Positronium-hydrogen elastic scattering: The electronic $S = 1$ state

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We have continued our investigation into the elastic scattering of positronium atoms by hydrogen atoms, extending the work to include the spin-one (triplet) state of the two electrons. Once again we have extracted the S-wave phase shifts from normalizable trial functions by examining the spatial behavior of the center-of-mass wave functions. An effective-range expansion linear in the positronium energy fits the results very well and leads to a scattering length $a^{(-)} \simeq 2.36 a_0$, compared with the static result $a^{(-)} = 2.476 a_0$ of Hara and Fraser. The S-wave total and ortho-para conversion cross sections are calculated by making use of both ^1S and ^3S results. In the ^3S case, we see no indication of any resonances below the excitation threshold at 5.1 eV.

I. INTRODUCTION

In this Addendum we extend our examination[1,2] of the system consisting of one proton, one positron, and two electrons, by considering the electronic triplet state. In Ref. 1 we used a generalized Hylleraas wave function to calculate singlet-spin, S-wave positronium-hydrogen (Ps-H) elastic scattering and compared the results with the static-exchange values of Hara and Fraser.[3] In the present work, the symmetric trial function of Ref. 1 was simply replaced by a similar but antisymmetric function, and the scattering calculations were repeated to give phase shifts for the triplet-spin S-wave case. Once these phase shifts were determined, they were combined with those of Ref. 1 to compute the S-wave total scattering cross sections and spin-exchange (Ps ortho-para conversion) cross sections for comparison with those of Hara and Fraser.

Since this Addendum is based so closely on the methods described in Ref. 1, we will not repeat the discussion contained there, and will only present new results. Specific references to parts of the earlier paper will be made as needed.

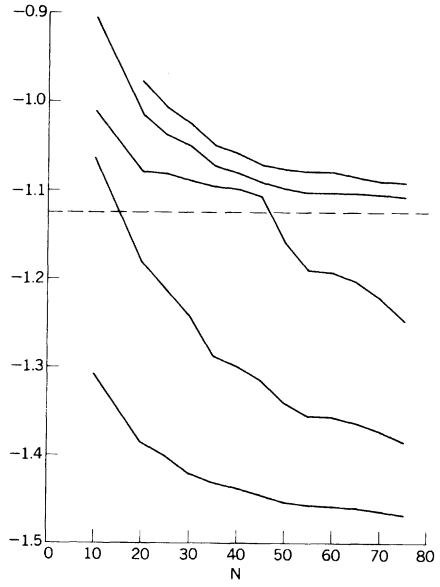

FIG. 1. First five triplet-spin eigenvalues of the Ps-H Hamiltonian plotted against expansion length N. Note the absence of a PsH bound state ($E < -1.5$) or any stabilized eigenvalues below the inelastic threshold at $E = -1.125$. The nonlinear parameters were $\alpha = 0.25$, $\beta = 0.5$, $\gamma = 1$; these are not necessarily optimum.

II. RESULTS

We diagonalized the Hamiltonian of the Ps-H system using the following S-wave basis functions:

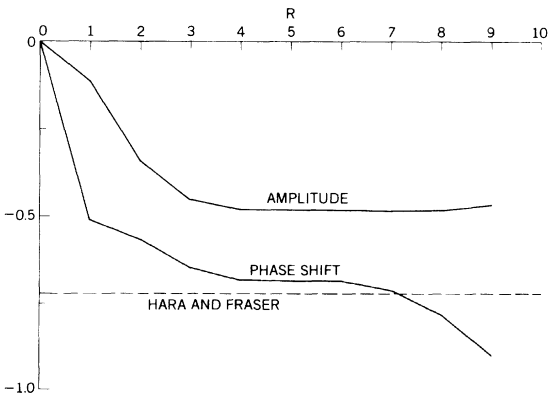

FIG. 2. Illustration of the method used to extract phase shifts from the center-of-mass wave functions: the best triplet-spin case. Here the "asymptotic" region extends over $R = 4$–6 ($N = 56$, $k = 0.2963$, $E = \frac{1}{2}k^2 = 0.597$ eV).

