Brief Reports

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Positron annihilation in positronium hydrides

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(Received 13 February 1986)

The two-photon annihilation rate for positronium hydride is calculated with the use of extensive Hylleraas-type wave functions in which all six interparticle coordinates are used. The binding energy against dissociation into a positronium atom and a hydrogen atom is improved upon the previous best value by about 3.8%. The two-photon annihilation rate, calculated with a wave function that gives a positron-electron cusp value of $-0.492a_0^{-1}$ (compared with the exact value of $-0.5a_0^{-1}$), is determined as 2.459 nsec^{-1}.

This work presents a theoretical study of positronium hydride, a system consisting of a positronium atom and a hydrogen atom. Ore[1] first showed that this system does form a bound system with a binding energy of about 0.1 eV. Over the years, there have been continuous theoretical studies[2–6] of this four-particle system, although it has yet to be observed experimentally. The best result[6] for the binding energy of PsH against dissociation into a positronium atom and a hydrogen atom is 1.0211 eV. Theoretical studies of the two-photon annihilation rate are also of interest. The most extensive calculation of the two-photon annihilation rate in the literature is by Page and Fraser.[5] The annihilation rate was not, however, calculated in Ref. 6. Other related problems that are of interest include scattering between positronium and hydrogen atoms.[7–9] Resonance states of PsH have also been studied theoretically. The resonance parameters for the lowest S-wave resonance state in Ps-H scattering have been studied by using the stabilization method[8] and a method of complex coordinates.[6,8] Higher resonance states of PsH were studied by Drachman[10] from the point of view that these are Rydberg states between a positively charged positron and a negatively charged H^- ion. The general properties of this system have been discussed in recent reviews.[11,12]

The present work is a continuation of the previous calculation.[6] The objective of this work is to provide a definitive nonrelativistic binding energy for PsH. Recently, there have been several theoretical methods to investigate possibilities of a positron binding to a many-electron atom (see Ref. 12 for example). To test the reliability of these methods, an accurate binding energy of PsH is needed to serve as a bench mark for these many-body calculations. This work presents such a calculation. Wave functions used in this work are of the Hylleraas type in which all six interparticle coordinates are included. Also, we calculate atomic properties for PsH such as two-photon annihilation rates, as well as various cusp values between different pairs of charged particles. These cusp values would give some measures of the qualities of the wave functions. In particular, the positron-electron cusp value would give some indication of the accuracy of the two-photon annihilation rates. For completeness, the average distances between different pairs of particles are also calculated.

The Hamiltonian for this system is

$$H=-\nabla_1^2-\nabla_2^2-\nabla_p^2-\frac{2}{r_1}-\frac{2}{r_2}+\frac{2}{r_p}-\frac{2}{r_{1p}}-\frac{2}{r_{2p}}+\frac{2}{r_{12}}\,, \tag{1}$$

where 1, 2, and p denote electrons 1, 2, and positron, respectively. The interparticle coordinate r_{1p} represents the distance between the electron 1 and the positron, and r_1 the electron 1 and the nucleus, etc. Atomic units are used in this work with energy expressed in rydbergs. A general form of wave function for positronium hydride is

$$\Psi=\sum_{\substack{i,j,k,\\ l,m,n}} C_{ijklmn}[r_1^i r_2^j r_p^k r_{2p}^l r_{1p}^m r_{12}^n e^{-\alpha r_1-\beta r_2-\gamma r_p}+(1\leftrightarrow 2)]\,, \tag{2}$$

where k, m, n, etc., are non-negative integers, with $\omega \le i+j+k+l+m+n$. In the previous investigation, the integer j is fixed at 0. Such a condition is also used here. However, in the present work, the integers l, m, and n can have nonzero values simultaneously. The reason is that we want the correlation effects between the two electrons and between the electron and positron to be taken into account as much as possible. The nonlinear parameters are optimized at $N=35$ terms. They are determined as $\alpha=0.65$, $\beta=1.00$, and $\gamma=0.59$. These values are the

TABLE I. Ground-state energies, cusp values, and two-photon positron annihilation rates for PsH calculated by using wave functions with different expansion lengths.

