

## Hydrogen-antihydrogen interactions

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Accurate quantum-mechanical calculations on the system hydrogen-antihydrogen ( $H\bar{H}$ ) are presented. The energy is calculated using the Ritz variational principle, and is obtained as a function of the proton-antiproton distance in the Born-Oppenheimer approximation. It is everywhere lower and therefore more accurate than that recently calculated by Junker and Bardsley. In particular, the maximum in the interatomic interaction reported by these authors is not seen in this calculation. The cross section for rearrangement annihilation is calculated and found to be uniformly larger than that reported by Junker and Bardsley.

### I. INTRODUCTION

Submicroscopic interactions between matter and antimatter have recently attracted some attention<sup>1,2</sup> because of the implications such interactions might have for various cosmological theories as well as speculations about antimatter meteorites and ball lightning.<sup>3</sup> An ambitious quantum-mechanical calculation on the simplest atom-antiatom pair (namely, hydrogen-antihydrogen,  $H\bar{H}$ ) recently reported by Junker and Bardsley<sup>1</sup> was extremely interesting because these authors found a small maximum in the interatomic interaction energy at a certain proton-antiproton distance, and they speculated that such a maximum would be found for all atom-antiatom pairs.

Junker and Bardsley calculated a very extensive configuration-interaction (CI) wave function (75 configurations) over a range of interbaryonic distances using the variational principle, the Born-Oppenheimer approximation, and the spinless non-relativistic Hamiltonian<sup>4</sup>

$$H(1; 2) = -\frac{1}{2}\nabla_1^2 - \frac{1}{2}\nabla_2^2 - \frac{1}{r_{a1}} - \frac{1}{r_{b2}} + \frac{1}{r_{a2}} + \frac{1}{r_{b1}} - \frac{1}{r_{12}} - \frac{1}{r_{ab}}. \quad (1)$$

Here, 1 denotes the electron, 2 the positron,  $a$  the proton, and  $b$  the antiproton.

In view of the need to represent accurately the correlation of the motions of electrons with positrons in energy calculations on mixed electron-

positron systems<sup>5</sup> and the well-known inability of CI wave functions to give a good account of purely electronic correlation,<sup>6</sup> we undertook a new calculation on  $H\bar{H}$  with a wave function which depends explicitly on the interleptonic distance  $r_{12}$ . CI wave functions do not depend explicitly on such coordinates and hence reproduce the correct behavior at short interleptonic distances (i.e., cusps) only in the limit of infinite expansions in a configuration basis. Suitably accurate cusps depend upon very large expansions, and in practice high accuracy in the cusps is almost always beyond reach because of realities of available computational resources. This limitation of the CI method does not disqualify it as a means of calculating accurate energies and other properties for koinoatoms and molecules, because the interleptonic cusps occur where the wave function is small and relatively unimportant. But in systems containing both electrons and positrons, cusps at electron-positron coalescence occur where the wave function is large; hence the CI method is inappropriate.<sup>5b</sup> For systems with many leptons and only one antilepton, the important interleptonic correlation effects can be accounted for satisfactorily using well-understood techniques.<sup>5a</sup> But for systems containing many leptons and many antileptons, accurate calculations are much more difficult.

### II. $H\bar{H}$ CALCULATION

The Hamiltonian commutes with the operators  $C_\phi$  and  $Q = \sigma_h P_{12}$ , where  $C_\phi$  rotates the leptons

through an angle  $\phi$  about the interbaryonic axis,  $\sigma_h$  reflects the leptonic coordinates in a plane which is the perpendicular bisector of the interbaryonic axis, and  $P_{12}$  exchanges leptons. Hence the wave function is either even or odd under  $Q$ , and has a rotational symmetry indicated by  $\Sigma$ ,  $\Pi$ ,  $\Delta$ , . . . . Assuming the ground state is even (thus allowing a nonzero wave function where the electron and positron coalesce) and  $\Sigma$ , and suppressing all spin coordinates (which are inconsequential here), we expand the wave function in a basis

$$\Psi = \sum_i c_i \Psi_i(1; 2), \quad (2)$$

where  $\Psi_i(1; 2)$  is the symmetry-adapted function,

$$\begin{aligned} \Psi_i = & (1/4\pi) [\exp(-\alpha_1 \xi_1 - \alpha_2 \xi_2 + \beta_1 \eta_1 + \beta_2 \eta_2) \xi_1^{r_i} \xi_2^{\bar{r}_i} \eta_1^{s_i} \eta_2^{\bar{s}_i} \rho^{\mu_i} \\ & + (-1)^{s_i + \bar{s}_i} \exp(-\alpha_2 \xi_1 - \alpha_1 \xi_2 - \beta_2 \eta_1 - \beta_1 \eta_2) \\ & \times \xi_1^{\bar{r}_i} \xi_2^{r_i} \eta_1^{\bar{s}_i} \eta_2^{s_i} \rho^{\mu_i}]. \end{aligned} \quad (3)$$