TABLE I. Triplet S-wave positronium-hydrogen scattering parameters. Errors are estimated from the slope of the plateau.

k^2	N	$\eta^{(-)}$	$k\cot\eta^{(-)}$	Eigenvalue number
0.0651	75	−0.591	-0.380 ± 0.011	1
0.0878	56	−0.6845	$-0.3630^{+0.0001}_{-0.0026}$	1
0.2315	75	−1.051	-0.275 ± 0.013	2
0.2898	56	−1.161	$-0.234^{+0.017}_{-0.021}$	2
0.5064	75	−1.445	$-0.090^{+0.021}_{-0.006}$	3

$$\phi_{lmn} = e^{-(\alpha x+\beta r_1+\gamma r_2)} x^l r_1^m \rho_1^n - (\vec{r}_1 \rightleftarrows \vec{r}_2), \qquad (1)$$

where the notation is defined in Ref. 1. [These functions differ from those in Eq. (2) of Ref. 1 only by having the opposite sign before the exchange term.] In Fig. 1 we show the five lowest eigenvalues plotted against expansion length. Notice the absence of a bound PsH triplet state ($E<-1.5$ Ry) or any sign of an elastic-scattering resonance, in contrast to the singlet case. (Compare Fig. 3 of Ref. 1.)

We then obtained the elastic-scattering S-wave phase shifts by projecting out the Ps-H center-of-mass wave function as suggested by Hazi and Taylor[4] and Temkin[5] and described in Eqs. (3)–(5) of Ref. 1. In Fig. 2 we plot the best single result of the present work, which should be compared with Fig. 1 of Ref. 1. In general, a longer expansion was necessary in the present case to obtain reasonable stability.

In Table I we list the triplet S-wave Ps-H scattering parameters obtained by this method, at five values of momentum k. (We emphasize that these values of k result from the numerical diagonalization of H and are not easily adjusted to the usual reporting values.) From the data in Table I we have plotted in Fig. 3 the effective-range function, $k\cot\eta^{(-)}$, against k^2. An excellent linear fit to the points can be made, yielding the following results for the triplet scattering length and effective range:

$$a^{(-)} = 2.36, \quad r_0^{(-)} = 1.31. \qquad (2)$$

This value of the scattering length is about 5% smaller than that of Ref. 3:

$$a^{(-)} = 2.476, \quad r_0^{(-)} = 1.44. \qquad (3)$$

[In Eq. (3) the effective range $r_0^{(-)}$ is obtained from the data of Ref. 3, fitted linearly and plotted in Fig. 3.]

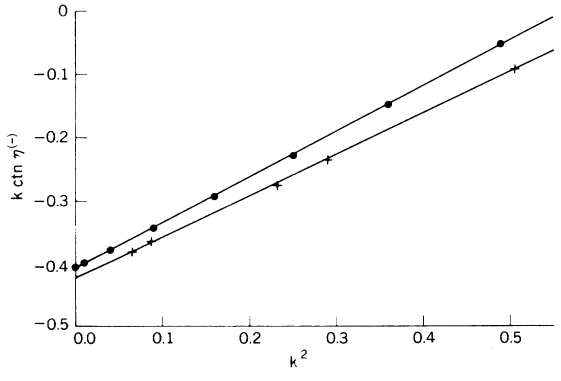

FIG. 3. Plot of the triplet-spin effective-range function $k\cot\eta^{(-)}$ as a function of k^2. The crosses are the five scattering results of this work, and the solid circles are from Ref. 3. The two curves are linear least-squares fits to the points for each calculation.

TABLE II. S-wave total cross section σ and ortho-para conversion cross section σ_c in units of πa_0^2 and their ratio $P=\sigma_c/\sigma$.

