nucleus or Born-Oppenheimer approximation. The atom-antiatom motion in this potential is treated classically and the turning point R_0 of the orbit is determined as a function of the impact parameter R_1 . If R_0 is less than R_c , the rearrangement will be assumed to occur.

For an interatomic potential energy V (V will be spherically symmetric for the cases we consider), R_0 is a function of R_1 and the collision energy E . The quantity E is the total kinetic energy in the center-of-mass frame of reference of the atom and antiatom treated as single particles. The quantity R_0 is determined by equating the initial collision energy and angular momentum to the energy and angular momentum at a turning point R_i , where the motion has no radial velocity. The resulting equation for the R_i is

$$[V(R_i) - E]R_i^2 = -ER_1^2, \quad (3.1)$$

where $V(R_i)$ is the value of the interatomic potential energy at R_i . There will be one or more roots of Eq. (3.1), depending on E and V . The value of R_0 is then the maximum R_i ,

$$R_0 = (R_i)_{\max}. \quad (3.2)$$

As R_1 is decreased R_0 decreases. In some cases R_0 is a discontinuous function of R_1 for fixed E . The value of R_1 at which R_0 becomes equal to R_c or suddenly drops below R_c , is designated R_{1c} . Rearrangement will occur only for $R_0 < R_c$ and the rearrangement cross section σ will be

$$\sigma = \pi R_{1c}^2. \quad (3.3)$$

In Sec. V the semiclassical method is applied to hydrogen-antihydrogen rearrangement scattering and in Sec. VI to antimuonium-argon rearrangement scattering.

If the semiclassical method is not applicable because the atom-antiatom motion is not classical, then an optical-potential method may be employed. In this method the atom-antiatom scattering is treated as two-particle scattering in the presence of a potential energy, which is the interatomic potential energy V plus a negative imaginary potential energy V_I . The quantity V_I results in absorption of the incoming wave, which corresponds to rearrangement. V_I is taken to be 0 for $R > R_c$, and its magnitude and form for $R < R_c$ are chosen to maximize the absorption cross section. This choice of V_I corresponds to the conclusion of the semiclassical discussion that rearrangement occurs only for $R < R_c$ and then with near unity probability. In the optical-potential method the rearrangement cross section is equal to the absorption cross section. In addition this method may be used to determine the scattering phase shifts. This method is used in Sec. VI to treat antihydrogen-argon scattering.

IV. HYDROGEN-ANTIHYDROGEN INTERATOMIC POTENTIAL ENERGY

A. Long Range

At long range ($R \geq 10a_0$) the perturbation potential energy v [Eq. (2.3)] is, on the average, quite small so it is convenient to use the perturbation expansion, Eqs. (2.7) and (2.8), to find the hydrogen (H) -antihydrogen (\bar{H}) interatomic potential energy V . We take both atoms to be in the ground state. We use the two-center multipole expansion²⁴ for v which is valid for $r_1 + r_2 < R$ (Fig. 1):

$$v = -\frac{e^2}{R} \sum_{\alpha=1}^{\infty} \sum_{\beta=1}^{\infty} \frac{r_1^{\alpha} r_2^{\beta}}{R^{\alpha+\beta}} \sum_{m=-\min(\alpha,\beta)}^{m=\min(\alpha,\beta)} \frac{(\alpha+\beta)!}{(\alpha+|m|)! (\beta+|m|)!} \times P_{\alpha}^{1|m|}(\cos\theta_1) P_{\beta}^{1|m|}(\cos\theta_2) \cos[m(\phi_1 + \phi_2)], \quad (4.1)$$

where the P 's are the associated Legendre polynomials and \min denotes the lesser of α and β . After the sum over m has been carried out for each combination of values of α and β , the $\alpha=1$, $\beta=1$ term is the dipole-dipole term of v , the $\alpha=1$, $\beta=2$ term is the dipole-quadrupole term of v , etc.

The first-order perturbation energy \mathcal{E}_1 is zero

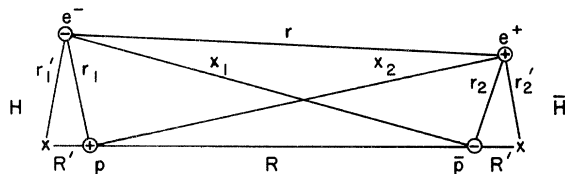


FIG. 1. Coordinates used in the definitions of the H- \bar{H} variational wave functions Ψ_{α} , Ψ_{β} , and Ψ_{γ} . The points x are the centers of the wave function Ψ_{γ} .

when evaluated by substituting Eq. (4.1) for v in Eqs. (2.6) and (2.8) due to the angular integrations. This is consistent with the discussion in Sec. II, indicating that \mathcal{E}_1 is negligible at long range for this case.

The second-order perturbation energy \mathcal{E}_2 for H-H has been evaluated²⁵ using Eq. (4.1) with the sign changed. The value of \mathcal{E}_2 for H- \bar{H} is equal to that of H-H, hence,

$$\mathcal{E}_2 = -6.50/R^6 - 124.4/R^8 - 3286/R^{10} - \dots \quad (4.2)$$

The R^{-6} term is the (dipole-dipole) \times (dipole-dipole) contribution, the R^{-8} term is the (dipole-quadrupole) \times (dipole-quadrupole) contribution, and the R^{-10} term is the sum of the (dipole-octupole) \times (dipole-octupole) and (quadrupole-quadrupole) \times (quadrupole-quadrupole) contributions.

The third-order perturbation energy \mathcal{E}_3 has a lowest-order term contribution of R^{-11} which comes from the (dipole-dipole) \times (dipole-dipole) \times (quadrupole-quadrupole) and (dipole-dipole) \times (dipole-quadrupole) \times (quadrupole-dipole) contributions associated with the first term of \mathcal{E}_3 in Eqs. (2.8). The second term of \mathcal{E}_3 is zero when Eq. (4.1) is used for v . The R^{-11} term of \mathcal{E}_3 for any two hydrogenlike atoms was calculated by Morgan²⁶ using a closure-expansion method. The result is in agreement with a more accurate variation-perturbation calculation of the same quantity by Chan and Dalgarno.²⁷