N[a]	E (Ry)	ν_{1p} (a_0^{-1})	ν_{12} (a_0^{-1})	ν_p (a_0^{-1})	ν_1 (a_0^{-1})	Γ (nsec^{-1})
126	−1.556 90	−0.488	0.0	1.026	−0.991	2.454
252	−1.577 40	−0.485	0.405	1.082	−1.008	2.435
312	−1.577 76	−0.483	0.502	1.066	−1.007	2.436
396	−1.577 89	−0.492	0.503	1.026	−1.010	2.459
Exact		−0.5	0.5	1.0	−1.0	

[a]See the text for details of wave functions.

same as those in Ref. 5. Results with extensive Hylleraas-type wave functions are shown in Table I. At first, we only include explicit correlation effects between electrons and positrons. The $N=126$-term wave function in Table I is constructed with $i+k+l+m \leq 5$, and $n=0$, i.e., no explicit electron-electron correlation terms are included in the wave functions. (We do have some correlation effects in the wave functions since the r_1 and r_2 factors are included.) Such effects are examined systematically as r_{12} factors when nonzero powers are added to the wave functions. For example, the $N=252$ terms are the sum of the 126 $n=0$ terms and 126 $n=1$ terms. One can see that with the r_{12} explicit correlation factors included, the binding energy improves significantly. The $N=312$ term wave function is the sum of the $N=252$ term wave function and 15 terms each for r_{12} factors with powers of 2, 3, 4, and 5 (a total of 60 terms). In other words, the 312 term wave function is the sum of 126 terms with $n=0$ and 186 terms of $n\neq 0$. The most extensive result occurs by using 396 terms. This wave function includes 210 terms with $n=0$ ($i+k+l+m \leq 6$), and the 186 terms of $n\neq 0$, as discussed above.

The final results for the ground-state energy of PsH calculated using the $N=396$ term wave function is $E=-1.577\,89$ Ry. This leads to a binding energy against dissociation into a positronium atom and a hydrogen atom of 0.077 89 Ry, or 1.0598 eV (1 Ry = 13.605 826 eV). The result represents an improvement over the previous calculation[6] by about 3.8%. It should be mentioned that the major difference between the present work and Ref. 6 is that we now include the previously omitted explicit product terms of r_{1p} and r_{2p}. In other words, we employ terms [see Eq. (2)] with nonzero integers of i, k, l, m, and n (we let $j=0$). As a result, the power factors of five interparticle coordinates are now explicitly included. Also, some effects of the sixth coordinate are taken into account in the exponential factors [α and β in Eq. (2) have nonzero values]. The inclusion of all the correlation effects between the four particles apparently enables us to improve the energy by a small but significant amount. It is further noted that since we use all six interparticle coordinates including products of r_{1p}, r_{2p}, and r_{12}, we can conclude that the results for the binding energy converge well.

One of the experimentally interesting parameters is the two-photon annihilation rate Γ, given in units of nsec^{-1}, which can be calculated by the following formula:[13]

$$\Gamma = 50.47n \frac{\langle \Psi \mid \delta r_{1p} \mid \Psi \rangle}{\langle \Psi \mid \Psi \rangle} , \tag{3}$$

where n is the number of electrons. ($n=2$ in the present work.) We also show results for annihilation rates in Table I. The result with the most extensive functions used in this work (the $N=396$ term function) indicates that the two-photon annihilation rate is of 2.459 nsec^{-1}. A comparison with previous calculations is shown in Table II.

To test the qualities of the wave functions, we have calculated the electron-electron and electron-positron cusp values. For a system interacting through Coulomb forces, the average value of the cusp condition between particles i and j is given by[14,15]

$$\nu_{ij} = \frac{\left\langle \Psi \left| \delta(r_{ij}) \frac{\partial}{\partial r_{ij}} \right| \Psi \right\rangle}{\langle \Psi \mid \delta(r_{ij}) \mid \Psi \rangle} , \tag{4}$$

and the exact value for ν_{ij} is

$$\nu_{ij} = Z_i Z_j \mu_{ij} , \tag{5}$$

TABLE II. Comparison with previous calculations for binding energies, positron-electron cusp values, and two-photon annihilation rates.