Energy (eV)	σ	σ_c	P (%)
0	45.2	2.20	4.9
1.115	17.5	0.65	3.7
1.686	13.2	0.50	3.8
2.704	8.9	0.34	3.8
3.801	6.3	0.25	3.9

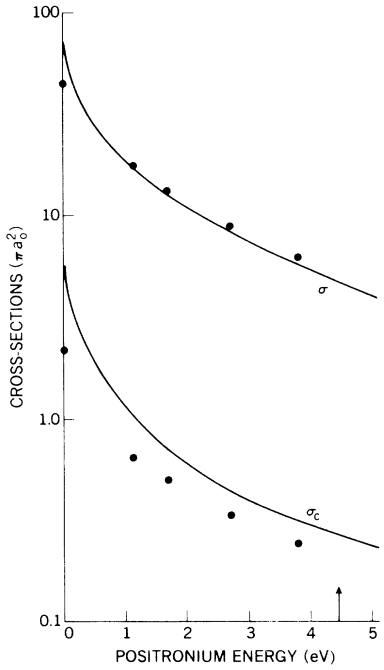

FIG. 4. S-wave triplet-spin Ps-H cross sections. The circles are the present results given in Table II, and the curves are from Ref. 3. Both total (σ) and ortho-para conversion (σ_c) cross sections are shown. The arrow indicates the position of the resonance reported in Ref. 1.

We calculated S-wave elastic cross sections σ and spin-exchange cross sections σ_c from the expressions given by Hara and Fraser[3]:

$$\sigma/(\pi a_0^2) = (\sin^2\eta^{(+)} + 3\sin^2\eta^{(-)})/k^2 , \quad (4)$$

$$\sigma_c/(\pi a_0^2) = \sin^2(\eta^{(+)} - \eta^{(-)})/(4k^2) . \quad (5)$$

[The spin-exchange cross section describes the probability that an ortho-Ps ($S=1$) atom will, by an exchange collision with the H atom, be converted into para-Ps ($S=0$). This represents a quenching process, since the para-Ps annihilation lifetime is about 10^3 times shorter than that of ortho-Ps.] Since the effective-range fit in the triplet case is so accurately linear in k^2 while the singlet case is not, we calculated the values of $\eta^{(-)}$ from the effective-range formula at the energies appropriate to the singlet calculation[6] (see Table I of Ref. 1.) The results are presented in Table II and are plotted, along with those of Hara and Fraser (HF),[3] in Fig. 4. We should point out that the ratio $P=\sigma_c/\sigma$ is lower at all energies in our calculation than in Ref. 3. At zero energy (where only S waves contribute) $P/P(\mathrm{HF})=0.605$, $\sigma/\sigma(\mathrm{HF})=0.633$, and $\sigma_c/\sigma_c(\mathrm{HF})=0.382$.

III. CONCLUSIONS

We have again shown the usefulness of the projection method[4,5] for extracting scattering phase shifts from normalizable, correlated trial functions. This work completes our program of calculations on the Ps-H system, since our restricted trial function and the character of the projection method are not capable of significant extension. To obtain real improvements, one should use more complete trial functions[7] and variationally correct scattering techniques. Judging from the scattering calculations presented here and in Ref. 1 as well as the bound singlet-state calculations,[7] it appears that the present triplet phase shifts are closer to the exact values than are the singlet phase shifts.

Note added in proof. B. A. P. Page [J. Phys. B 9, 1111 (1976)] has recently carried out a Kohn variational calculation at zero energy using a correlation function similar to Eq. (1). With $N=35$ the results are $a^{(+)}=5.844$ and $a^{(-)}=2.319$.

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[1]R. J. Drachman and S. K. Houston, Phys. Rev. A 12, 885 (1975).
[2]S. K. Houston and R. J. Drachman, Phys. Rev. A 7, 819 (1973).
[3]S. Hara and P. A. Fraser, J. Phys. B 8, L472 (1975).
[4]A. U. Hazi and H. S. Taylor, Phys. Rev. A 1, 1109 (1970).
[5]A. Temkin, in *Autoionization*, edited by A. Temkin (Mono, New York, 1966), p. 67.
[6]In Table II of Ref. 1 we illustrated an extrapolation technique intended to provide improved values of $a^{(+)}$ and $r_0^{(+)}$. Since the method is based on the existence of a bound PsH singlet state, it cannot be used to improve the triplet results. For that reason we preferred to calculate σ and σ_c using uncorrected values of the phase shifts.
[7]B. A. P. Page and P. A. Fraser, J. Phys. B 7, L389 (1974).