A brief description of the closure-expansion method as applied to the R^{-11} term of \mathcal{E}_3 follows. The first term of \mathcal{E}_3 [Eqs. (2.8)] can be written as

$$\mathcal{E}_3 = \sum_{m=0}^2 \sum_{n=0}^2 E_{3mn} + \sum_{m=0}^3 R_m, \quad (4.3)$$

in which

$$E_{3mn} = E_0^{-2} \sum_{\substack{k \neq 0 \\ l \neq 0}} \left(\frac{E_k}{E_0} \right)^m \left(\frac{E_l}{E_0} \right)^n A_{0k} A_{kl} A_{l0}, \quad (4.3a)$$

$$R_m = 2E_0^{-4} \sum_{\substack{k \neq 0 \\ l \neq 0}} \frac{E_k^3}{(E_0 - E_k)} \left(\frac{E_l}{E_0} \right)^m A_{0k} A_{kl} A_{l0} \quad \text{for } m \neq 3, \quad (4.3b)$$

$$R_3 = E_0^{-6} \sum_{\substack{k \neq 0 \\ l \neq 0}} \frac{E_k^3 E_l^3}{(E_0 - E_k)(E_0 - E_l)} A_{0k} A_{kl} A_{l0}. \quad (4.3c)$$

Closure may be used to calculate each of the E_{3mn} . The indices m and n in E_{3mn} are restricted to be no greater than 2, since otherwise divergences result. To calculate the E_{3mn} using closure we use Eq. (2.4) and write

$$E_k^m E_l^n A_{kl} = \int E_k^m \psi_k^* v E_l^n \psi_l d\tau = \int (H_0^m \psi_k^*) v H_0^n \psi_l d\tau. \quad (4.4)$$

The closure relation

$$\sum_{k \neq 0} \psi_k(\vec{r}) \psi_k^*(\vec{r}') = \delta(\vec{r} - \vec{r}') - \psi_0^*(\vec{r}') \psi_0(\vec{r}) \quad (4.5)$$

is then used to perform the two summations in each of the E_{3mn} . Using the Hermitian properties of H_0^n and neglecting terms that have A_{00} as a factor, we obtain

$$E_{3mn} = E_0^{-(2+m+n)} \int v(H_0^n v \psi_0) (H_0^n v \psi_0) d\tau. \quad (4.6)$$

The values of the R^{-11} terms of the E_{3mn} are found by substituting the various relevant terms in the multipole expansion for v , Eq. (4.1), into Eq. (4.6) and performing the integrations. These values are first used to obtain knowledge of the dependence of the matrix-element product $A_{0k} A_{kl} A_{l0}$ on E_k and E_l when $A_{0k} A_{kl} A_{l0}$ is considered as a function of these variables. This knowledge allows the values of the R_m to be placed within fairly definite limits.²⁶ With the values of the E_{3mn} and the allowed ranges of the R_m , Eq. (4.3) gives

$$\mathcal{E}_3 = -(3700 \pm 17\%)R^{-11} + O(R^{-13}). \quad (4.7)$$

From the result of Chan and Dalgarno²⁷ we find

$$\mathcal{E}_3 = -3986R^{-11} + O(R^{-13}), \quad (4.8)$$

which falls within the range of error given in Eq. (4.7). The quantity \mathcal{E}_3 is small compared to \mathcal{E}_2 at long range. The long-range interatomic potential energy of H- \bar{H} may therefore be taken to be \mathcal{E}_2 of Eq. (4.2). The principal significance of \mathcal{E}_3 is that it leads to a difference in the H- \bar{H} and H-H long-range nonrelativistic interatomic potential energies. From Eq. (4.8) this difference is

$$V_{H-H} - V_{H-\bar{H}} = 7972R^{-11} + O(R^{-13}). \quad (4.9)$$

B. Short and Intermediate Range

For values of $R \lesssim 10a_0$ the multipole expansion Eq. (4.1) becomes inaccurate and also use of the perturbation expansion for V [Eq. (2.7)] is questionable. Hence we use a variational method to determine V .

Four variational wave functions were used [Fig. 1 and Eq. (2.6)]:

$$\Psi_\alpha = \psi_0 = \pi^{-1} e^{-r_1 - r_2}, \quad (4.10)$$

$$\Psi_\beta = e^{-a(r_1 + r_2)} - b r, \quad (4.11)$$

$$\Psi_\gamma = e^{-a'(r_1 + r_2')}, \quad (4.12)$$

$$\Psi_\delta = \psi_0 + \sum_{k \neq 0} \frac{A_{0k} \psi_k}{\mathcal{E} - E_k}. \quad (4.13)$$

The first variational wave function Ψ_α is the unperturbed wave function; Ψ_β and Ψ_γ are two-parameter variational wave functions; Ψ_δ is the wave function through first order in v in the Lennard-Jones-Brillouin-Wigner perturbation expansion.¹⁵ Each wave function is used in the variational expression for the energy,

$$\mathcal{E} = \int \Psi H \Psi d\tau / \int \Psi^2 d\tau. \quad (4.14)$$

For Ψ_β and Ψ_γ , \mathcal{E} is minimized with respect to variations of their parameters. From Eq. (2.5), the interatomic potential energy V is given by

$$V = \mathcal{E} - E_0 = \mathcal{E} + 1. \quad (4.15)$$

For Ψ_α , Ψ_β , and Ψ_γ , Eq. (4.14) is evaluated exactly resulting in an upper bound to \mathcal{E} and hence V . For Ψ_δ the closure approximation is used in the evaluation of Eq. (4.14) and an approximate upper bound to V is obtained.

The results for V for the different trial wave functions are shown in Fig. 2. Also shown in Fig. 2 are the interatomic potential energies for the rearranged states. Curve I shows $V + \frac{3}{4}$ for the state in which e^- and e^+ are in the ground state of positronium with zero kinetic energy, and curve II shows $V + 1$ for the state in which e^- and e^+ are free particles with zero kinetic energy. The critical radii R_{cI} and R_{cII} , as defined in Sec. III, are the values of R at which curves I and II cross the curves for V and are given in Table I.

The wave function Ψ_β of Eq. (4.11) is exact in the limits $R = \infty$ ($a = 1$, $b = 0$) and $R = 0$ ($a = 0$, $b = \frac{1}{2}$) corresponding to free positronium. The integrals in Eq. (4.14) for Ψ_β can all be evaluated analytically. The values of a and b that minimize \mathcal{E} show little tendency to approach their $R = 0$ values as R decreases, and indeed the minimum of \mathcal{E} disappears for $R < 1.2a_0$. The negative values of b in Fig. 3 show a tendency of the electron and positron to be farther apart on the average than in the unperturbed state.