Binding energy (Ry)	ν_{1p} (a_0^{-1})	Γ (nsec^{-1})	Reference
0.0494	−0.477	2.459	4
0.0584	−0.440	2.22	3
0.073 58	−0.455	2.327	5
0.075 05			6
0.077 89	−0.492	2.459	Present work

TABLE III. Average distances between various pairs of charged particles (units in a_0).

$\langle r_1 \rangle$	$\langle r_p \rangle$	$\langle r_{1p} \rangle$	$\langle r_{12} \rangle$
2.993	3.644	3.849	3.556

where Z_i is the charge for the particle i and μ_{ij} is the reduced mass for the particles i and j. The exact values for the electron-electron and electron-positron conditions are hence $+0.5a_0^{-1}$ and $-0.5a_0^{-1}$, respectively. Similarly, the exact cusp values for electron-nucleus and positron-nucleus would be $-1.0a_0^{-1}$ and $+1.0a_0^{-1}$, respectively (assuming the nucleus is infinitely heavy). The cusp values are also shown in Table I. The positron-electron cusp value would give a qualitative measure of the accuracy of the positron annihilation rates. It is seen that all the cusp values are very close to the exact values, with the most uncertainty being less than 3%.

Table II shows a comparison of two-photon annihilation rates with previous calculations. It is noted that although the binding energy of PsH calculated in some of these references differs substantially from the accurate binding energy, the two-photon annihilation rates would nevertheless agree very well with the present elaborate calculation if the electron-positron cusp values are good. It indicates that the positron-electron cusp value does serve a qualitative measure of annihilation rates.

This work also reports a calculation of all average distances between various particles. The results shown in Table III indicate that this system is fairly large, but not as large as a positronium negative ion.[16] For example, in Ps^- the average electron-electron distance is $8.55a_0$ and the average electron-positron distance is $5.49a_0$. These compare with the values of $3.56a_0$ and $3.85a_0$, respectively, for PsH.

In summary, we have calculated an improved binding energy of positronium hydrides. The binding energy of 1.0598 eV represents an improvement of about 3.8% over the previous best value of 1.0211 eV. It is believed that the results can be used as reference for nonrelativistic binding energy of PsH. This work also reports a calculation of positron annihilation into two photons. The annihilation rate is determined as 2.459 nsec^{-1}. The excellent agreements between the calculated cusp values and the exact ones indicate that the overall quality of the wave functions is good. Such agreements also support the reliability of the two-photon annihilation rate. The calculated average interparticle distances show that this system is fairly large, but not as large as positronium negative ions.

[1]A. Ore, Phys. Rev. **83**, 665 (1951).
[2]S. Neamtan, G. Darewych, and G. Oczkowski, Phys. Rev. **126**, 193 (1962).
[3]P. B. Navin, D. M. Schrader, and C. F. Lebade, Phys. Rev. A **9**, 2248 (1947).
[4]S. K. Houston and R. J. Drachman, Phys. Rev. A **7**, 819 (1973).
[5]B. A. P. Page and P. A. Fraser, J. Phys. B **7**, 1389 (1974).
[6]Y. K. Ho, Phys. Rev. A **17**, 1675 (1978).
[7]P. A. Fraser, Proc. Phys. Soc. London **78**, 329 (1961); S. Hara and P. A. Fraser, J. Phys. B **8**, L472 (1975).
[8]R. J. Drachman and S. K. Houston, Phys. Rev. A **12**, 885 (1975).
[9]R. J. Drachman and S. K. Houston, Phys. Rev. A **14**, 894 (1976).
[10]R. J. Drachman, Phys. Rev. A **19**, 1900 (1979).
[11]R. J. Drachman, Can. J. Phys. **60**, 494 (1982).
[12]D. M. Schrader, in *Positron Annihilation*, edited by P. G. Coleman, S. C. Sharma, and L. M. Diana (North-Holland, Amsterdam, 1982), p. 71.
[13]Chang Lee, Zh. Eksp. Teor. Fiz. **33**, 365 (1958) [Sov. Phys.—JETP **6**, 281 (1958)].
[14]T. Kato, Commun. Pure Appl. Math. **10**, 151 (1957).
[15]D. P. Chong and D. M. Schrader, Mol. Phys. **16**, 137 (1969).
[16]Y. K. Ho, J. Phys. B **16**, 1530 (1983).