In the above,  $\xi$  and  $\eta$  denote the elliptic coordinates,<sup>7</sup>  $\rho = 2r_{12}/r_{ab}$ , and  $r_i$ ,  $\bar{r}_i$ ,  $s_i$ ,  $\bar{s}_i$ , and  $\mu_i$  are integers. The coefficients  $c_i$  and exponents  $\alpha_k$ ,  $\beta_k$  ( $k=1, 2$ ) are variational parameters.

The matrix elements and integrals needed to solve the eigenvalue problem,

$$(\underline{H} - E\underline{S})\underline{c} = 0, \quad (4)$$

are computed using a method described previously.<sup>7</sup> All matrix elements as well as the energy  $E$  and eigenvector  $\underline{c}$  are functions of  $r_{ab}$ . The computations were carried out on an IBM 360/91 computer at the Max Planck Institute for Physics and Astrophysics in Munich.

To select the most important terms in the expansion

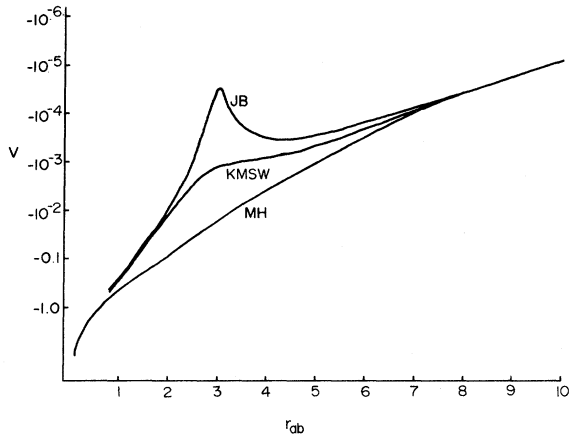


FIG. 1. Interatomic potential  $V$  from Ref. 1 (curve JB), Ref. 2 (curve MH), and the present work (curve KMSW) as a function of the interbaryonic distance  $r_{ab}$ .  $V$  is related to  $E$ , the total energy of the system  $\text{H}\bar{\text{H}}$ , by  $V = E + 1$ .

sion (2) the exponents were first optimized in an 18-term expansion for  $r_{ab} = 1, 3.1, \text{ and } 6$  a.u., and for these internuclear distances test runs were made using the basis functions (3) with  $r_i$ ,  $\bar{r}_i$ ,  $s_i$ ,  $\bar{s}_i \leq 5$ , and  $\mu_i \leq 2$ . Next, a 35-term wave function was constructed which included terms that were the most important ones for all three internuclear distances. In this wave function the exponents were optimized for  $r_{ab} = 0.95, 1, 3, \text{ and } 6$  a.u. Since the exponents were approximately linear functions of the internuclear distance, for intermediate separations their values were obtained by linear interpolation. For  $r_{ab} > 6$  they were also interpolated assuming for  $r_{ab} = 12$  the asymptotic values  $\alpha_1 = \alpha_2 = \beta_1 = -\beta_2 = 6$ . In the case of  $\beta_2$ , two additional optimizations were made for  $r_{ab} = 5$  and 8 a.u. In the final runs, the 35-term expansion was augmented with 42 additional basis functions, different for different regions of  $r_{ab}$ : One set of 42 additional functions was used for  $r_{ab} \geq 3$  a.u., and another for  $r_{ab} < 3$  a.u. A total of 77 basis functions were thus used for all interbaryonic distances except  $r_{ab} = 10$ , where the final run was made with a 50-term expansion due to an almost linear dependence of some of the basis functions.

The accuracy of the energy, being very high for large  $r_{ab}$ , deteriorates with decreasing interbaryonic distance. In the vicinity of  $r_{ab} = 3$  the total energy has probably converged to six significant figures. At smaller  $r_{ab}$  not more than four figures in the total energy are likely to be reliable.

### III. RESULTS

The energy  $E$  is given in terms of the interatomic potential  $V = E + 1$  in Fig. 1. The curve labeled KMSW is the present results, which are to

TABLE I. Interatomic interaction energy  $V^a$  of  $\text{H}\bar{\text{H}}$ .