The wave function Ψ_γ through the parameter R' allows the centers of the electron and positron charge distributions to be shifted by the same amount away from the opposite nucleus. The integrals in Eq. (4.14) are easily determined. For small R' , Ψ_γ approximates a generalization of the wave function that Wightman found²³ gave a good approximation to the energy of the π^- -H system. Figure 4 shows the values of the variational parameters a' , R' as functions of R .

The trial functions Ψ_α , Ψ_β , and Ψ_γ are not capable of giving the negative long-range van der Waals energy of H- \bar{H} and indeed give positive val-

TABLE I. Values of the critical radii R_{cI} and R_{cII} for the trial wave functions Ψ_α , Ψ_β , Ψ_γ , and Ψ_δ .

Wave function	R_{cI}	R_{cII}
Ψ_α	$1.31a_0$	$0.83a_0$
Ψ_β	$1.28a_0$	undefined
Ψ_γ	$1.21a_0$	$0.62a_0$
Ψ_δ	$0.5a_0$	$0.2a_0$

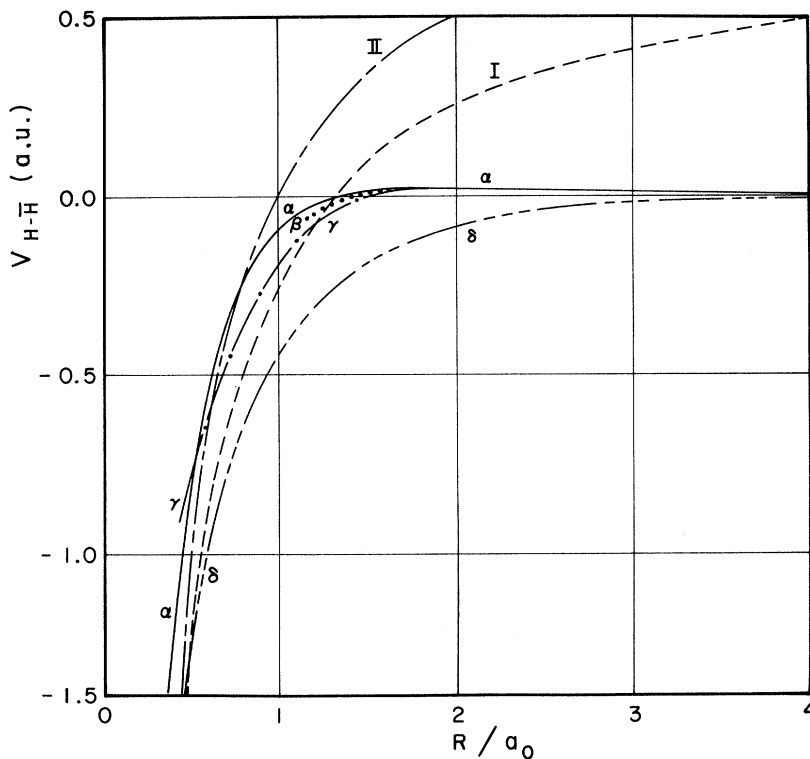


FIG. 2. H-H̄ interatomic potential energy V as a function of nucleus-antinucleus separation R in units of a_0 . Curves α , β , γ , and δ are approximations to V in the initial state. Curve I is $V + \frac{3}{4}$ for the rearranged state when the e^+ and e^- are emitted as an atom of ground-state positronium with zero kinetic energy. Curve II is $V + 1$ in the rearranged state when the e^+ and e^- are emitted as free particles with zero kinetic energy.

ues of V for $R \geq 1.6a_0$ (Fig. 2). These variational wave functions do not include the correlation in the positions of the electron and positron that lead to the van der Waals energy.

The wave function Ψ_6 [Eq. (4.13)] is the wave function for H-H̄ in the Lennard-Jones-Brillouin-Wigner perturbation expansion taken through first order in v and includes correlation. When it is used in Eq. (4.14), \mathcal{E} is the Lennard-Jones-Brillouin-Wigner expansion for the energy carried through third order in v . The result for V is

$$V = A_{00} + \sum_{k \neq 0} \frac{A_{0k} A_{k0}}{V - 1 - E_k} + \sum_{\substack{k \neq 0 \\ l \neq 0}} \frac{A_{0k} A_{kl} A_{l0}}{(V - 1 - E_k)(V - 1 - E_l)}, \quad (4.16)$$

where the A_{kl} are given by Eq. (2.6). Note that in Eq. (4.16), V appears in the denominators of the sums as a result of the form of Ψ_6 . In practice this usually requires that V be obtained by an iterative solution. To avoid the difficulty in calculating and using A_{kl} we drop the third term on the right-hand side and make a closure approximation for the second term. We write

$$\sum_{k \neq 0} \frac{A_{0k} A_{k0}}{V - 1 - E_k} = \frac{1}{V - 1} \sum_{k \neq 0} A_{0k} A_{k0} + \frac{1}{V - 1} \sum_{k \neq 0} \frac{E_k A_{0k} A_{k0}}{V - 1 - E_k} \equiv E_{20} + E'_2. \quad (4.17)$$

We drop the term E'_2 and apply the closure relation, Eq. (4.5), to obtain

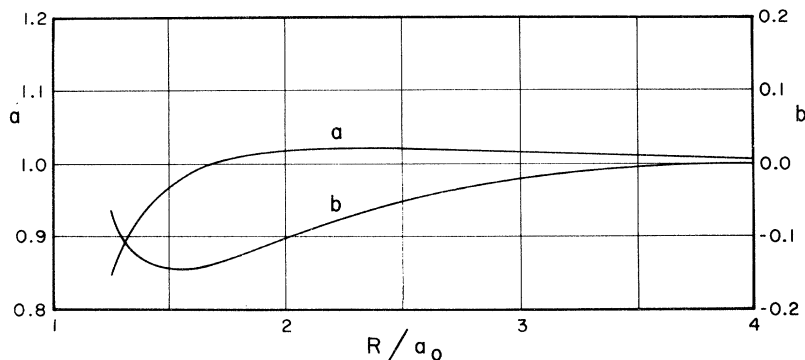


FIG. 3. Values of the variational parameters a and b of Ψ_6 as functions of R in units of a_0 .

