HYDROGEN–ANTIHYDROGEN INTERACTION POTENTIAL

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The peak which appeared in the H–$\bar{\text{H}}$ interaction potential calculated by Junker and Bardsley was proven by Kołos et al. to be a spurious maximum due to inefficacy of the standard molecular calculations in dealing with short-range effects. Using a different computational technique and a trial function much simpler than in the previous calculations we obtained H–$\bar{\text{H}}$ interaction energies in very good agreement with the results of Kołos et al.

1. Introduction. Ball lightning is one of the astrophysical observations which may support the idea of cosmic antimatter [1]. A theoretical explanation for this phenomenon could be the existence of a small positive barrier in the interaction potential between an atom and an anti-atom. Several papers investigated this possibility on the simplest systems of this type. The results obtained by Puget [2] for H–$\bar{\text{H}}$ were encouraging for the supporters of the antimatter origin of the ball lightning, as he found a positive barrier at the p–$\bar{\text{p}}$ interdistance $R = 1.8a_0$. Then Junker and Bardsley [3] showed that this barrier is actually below the dissociation energy of the system. To prove this they employed a trial function with up to 75 Slater atomic orbitals and standard elliptical orbitals, which are currently employed in molecular calculations. The explicit inclusion of the interleptonic distance r_{12} was made by Kołos et al. [4] and brought an expected improvement of the results at short interparticle distances. Like in all the other calculations they employed the Rayleigh–Ritz variational principle, with the Born–Oppenheimer approximation and obtained lower and therefore more accurate results than the previous papers. In the final runs they used 77 basis functions containing powers of r_{12} up to 2. With this computational effort the barrier disappeared and consequently it was interpreted as an effect of the theoretical inaccuracy in the low-R region. The calculation of Kołos et al. [4] showed the necessity of the explicit inclusion of the interleptonic distances in systems containing positrons, but in a way shaded its effectiveness by using such an elaborate trial wave function. The purpose of our paper is to show that even if one uses a much simpler Hylleraas-type trial function the effect of the r_{12} inclusion on the potential energy accuracy will be crucial.

2. Theory. Our approach is similar to that of refs. [2–4], that is the Ritz variational method with the Born–Oppenheimer approximation. We employ a trial function of the form

$$\psi = \sum_{i=1}^{n} c_i \exp(-\alpha r_{\mathrm{A}1} - \beta r_{\mathrm{B}2})\, \lambda_1^{p_i} \mu_1^{q_i} \lambda_2^{s_i} \mu_2^{t_i} r_{12}^{m_i} \tag{1}$$

with p_i, q_i, s_i, t_i, m_i nonnegative integers. The variational method leads to the well-known eigenvalue problem:

$$(\tilde{H} - E\tilde{S})\,\tilde{C} = 0, \tag{2}$$

where the matrix elements H_{ij} and S_{ij} are multiple integrals calculated with a procedure different from the one employed by Kołos et al. [4,5].

Let us now discuss in more detail our method. The trial wave function (1) has the correct asymptotic behaviour for $\alpha = \beta = 1$, when electron 1 is bounded to proton A and positron 2 is bounded to antiproton B. Using el-

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liptical coordinates, ψ can be rewritten,

$$\psi = \sum_{i=1}^{n} c_i \exp[-\alpha(\lambda_1 + \lambda_2) - \beta(\mu_1 - \mu_2)]\, \lambda_1^{p_i}\mu_1^{q_i}\lambda_2^{s_i}\mu_2^{t_i} r_{12}^{m_i}, \tag{3}$$

where the parameters α and β are now different from those which appear in the function (1). With the new nonlinear parameters the asymptotic behaviour is given by

$$\alpha = \beta = \tfrac{1}{2}R. \tag{4}$$

After applying the hamiltonian in elliptical coordinates on the trial function (3) we obtained the following matrix elements:

$$S_{ij} = 2\pi(\tfrac{1}{2}R)^6(\lambda_1^2 - \mu_1^2)(\lambda_2^2 - \mu_2^2)\exp[-2\alpha(\mu_1 - \mu_2)]\, \lambda_1^{p_i+p_j}\mu_1^{q_i+q_j}\lambda_2^{s_i+s_j}\mu_2^{t_i+t_j} r_{12}^{m_i+m_j},$$

$$H_{ij} = 2\pi(\tfrac{1}{2}R)^6(\lambda_1^2 - \mu_1^2)(\lambda_2^2 - \mu_2^2)\exp[-2\alpha(\mu_1 - \mu_2)]\, \lambda_1^{p_i+p_j}\mu_1^{q_i+q_j}\lambda_2^{s_i+s_j}\mu_2^{t_i+t_j} r_{12}^{m_i+m_j}\Bigg\{ r_{12}^{m_i+m_j}$$