$r_{ab}$	$V_{\text{JB}}$ (Ref. 2)	$V_{\text{KMSW}}$ (present work)
0.95		-0.314 522
0.975	-0.277 201	
1.0	-0.257 076	-0.271 095
1.5	-0.055 216	-0.060 540
2.0	-0.010 219	-0.013 221
2.5	-0.001 244	-0.003 149
3.0	-0.000 040	-0.001 280
3.05	-0.000 033	
3.1	-0.000 031	-0.001 173
3.15	-0.000 039	
3.5	-0.000 165	-0.000 967
4.0	-0.000 301	-0.000 817
5.0	-0.000 280	-0.000 463
6.0	-0.000 154	-0.000 208
8.0	-0.000 037	-0.000 037
10.0	-0.000 008	-0.000 008

<sup>a</sup>  $V = E + 1$ , where  $E$  is the total energy of  $\text{H}\bar{\text{H}}$ .

be compared with the results of Junker and Bardsley<sup>1</sup> (curve JB) and Morgan and Hughes<sup>2</sup> (curve MH). The latter potential was deduced from second-order perturbation theory and known limiting forms for large and small  $r_{ab}$ . Unlike  $V_{\text{KMSW}}$  and  $V_{\text{JB}}$ ,  $V_{\text{MH}}$  is not bounded by the true potential. The most salient feature of our results is the absence of a maximum. Table I lists our results for  $V$ .

The cross section for the rearrangement from  $\text{H}\bar{\text{H}}$  to protonium (Pn) and positronium (Ps), which is sensibly also the cross section for annihilation, was calculated using our interatomic potential curve and the classical method of Purcell and Field.<sup>8</sup> It is displayed in Fig. 2 along with the results of Morgan and Hughes, and the extended results of Junker and Bardsley (both groups used the method of Purcell and Field also). The present results are similar to those of Junker and Bardsley for collision energies larger than about 1 eV, and nearly coincide with the results of Morgan and Hughes at energies lower than 0.0086 eV. The present cross section, as well as that of Junker and Bardsley (extended by the present authors), is not a smooth function of the collision energy. This point is discussed in Sec. IV.

#### IV. DISCUSSION

The semiclassical method of calculation of the cross section involves the concept of a critical interbaryonic distance  $R_c$ : If the interbaryonic

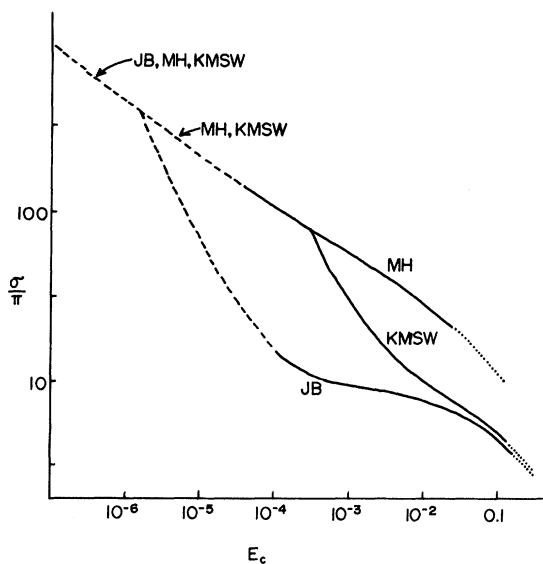


FIG. 2. Rearrangement/annihilation cross section  $\sigma$  as a function of  $E_c$ , the collision energy of H and  $\bar{\text{H}}$  in the center-of-mass system. The curves are from Ref. 1 (curve MH), Ref. 2 (curve JB), and the present results (curve KMSW).

distance  $r_{ab}$  falls below  $R_c$  during a collision, then the dipole is too weak to bind Ps and the rearrangement takes place. An accurate determination of  $R_c$  is therefore of some interest.

The electronic energy of the one-electron system  $\text{H}\bar{p}$  (hydrogen atom-antiproton) as a function of  $r_{ab}$  is shown as curve W on Fig. 3, after the work of Wightman.<sup>9,10</sup> Obviously the same curve results if the electron is replaced by a positron. A significant feature of the system shown by curve W is the small binding energy of the lepton as  $r_{ab}$  approaches the critical binding distance<sup>11,12</sup> from above. The arrow pointing up is at the critical binding distance. The approximations of the leptonic energy of  $\text{H}\bar{\text{H}}$ ,  $E + (1/r_{ab})$ , are also shown in Fig. 3 as curves JB,<sup>1</sup> MH,<sup>2</sup> and KMSW (present work). Clearly, one should not attempt to estimate  $R_c$  for  $\text{H}\bar{\text{H}}$  by extrapolation. Low-order perturbation theory is not of much help either; the energy of  $\text{H}\bar{p}$  correct to second order (with the electron-antiproton interaction taken to be the perturbation) gives 1.25 as the critical binding distance for  $\text{H}\bar{p}$ .<sup>13</sup>