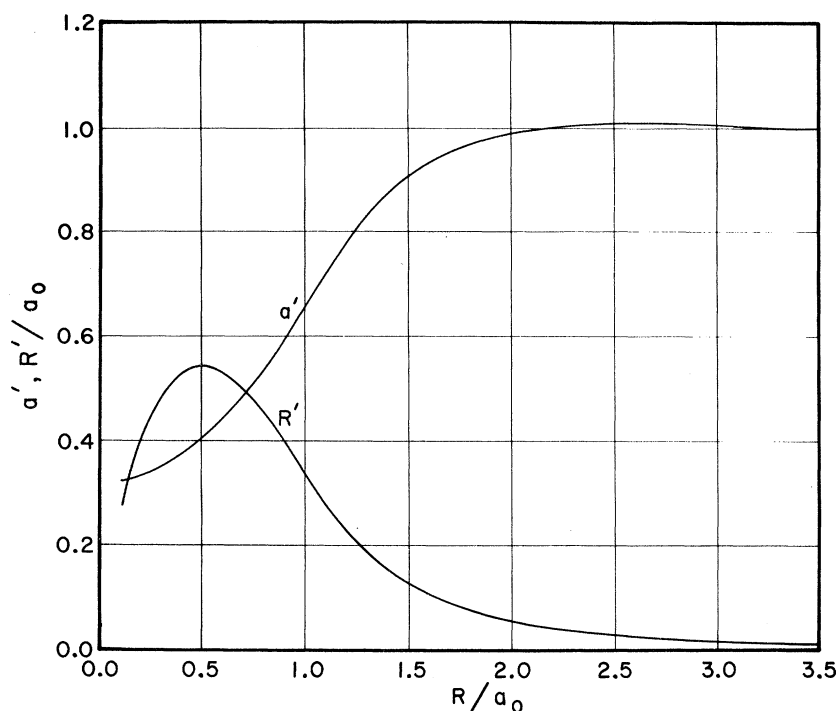


FIG. 4. Values of the variational parameters a' and R' of Ψ_γ as functions of R in units of a_0 .

$$E_{20} = \frac{1}{V-1} \left(\int \psi_0^2 v^2 d\tau - A_{00}^2 \right), \quad (4.18)$$

where

$$v = 1/x_1 + 1/x_2 - 1/r - 1/R \quad (4.19)$$

and

$$A_{00} = (1/R)e^{-2R} \left(-1 - \frac{5}{3}R + \frac{3}{4}R^2 + \frac{1}{8}R^3 \right). \quad (4.20)$$

Using Eqs. (4.16)–(4.18), we obtain a quadratic equation for V whose solution is

$$V = \frac{1}{2}(A_{00} + 1) - \frac{1}{2} \left[(A_{00} - 1)^2 + 4 \left(\int \psi_0^2 v^2 d\tau - A_{00}^2 \right) \right]^{1/2}. \quad (4.21)$$

The integration can be done analytically. Divergent integrals are obtained if closure is used for the third term of Eq. (4.16) or for E'_2 in Eq. (4.17). The solution for V obtained from Eq. (4.21) is shown as curve δ in Fig. 2, and given in Table II.

Estimates of the values of the terms neglected in Eq. (4.16) to obtain Eq. (4.21) can be made as follows. At long range the third term of Eq. (4.16) is given by Eq. (4.7) which is small compared to V from Eq. (4.21) for $R > 3a_0$. An estimate of E'_2 at long range can be made by comparing the asymptotic expansion of the left-hand side of Eq. (4.17), given by Eq. (4.2), with the asymptotic expansion of E_{20} obtained from Eq. (4.21) as

$$V = E_{20} = -6R^{-6} - 135R^{-8} - 3937.5R^{-10} - \dots \quad (4.22)$$

These two expansions determine $E'_2 = -0.5R^{-6} + \dots$,

which equals about 8% of V from Eq. (4.2).

To ascertain better the effect of the neglect of E'_2 we have calculated V for H-H neglecting exchange

TABLE II. Values of the interatomic potential energy V for H-H in atomic units as a function of nucleus-anti-nucleus separation R . In column δ are the values of V obtained by the use of Ψ_0 and closure. In column J-B are the values obtained by Junker and Bardsley by the use of a 75-term variational wave function (Ref. 29).

R	δ	V	J-B
$0.1a_0$	-8.807		
$0.2a_0$	-3.970		
$0.5a_0$	-1.266		
$0.8a_0$	-0.643		
$0.975a_0$			-0.277 201
$1.0a_0$	-0.442		-0.257 076
$1.2a_0$	-0.312		
$1.5a_0$	-0.1894		-0.055 216
$2.0a_0$	-0.0843		-0.010 219
$2.4a_0$	-0.0446		
$2.5a_0$			-0.001 244
$3.0a_0$	-0.017 57		-0.000 040
$3.05a_0$			-0.000 033
$3.10a_0$			-0.000 031
$3.15a_0$			-0.000 039
$3.4a_0$	-0.009 67		
$3.5a_0$			-0.000 165
$4.0a_0$	-0.004 10		-0.000 301
$5.0a_0$	-0.001 077		-0.000 208
$6.0a_0$	-0.000 315		-0.000 154
$8.0a_0$	-0.000 038 7		
$10.0a_0$	-0.000 007 96		-0.000 008

using Eq. (4.21) with the appropriate v for H-H:

$$v = -1/x_1 - 1/x_2 + 1/r + 1/R. \quad (4.23)$$

Curve 2 of Fig. 5 shows the result. Curve 1 of Fig. 5 shows accurately calculated values of V .²⁸ At $R = 3a_0$, curve 2 lies above curve 1 by an amount that is somewhat in excess of the exchange contribution to the energy of H-H as given by Heitler-London theory. Hence the neglect of E'_2 is justified for H-H for $R > 3a_0$. We conclude that use of Eq. (4.21) gives a reasonably accurate value of V for \bar{H} -H for $R > 3a_0$.

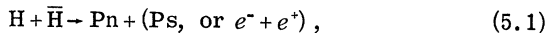
For $R \lesssim 0.5a_0$ the dominant term in v of Eq. (4.19) is $-1/R$. Hence V is obtained from Eq. (4.21) to a good approximation.

C. Summary of Results

Tables II and III and Fig. 6 summarize our results for V for \bar{H} -H for the different ranges of R . Also Table II and curve J-B of Fig. 6 give results of a recent calculation by Junker and Bardsley²⁹ based on the use of a 75-term variational wave function. Our curves α , β , and γ and the J-B curve are derived variationally and provide upper bounds to V . Our curve δ is an upper bound if E'_2 in Eq. (4.17) and the third term in Eq. (4.16) can be neglected; we have argued that the curve δ is indeed an upper bound for $R > 3a_0$.

V. \bar{H} -H AND \bar{p} -H SCATTERING

Using the interatomic potential energy V obtained from Sec. IV, we apply the semiclassical method discussed in Sec. III to calculate the total cross section for the rearrangement collision:



where Pn denotes a protonium atom (bound p , \bar{p}) and Ps is a positronium atom.