$$\times\left[\frac{2}{R^2}\left(-\frac{1}{\lambda_1^2-\mu_1^2}[R_{\alpha p_i m_i}(\lambda_1) - R_{\beta q_i m_i}(\mu_1) - 2R\mu_1] - \frac{1}{\lambda_2^2-\mu_2^2}[R_{\alpha s_i m_i}(\lambda_2) - R_{-\beta t_i m_i}(\mu_2) + 2R\mu_2]\right) - \frac{1}{R}\right]$$

$$- r_{12}^{m_i+m_j-1} + r_{12}^{m_i+m_j-2} m_i\left[m_i + 1 + \frac{1}{2(\lambda_1^2-\mu_1^2)}(S_{\alpha p_i m_i} - S_{\beta q_i m_i}) + \frac{1}{2(\lambda_2^2-\mu_2^2)}(S_{\alpha s_i m_i} - S_{-\beta t_i m_i})\right]\Bigg\}, \tag{5}$$

where

$$R_{abc}(\xi) = (\xi^2 - 1)[a^2 - 2ab/\xi + b(b-1)/\xi^2] + (c+2)(b - a\xi),$$

$$S_{abc} = (b - a\lambda_1)(\lambda_1^2 - \lambda_2^2 - \mu_1^2 - \mu_2^2 + 2\mu_1\mu_2\lambda_2/\lambda_1).$$

The integration of the matrix elements (5) was carried out by employing a gaussian quadrature method shown explicitly by Goodisman [6]. Similar to the work of Kołos et al. [4], an initial search with a five-term trial function was made to determine the nonlinear parameters α and β. As we intended to use for less terms than Kołos et al., this search was made more carefully than in their case. We also noticed that the most important terms were those in which $p_i = s_i$ and $q_i = t_i$, as one would expect from the system symmetry. In the final runs we employed only those terms, with $p_i \leqslant 2$, $q_i \leqslant 2$ and $m_i \leqslant 1$.

The explicit inclusion of the interleptonic distance r_{12} produced nonpolynomial integrands and consequently an important search was made to determine the best set of gaussian points. The increase in the number of Gauss–Legendre and Gauss–Laguerre points, employed in the μ and λ integration respectively, had an opposite effect on the values of the interaction energy. Therefore the values of energy obtained with 9, 8, 10, 10 integration points on the $\lambda_1, \lambda_2, \mu_1, \mu_2$ coordinates were not too different from the values obtained with 4, 3, 8, 8 points; the differences were smaller than 10^{-6} au at large R, while for $R = 3\,a_0$ and $R = 1\,a_0$ they were 4×10^{-4} and 7×10^{-3} au, respectively. The final runs were performed with 9, 8, 10, 10 integration points and we expect the results to be reliable to 6 or 5 figures at $R = 3\,a_0$ and to about 4 figures at $R = 1\,a_0$.

3. Results and discussion. Fig. 1 shows the variation with R of the nonlinear parameters α and β, while the explicit values can be found in table 1. It appears from fig. 1 that after $R = 4\,a_0$ the system tends to shape itself in an asymptotic form, as the nonlinear parameters take values very close to their asymptotic behaviour (4). The oscillations in this range might indicate that the five-term trial function used in the initial search was not flexible enough.

In fig. 2 and table 1 the H–$\bar{\text{H}}$ interaction energy obtained for different values of R is compared with the re-

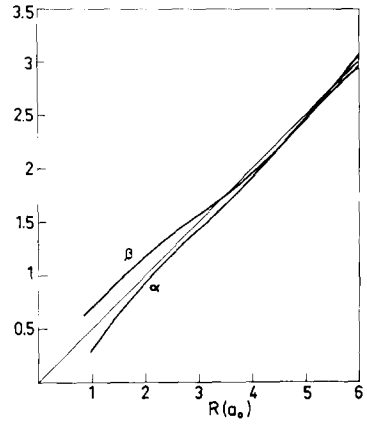

Fig. 1. Variation with the interbaryonic distance R of the nonlinear parameters employed in the present work.