Why did Junker and Bardsley get a maximum in  $V$ ? We should first note that their barrier is very small. The difference in the Junker-Bardsley interatomic potential  $V$  between its maximum at  $r_{ab} = 3.1$  a.u. and its minimum at  $r_{ab} \sim 4.4$  a.u. is only 0.0088 eV. Indeed, the barrier height is less than the width of the line in Fig. 4, which is a linear plot of  $E = V - 1$  versus  $r_{ab}$ . Junker and Bardsley's maximum is at the arrow pointing up

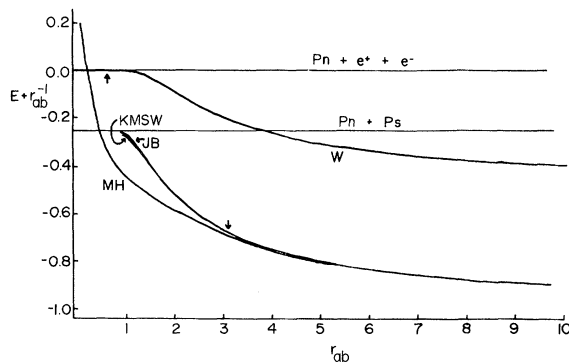


FIG. 3. Leptonic energy  $E + 1/r_{ab}$  for the systems  $\text{H}\bar{\text{H}}$  (curves MH, JB, and KMSW from Refs. 1 and 2 and the present work, respectively), and  $\text{H}\bar{p}$  (or  $\bar{\text{H}}p$ , curve W from Refs. 9 and 10) as a function of the interbaryonic distance  $r_{ab}$ . The arrow pointing down shows where Junker and Bardsley found a maximum in  $V = E + 1$ , and the arrow pointing up is at the critical binding interbaryonic distance for  $\text{H}\bar{p}$ . The horizontal lines show the energies of the two systems with the leptons unbound from the baryons and at rest at a large distance from them.

on the curve  $\overline{H\bar{H}}$ , and the minimum is at the arrow pointing down. Moreover, the leptonic binding energy (curve JB, Fig. 3) has no barrier at all because the curve is monotonic. Second, we note that the difference between Junker and Bardsley's interatomic interaction energy and our more accurate results at their maximum is not large either—0.031 eV. The energy calculated by Junker and Bardsley is distinguishable from ours in Fig. 3 only close to  $R_c$ , and not at all in Fig. 4. The difference between Junker and Bardsley's energy and ours is shown in Fig. 5.

Figure 5 suggests an answer to our question. Junker and Bardsley's results are accurate for large interbaryonic distances, where even a compact CI function would be quite accurate. But as  $r_{ab}$  gets smaller than 3.1, the error in their energy begins to grow rapidly. For large  $r_{ab}$  ( $\sim 10$ ) the system is two atoms interacting via weak long-range polarization forces, but for  $r_{ab}$  approaching  $R_c$  from above, the system becomes positronium weakly bound by a dipole; i.e., the interleptonic interaction becomes predominantly short-range correlation. Everywhere on the  $r_{ab}$  axis for  $r_{ab} \approx R_c$ , the wave function may be regarded as a mixture of these two "configurations,"  $\overline{H\bar{H}}$  and PnPs, and the contribution of the PnPs-like "configuration" changes from zero to one as  $r_{ab}$  decreases from infinity to  $R_c$ . It is easy to show that

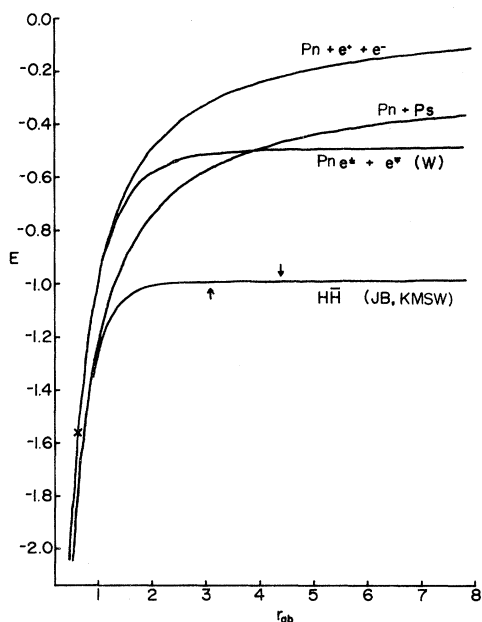


FIG. 4. Total energy  $E$  for the four systems  $\overline{H\bar{H}}$  (present work), Pn + Ps (i.e.,  $\overline{H\bar{H}}$  with the leptons free and at rest;  $E = 1/-r_{ab} - \frac{1}{4}$ ),  $\overline{H\bar{H}}$  (Refs. 9 and 10), Pn +  $e^+ + e^-$  ( $E = -1/-r_{ab}$ ).  $\times$  marks the critical binding interbaryonic distance for  $\overline{H\bar{H}}$ .