Using V as specified in Table IV we determine the turning point R_0 of the classical orbit as a

TABLE III. Results for interatomic potential energy V of H-H as a function of internuclear distance R .

R	$V_{\bar{H}-\bar{H}}$
$R \geq 10a_0$	Equation (4.2)
$10a_0 \geq R > 3a_0$	Equation (4.21)
$3a_0 \gtrsim R \gtrsim 0.5a_0$	Uncertain
$0.5a_0 > R$	Equation (4.21)

function of the impact parameter R_1 and collision energy E by solving Eqs. (3.1) and (3.2). A graphical solution is illustrated in Fig. 7. The functions $-ER^2$ and $(V-E)R^2$ are plotted vs R for a low-energy collision. If a horizontal line is drawn that intersects the upper curve at $R = R_1$, then the largest value of R at which this line intersects the lower curve is R_0 . R_0 is a discontinuous function of R_1 due to the maximum in the $(V-E)R^2$ curve at $R = R_m$. The value of R_1 that gives $R_0 = R_m$ is R_{1c} since $R_0 < R_c$ for $R_1 < R_{1c}$, as applied to either final state in Eq. (5.1). In our calculation R_m is determined numerically for each E and then R_{1c} is obtained.

The total rearrangement cross section σ including both final states in Eq. (5.1) is given by Eq. (3.3) and is shown as curve 1 in Fig. 8 and tabulated in Table V. Also shown as curve 2 in Fig. 8 are the results of Junker and Bardsley²⁹ for the cross section. Curve 1 is valid for E between 3×10^{-5} (10^{-3} eV) and 3×10^{-2} (1 eV). For $E \lesssim 3 \times 10^{-5}$ the classical-orbit approximation is not valid, and for $E \gtrsim 3 \times 10^{-2}$, values of V for $R < 3a_0$ (where a_0 is the Bohr radius) are required but in this region V is uncertain. An accurate power-law fit to the solid portion of curve 1 is given by

$$\sigma = 5.0E^{-0.32}\pi a_0^2. \quad (5.2)$$

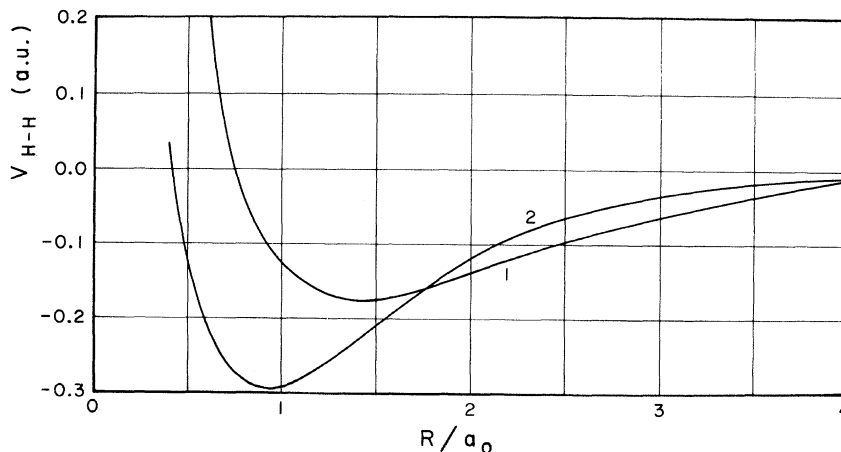


FIG. 5. H-H interatomic potential energy V as a function of R in units of a_0 . Curve 1 is an accurate form of V from the work of Kolos and Roothaan (Ref. 28) Curve 2 is an approximation to V using a wave function similar to Ψ_6 and closure.

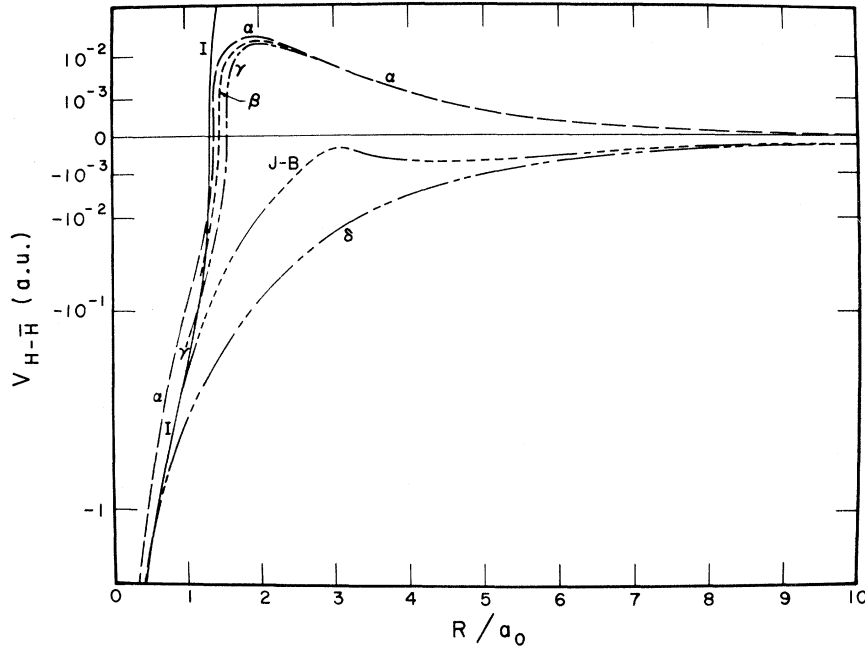


FIG. 6. $H-\bar{H}$ interatomic potential energy as a function of nucleus-antinucleus separation R in units of a_0 . Curves α , β , γ , δ , I, and II are defined as in Fig. 2; curve J-B is the result of the use of a 75-term wavefunction by Junker and Bardsley (Ref. 29). A cube-root scale has been used along the vertical axis to illustrate the peak in curve J-B at $3.1a_0$ and to allow all curves to be shown.

The relative probability for formation of the two final states in Eq. (5.1) is difficult to determine. The relative probability for Ps formation is made greater by the fact that $R_{cI} > R_{cII}$, but it is made less by the greater phase-space restriction imposed on Ps formation.

The elastic-scattering cross section for $\bar{H}+H$ at low energy is approximately equal to σ since several angular-momentum waves are involved in the collision which is highly absorptive.