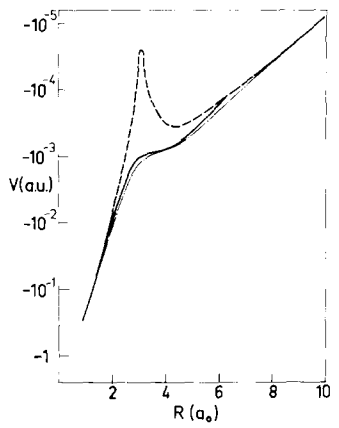

Fig. 2. Interatomic potential V of the H–$\bar{\text{H}}$ system: — present results; – – – results of Junker and Bardsley [3]; –.–.– results of Kołos et al. [4].

sults of Junker and Bardsley [3] and of Kołos et al. [4]. The most important point in this comparison is the obvious success of our calculation using only 14 terms in the Hylleraas-type trial function. Except for the energies obtained at $R = 5\,a_0$ and $R = 6\,a_0$, in error because of incorrect nonlinear parameters, the agreement with the extensive calculation of ref. [4] is quite impressive and shows the importance of the accurate nonlinear parameters.

The differences to the results of Kołos et al. [4] are shown more explicitly in fig. 3, together with the differences between the energies of ref. [3] and ref. [4]. Kołos et al. [4] attributed the differences between their results and those of Junker and Bardsley [3] to the inefficacy of the latter calculation in dealing with the short-range correlations. More exactly, it is the virtual positronium formation which has to be taken into account; the positronium wave function $\exp(-\frac{1}{2}r_{12})$ is included in the trial function of ref. [4] through powers of r_{12} up to $m_i = 2$. Our trial function contains powers of r_{12} only up to $m_i = 1$. The explicit inclusion of r_{12} in 7 of the 14 terms (see table 2) was sufficient to approximate $\exp(-\frac{1}{2}r_{12})$ in the vicinity of $R = 3\,a_0$ and consequently the spurious maximum disappeared. The use of a trial function containing only the first 8 terms of table 2, with 3 of them with $m_i = 1$, gave a pronounced maximum above the dissociation limit at $R = 3\,a_0$. Our results in the vicinity of $R = 1\,a_0$ are about 5% higher than the results of Kołos et al. [4] implying that our wave function is not flexible enough at very short range; however, judging from the efficiency of our method, we believe that the re-

Table 1
The variation with the interbaryonic distance R of the nonlinear parameters α and β and of the H–$\bar{\text{H}}$ interaction energy $V = E + 1$, E being the total energy of the system in atomic units.

R (a_0)	α	β	V_{CB} (present work)	V_{JB} [3]	V_{KMSW} [4]
1.0	0.320	0.700	−0.257521	−0.257076	−0.271095
2.0	0.920	1.170	−0.011152	−0.010219	−0.013221
3.0	1.430	1.565	−0.001113	−0.000040	−0.001280
3.05	1.450	1.580	−0.001042	−0.000033	–
3.1	1.470	1.600	−0.001008	−0.000031	−0.001173
3.5	1.650	1.750	−0.000910	−0.000165	−0.000967
4.0	1.920	1.970	−0.000801	−0.000301	−0.000817
5.0	2.470	2.460	−0.000428	−0.000280	−0.000463
6.0	2.970	3.070	−0.000183	−0.000154	−0.000208

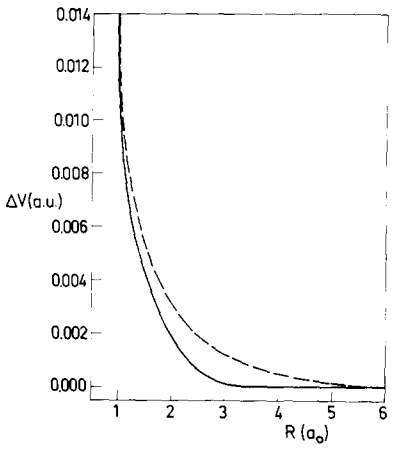

Fig. 3. Differences between H–$\bar{H}$ interatomic potentials calculated by various authors: —— V_{CB} (present work) – V_{KMSW} [4]; – – – V_{JB} [3] – V_{KMSW} [4].

Table 2
The set of powers $p_i = s_i, q_i = t_i, m_i$ employed in our 14-term Hylleraas-type trial function.

p_i	q_i	m_i	i	p_i	q_i	m_i	i	p_i	q_i	m_i	i
0	0	0	1	1	1	1	6	2	1	1	11
1	0	0	2	2	0	0	7	1	2	1	12
0	1	0	3	0	2	0	8	1	0	1	13
1	1	1	4	2	1	0	9	0	1	1	14
0	0	1	5	1	2	0	10				

sults of Kołos et al. can be reproduced for all the values of R with a relatively small number of terms in the trial function.

Variational studies on other atom–anti-atom systems were performed only by Junker and Bardsley [3,7] and did not show features different from those encountered in the H–$\bar{H}$ case.

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