a trial wave function corresponding to noninteracting atoms, namely,  $e^{-r_{a1}}e^{-r_{b2}}$ , gives a very pronounced maximum in the interatomic interaction energy of about 0.02 a.u. at  $r_{ab} \approx 2$  a.u. Junker and Bardsley's wave function is simply not accurate enough to suppress this spurious maximum, presumably because of the inefficacy of the CI method in dealing with short-range correlation.

Another simple CI-type trial wave function,  $(1 + \alpha z_{a1} z_{b2})e^{-r_{a1}}e^{-r_{b2}}$ , contains the main part of the long-range polarization effect (the  $z$  axis coincides with the interbaryonic axis). It is found that the optimum value of the parameter  $\alpha$  passes through zero very close to the Junker-Bardsley maximum, which illustrates the inadvisability of using the CI method on systems for which short-range correlation is important. In order to represent the PnPs contribution to the wave function, one needs a basis function to reflect virtual positronium, namely,  $e^{-r_{12}/2}$ . Our wave function does this by virtue of having powers of  $r_{12}$  in the basis set. The variational principle presumably arranges these powers to approximate  $e^{-r_{12}/2}$ .

In the method of Purcell and Field for determining the cross section, one calculates, for a given collision energy  $E_c$ , the largest impact parameter  $R_1$  which generates an interbaryonic trajectory such that the classical turning point  $R_0$  is less than the critical distance  $R_c$ . The cross section is then  $\pi R_1^2$ . The method, which has been described in detail by Morgan and Hughes depends upon finding the value of  $r_{ab}$  (other than zero) which maximizes the function  $r_{ab}^2(V - E_c)$ . The method is very straightforward for moderate values of  $E_c$  because  $R_0$  varies discontinuously with the

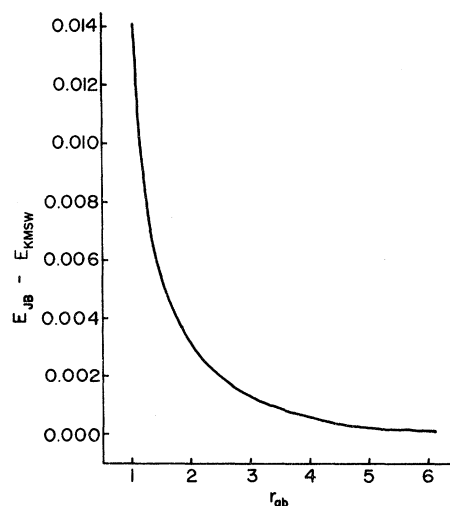


FIG. 5. Difference between the total energy obtained by Junker and Bardsley and that obtained in the present work.

impact parameter such that it jumps over a segment of interbaryonic distance which surely contains  $R_c$ . The value of the impact parameter where  $R_0$  has this fortuitous discontinuity may therefore unambiguously be taken to be the critical value  $R_1$ , and the cross section may be calculated without benefit of an accurate determination of  $R_c$ . However, as  $E_c$  increases, the "jump" taken by  $R_0$  decreases in size, and one begins to lose confidence that  $R_c$  lies on the jumped segment. Some uncertainty in the calculated value of the cross section results. In Fig. 2 the dotted portions of the Junker-Bardsley and present cross sections are in this high-energy region and should therefore be regarded as tentative until  $R_c$  can be accurately determined.

The dotted part of the Morgan-Hughes cross section represents a part of the curve for which

the potential presented by these authors is probably not very accurate, according to their estimate.<sup>2</sup>

The function  $\gamma_{ab}^2(V - E_c)$  may have more than one local maximum and the correct choice is the largest of these. The interatomic potentials of Junker and Bardsley and of the present authors give rise to two local maxima for certain ranges of collision energy, and the correct choice of these switches from one to the other as  $E_c$  varies. As a consequence, the cross sections are not a smooth function of  $E_c$ .

The dashed portions of the curves in Fig. 2 correspond to collision energies so low that no more than two partial waves would contribute significantly to a quantum-mechanical calculation of the baryonic scattering system; the classical theory used for the dashed portions is thus of questionable validity.

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