The semiclassical method can be applied to calculate the rearrangement cross section for

$$\bar{p}+H \rightarrow Pn+e^- . \quad (5.3)$$

The $\bar{p}-H$ (or $p-\bar{H}$) interatomic potential energy V can be determined for different ranges of R as follows:

(i) For $R \leq a_0$ we use the V determined by Wightman²³ for the π^-H system.

(ii) For $a_0 \leq R \leq 4.5a_0$ we use Bates's calculation³⁰ of the electron binding energy of $\bar{p}-H$.

(iii) For $4.5a_0 \leq R \leq 20a_0$ we use a form for V that joins smoothly with V in regions (ii) and (iv).

(iv) For $R \geq 20a_0$ we use the long-range monopole-induced dipole energy^{18,19} given by

$$V = -2.251R^{-4} . \quad (5.4)$$

The resulting V is shown as curve I in Fig. 9 and is given in Table VI. The critical radius R_c is equal to $0.639a_0$.²³

The semiclassical method is applied in the same manner as for $H-\bar{H}$ and the resulting cross section is shown as curve I of Fig. 10 and in Table VII. The cross section is valid for 3×10^{-7} (10^{-5} eV) $\lesssim E$

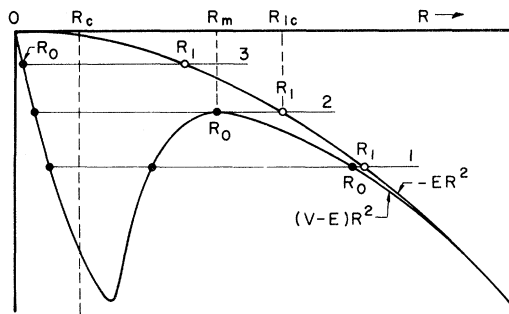


FIG. 7. Illustration of the solution of Eqs. (3.1) and (3.2) and a determination of R_{1c} for an interatomic potential energy similar to that found for $H-\bar{H}$ by the use of Ψ_0 and closure.

TABLE IV. Detailed form used for the interatomic potential energy V for the calculation of the $H-\bar{H}$ rearrangement cross section for various ranges of nucleus-antinucleus separation R .

R	V
$R \geq 11a_0$	Equation (4.2)
$11a_0 \geq R \geq 9a_0$	Smooth interpolation of above and below forms
$9a_0 \geq R \geq 3a_0$	Equation (4.21)
$3a_0 \geq R \geq 0.5a_0$	Any smooth interpolation of above and below forms
$0.5a_0 \geq R$	Equation (4.21)

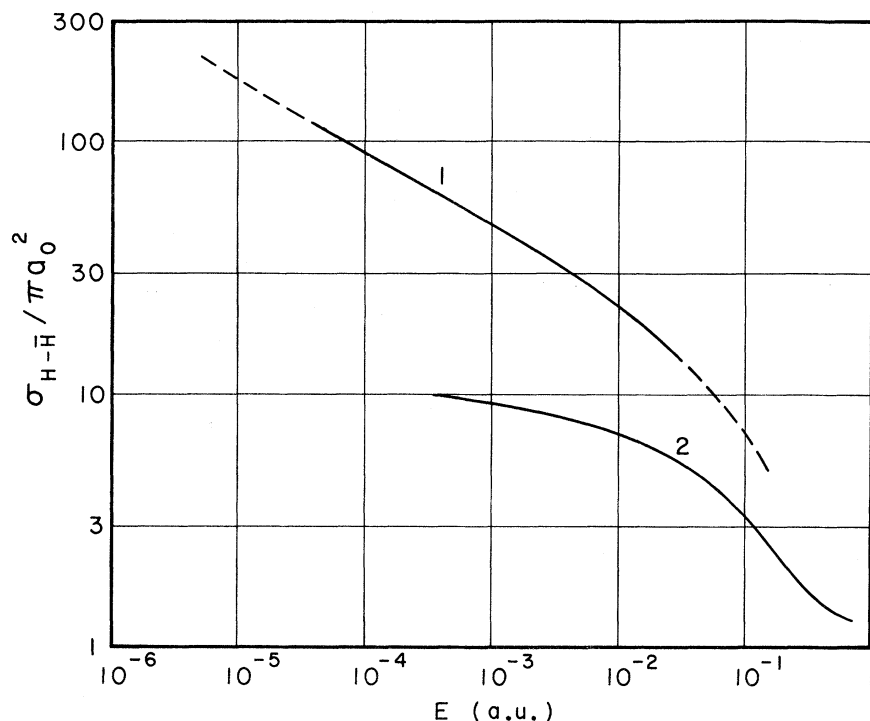


FIG. 8. $H-\bar{H}$ rearrangement cross section in units of πa_0^2 as a function of collision energy in atomic units, obtained by the semiclassical method. Curve 1 shows the results obtained in the text; curve 2 shows the results of Junker and Bardsley (Ref. 29).

$\approx 3 \times 10^{-2}$ (1 eV). For lower energies the classical orbits are not valid and for higher energies the method we use has limited accuracy.

In view of the difference in the $H-\bar{H}$ rearrangement cross section determined here from Ψ_6 and that of $J-B^{29}$ and of the astrophysical importance of

this cross section,⁶ it would be valuable to have further calculations of $V_{H-\bar{H}}$ and a more fully quantum-mechanical calculation of the rearrangement collision.

VI. ANTIMUONIUM-ARGON SCATTERING

The scattering of an atom of antimuonium (\bar{M} , bound μ^+ , e^-) by an atom of argon (Ar) is important to the possible conversion of muonium (\bar{M} , bound μ^+ , e^-) to antimuonium as it may occur in argon gas.³¹ The rearrangement cross section and the elastic scattering cross section for \bar{M} -Ar are important to the probability of this conversion.^{26,32}

The \bar{M} -Ar interatomic potential energy is equal to that of \bar{H} -Ar. Because of the complexity of the

TABLE V. The hydrogen-antihydrogen rearrangement cross section σ , determined from V as given in Table IV, in units of πa_0^2 as a function of collision energy E in atomic units.

E	σ
5.00×10^{-6}	216
8.00×10^{-6}	186
1.25×10^{-5}	162
2.00×10^{-5}	140
3.15×10^{-5}	123
5.00×10^{-5}	107
8.00×10^{-5}	94
1.25×10^{-4}	83
2.00×10^{-4}	73
3.15×10^{-4}	65
5.00×10^{-4}	57
8.00×10^{-4}	50
1.25×10^{-3}	44
2.00×10^{-3}	38
3.15×10^{-3}	33
5.00×10^{-3}	28.6
8.00×10^{-3}	24.2
1.25×10^{-2}	20.4
2.00×10^{-2}	16.8
3.15×10^{-2}	13.7

TABLE VI. Interatomic potential energy V for \bar{p} -H in atomic units as a function of internuclear separation R . The sources of the values are given in the text.

R	V
$0.1a_0$	-9.50
$0.2a_0$	-4.50
$0.4a_0$	-2.00
$0.7a_0$	-0.929
$1.0a_0$	-0.510
$2.0a_0$	-0.087
$4.0a_0$	-0.0091
$7.0a_0$	-0.00136
$10.0a_0$	-0.000310
$20.0a_0$	-0.0000141

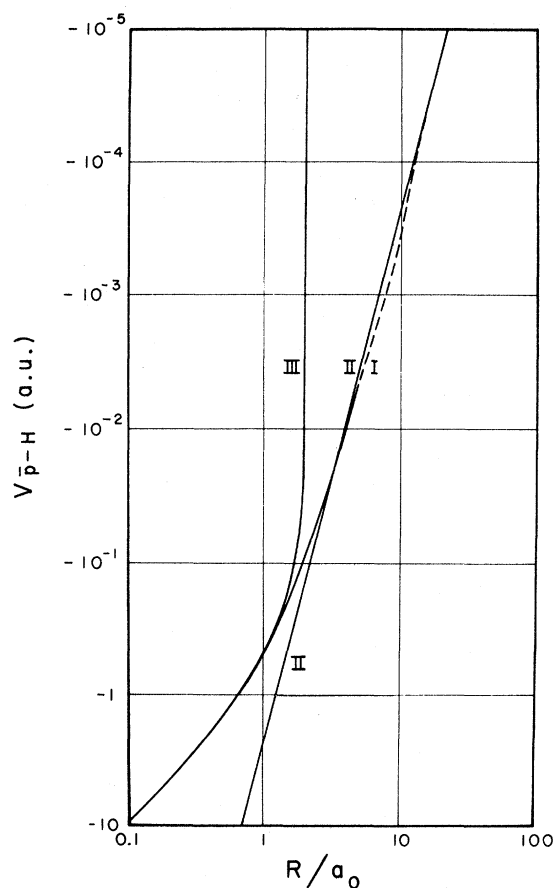


FIG. 9. Interatomic potential energy of \bar{p} -H in atomic units as a function of nucleus-antinucleus separation R in units of a_0 . Curve I is a plot of V as given in Table V; curve II is a plot of Eq. (5.4); curve III is $V + \frac{1}{2}$ for the rearranged state of Eq. (5.3).

argon atom, there is no simple method that will allow a direct and reasonably accurate determination of the \bar{M} -Ar interatomic potential energy V . We have employed a variety of methods that are applicable for different values of R , and have combined them to give a single analytic formula as a reasonable estimate for V ²⁶:

$$V = \mathcal{E}_1 + \mathcal{E}_2, \quad (6.1)$$

$$\mathcal{E}_1 = - (8/R)e^{-KR} + A\mathcal{E}_2, \quad (6.1a)$$

where

$$\begin{aligned} \mathcal{E}_2 = & - (1 - e^{-(K_8 R)^8}) C_8 R^{-8} \\ & - (1 - e^{-(K_8 R)^8}) C_8 R^{-8} \\ & - (1 - e^{-(K_{10} R)^{10}}) C_{10} R^{-10}, \end{aligned} \quad (6.1b)$$

$$\begin{aligned} A = & [-0.21 - 0.068(R - R_0) \\ & + 0.0122(6.35 - R)^2] e^{-(R/8.3)^{22}}, \end{aligned} \quad (6.1c)$$

and

$$K = 2.6, \quad K_8 = 0.530, \quad K_{10} = 0.305,$$

$$\begin{aligned} K_{10} &= 0.200, \quad C_8 = 20.2, \quad C_8 = 485, \\ C_{10} &= 39\,000. \end{aligned} \quad (6.1d)$$

Equation (6.1) expresses V as being roughly the sum of the first-order energy \mathcal{E}_1 and the second-order energy \mathcal{E}_2 .

The first term on the right-hand side of Eq. (6.1a) is an approximation to \mathcal{E}_1 for $R \lesssim a_0$ and is the potential energy between the μ^- and the Ar core of the nucleus plus the ten inner electrons screened by the outer eight electrons. The second term is an approximation to \mathcal{E}_1 for $R \gtrsim 2a_0$. The quantity A for \bar{M} -Ar can be computed for $R > 6a_0$ by using the Hartree-Hartree wave function³³ for Ar to determine \mathcal{E}_1 and using Eq. (6.1b) for \mathcal{E}_2 , and it is given in Eq. (6.1c). The quantity A for H- \bar{H} can be determined from the results of Sec. IV. It is observed that $A_{\bar{M}\text{-Ar}}/A_{\text{H-}\bar{H}}$ is independent of R for $R > 6a_0$. Hence we assume that Eq. (6.1c) can be applied for all R .

Equation (6.1b) gives \mathcal{E}_2 as a sum of the R^{-6} , R^{-8} , and R^{-10} long-range contributions to \mathcal{E}_2 , and each term is multiplied by an appropriate cutoff factor to improve the accuracy for small values of R . The values of C_8 , C_8 , and C_{10} are equal to the corresponding quantities for H-Ar. C_8 has been accurately calculated,¹⁶ and we have determined C_8 and C_{10} from the known polarizabilities of H and Ar and a harmonic-oscillator-model equation for the C' 's.¹⁷ The oscillator energies are chosen to fit the values of C_8 for H-H, H-Ar, and Ar-Ar.¹⁶ The value of C_{10} has been increased to take into account the R^{-12} and higher terms of \mathcal{E}_2 . The parameters K_8 , K_8 , and K_{10} are determined by comparison with H- \bar{H} and from the properties of a Poincaré-type asymptotic expansion.³⁴

We estimate the uncertainty in $V_{\bar{M}\text{-Ar}}$ of Eq. (6.1) to be about $\pm 10\%$ for $R \gtrsim 10a_0$, and to increase to a factor of 2 for $a_0 \lesssim R \lesssim 3a_0$.²⁸ A fit to Eq. (6.1) which is correct to within about 20% for $5a_0 < R < 15a_0$ is given by

TABLE VII. Antiproton-hydrogen rearrangement cross section σ in units of πa_0^2 as a function of collision energy E in atomic units.

E	σ
10^{-6}	4240
3×10^{-6}	1700
10^{-5}	930
3×10^{-5}	555
10^{-4}	315
3×10^{-4}	200
10^{-3}	115
3×10^{-3}	60.0
10^{-2}	29.5
3×10^{-2}	15.0

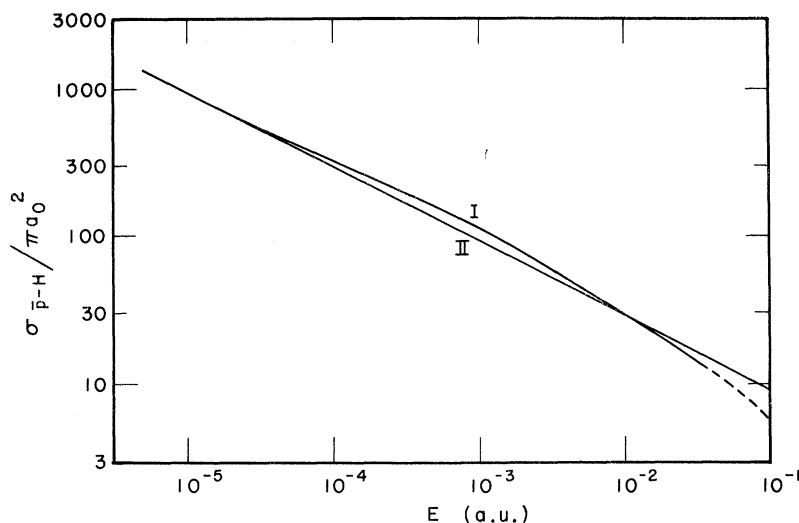
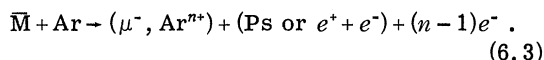


FIG. 10. \bar{p} -H rearrangement cross section σ as a function of collision energy E determined by the semiclassical method. For curve I the V of Table V is used. For curve II the V of Eq. (5.4) and σ of Eq. (7.4) are used.

$$V = -240R^{-6.91}. \quad (6.2)$$

The semiclassical method can be used to determine the total cross section for the rearrangement collision:



We estimate that the critical radii for the final states for $n=1$ or 2 in Eq. (6.3) lie between $0.5a_0$ and $1.5a_0$. These critical radii are greater than the turning points of classical \bar{M} -Ar orbits for low collision energies. Using the method of solution of Sec. V and Eq. (6.2) for V with the above estimates of uncertainty, we find

$$\sigma_{\bar{M}-\text{Ar}} = 55\pi a_0^2 (293 \text{ K}/T)^{0.289} \pm 20\%, \quad (6.4)$$

in which T is the temperature. Equation (6.4) is not valid for $T < 1$ K where the classical-orbit approximation is not applicable, and for $T > 2000$ K where $R_m < 5a_0$. Within most of the range $1 \text{ K} < T < 2000 \text{ K}$ several angular-momentum waves are involved in Eq. (6.3), and the elastic scattering cross section will be roughly equal to $\sigma_{\bar{M}-\text{Ar}}$.

We have employed the optical-model method discussed in Sec. III to calculate $\sigma_{\bar{M}-\text{Ar}}$ for a collision energy of 1.86×10^{-3} (mean collision energy of \bar{M} and Ar at $T=293 \text{ K}$). The real part of V is given by Eq. (6.1) and the imaginary part, V_I , was chosen in accordance with the prescriptions of Sec. III. It was found that there is a large range of depths and forms of V_I which lead to a nearly constant and maximum $\sigma_{\bar{M}-\text{Ar}}$. We find

$$\sigma_{\bar{M}-\text{Ar}} = 56.5\pi a_0^2 \pm 5\% \quad (6.5)$$

and

$$\sigma_{\text{elastic}} = 48\pi a_0^2 \pm 10\%, \quad (6.6)$$

in good agreement with the results of the semi-

classical method for $T=293 \text{ K}$. The uncertainties result from the uncertainties in V and R_c .

It should be noted that when V was reduced in magnitude by more than a factor of 2 around $R \approx 2a_0$ or increased in magnitude by more than a factor of 3 around $R \approx 2a_0$, $\sigma_{\bar{M}-\text{Ar}}$ was considerably reduced.

VII. REARRANGEMENT CROSS SECTIONS IN OTHER LOW-ENERGY ATOM-ANTIATOM COLLISIONS

General approximate formulas for the atom-antiatom rearrangement cross section at low energies may be derived for two cases using the semiclassical method. The first case involves atoms and antiatoms for which the interatomic potential energy V is negative and proportional to $R^{-\mu}$, where $\mu > 2$, for large R . The second case applies when the atom and antiatom are both ionized.

In the first case R_0 is a discontinuous function of R_1 , and there is the additional requirement that V be sufficiently negative for small R to ensure that $R_0 < R_c$ for $R_1 < R_{1c}$, where R_{1c} is determined from R_m according to the procedure used in Sec. V. Then the rearrangement cross section depends principally on V for large R ($R \gtrsim 5a_0$). We take

$$V = -CR^{-\mu}. \quad (7.1)$$

Using the semiclassical method as applied in Sec. V, we obtain

$$R_m = ((\mu - 2)C/2E)^{1/\mu} \quad (7.2)$$

and

$$\sigma = \mu(\mu - 2)^{(2/\mu)-1} (C/2E)^{2/\mu} \pi a_0^2, \quad (7.3)$$

which is valid when R_m lies in a region where Eq. (7.1) gives V approximately. Equation (7.3) can be applied to atom-antiatom collisions in which one member is neutral and the other ionized. Taking

$\mu = 4$ and $C = \frac{1}{2}\alpha$, where α is the polarizability of the neutral member, we obtain

$$\sigma = (2\alpha/E)^{1/2} \pi a_0^2. \quad (7.4)$$

For \bar{p} -H ($\alpha = 4.502$), Eq. (7.4) gives curve II of Fig. 10, which is a good approximation to the accurate values of σ given by curve I.

In the second case we take

$$V = -Z\bar{Z}/R \quad (7.5)$$

for all $R \geq R_c$. The quantities Z and \bar{Z} are the magnitudes of the charges on the ion and anti-ion. We apply the semiclassical method by determining as R_{1c} the value of R_1 which gives $R_0 = R_c$. Hence, we find

$$\sigma = (1 + Z\bar{Z}/R_c E) \pi R_c^2. \quad (7.6)$$

For singly ionized species, $Z = \bar{Z} = 1$ and, in general, $R_c \approx 0.5 a_0$.

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