Scattering of Positronium by Atomic Hydrogen

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Extensive new calculations, in the coupled-pseudostate formalism, are reported for o-Ps($1s$) scattering by H($1s$) in the energy range 0 to 40 eV. An S-wave resonance first predicted by Drachman and Houston [Phys. Rev. A **12**, 885 (1975)] is confirmed and new resonances are found in the P, D, F, G, and H waves. The cross section for o-Ps($1s$) to p-Ps($1s$) conversion is shown to have significant structure. Results for the total cross section and its components indicate that Ps ionization is the main process at the higher energies. Excitation of the H atom becomes increasingly important above 20 eV. [S0031-9007(98)06224-3]

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The positronium-atomic hydrogen, Ps-H, system is one of the fundamental collision systems of atomic physics. Yet, because of computational and experimental difficulties, it has remained largely unexplored [1]. However, as a result of recently acquired capability to perform atomic scattering experiments with Ps beams [2], the need to understand this most basic of such systems has become of paramount importance. Ps can exist either in a spin singlet [para (p)] state or a spin triplet [ortho (o)] state. In its ground level, Ps($1s$), these states have lifetimes of 0.125 and 142 ns, respectively [1], before decaying (predominantly) into two and three photons, respectively. Consequently, only the o-Ps($1s$) state is sufficiently long-lived to be used as a laboratory projectile. Our interest here, therefore, centers upon collisions of o-Ps($1s$) with ground state atomic hydrogen.

Until now, and with the exception of S-wave scattering [3], theoretical studies of Ps-H scattering have been restricted to relatively elementary approximations such as the first Born approximation [4,5], the static-exchange approximation [6] and, most recently, a three-state Ps($1s, 2s, 2p$) + H($1s$) calculation [7]. For S-wave scattering we have somewhat more sophisticated information gleaned from what are essentially bound state-type approximations. Thus, we have fairly good values for the scattering lengths and effective ranges as well as good estimates of the S-wave scattering phase shifts at a few isolated low energies [8,9]. In addition, we know that the Ps-H system has a bound state [10] of binding energy 1.067 eV [11], as well as a resonance at 4.01 eV of width 0.075 eV [12], both bound state and resonance being S-wave with total electronic spin zero.

In this Letter we announce extensive new calculations based upon the coupled-pseudostate formalism, an approach which has been applied with considerable success to e^+-atom and e^--atom scattering [13–15]. In this form of approximation discrete pseudostates are used to represent the continuum of the Ps and/or H atom. A great advantage of the pseudostate method is that it provides a complete and internally consistent picture of all the main processes, i.e., elastic scattering, discrete excitations, ionization, and total scattering. In this approximation the system wave function Ψ for Ps-H scattering is expanded as [16]

$$\Psi = \sum_{a,b} [G_{ab}(\mathbf{R}_1)\phi_a(\mathbf{t}_1)\psi_b(\mathbf{r}_2) + (-1)^S G_{ab}(\mathbf{R}_2)\phi_a(\mathbf{t}_2)\psi_b(\mathbf{r}_1)], \quad (1)$$

where $\mathbf{R}_i \equiv (\mathbf{r}_p + \mathbf{r}_i)/2$ is the position vector of the Ps center of mass, $\mathbf{t}_i \equiv \mathbf{r}_p - \mathbf{r}_i$ is the Ps internal coordinate, and $\mathbf{r}_p$ ($\mathbf{r}_i$) is the position vector of the positron (ith electron), all position vectors being referred to the atomic nucleus as origin. S specifies the total electronic spin. The Ps (H) states ϕ_a (ψ_b) diagonalize the Ps (H) Hamiltonian and may be either eigenstates or pseudostates [5,13,14]. Substituting (1) into the Schrödinger equation and projecting with $\phi_a(\mathbf{t}_1)\psi_b(\mathbf{r}_2)$ leads to coupled equations of the form

$$(\nabla_R^2 + p_{ab}^2)G_{ab}(\mathbf{R}) = 4\sum_{a'b'}\left[V_{ab,a'b'}(\mathbf{R})G_{a'b'}(\mathbf{R}) + (-1)^S \int_0^\infty L_{ab,a'b'}(\mathbf{R},\mathbf{R}')G_{a'b'}(\mathbf{R}')d\mathbf{R}'\right], \quad (2)$$

where p_{ab} is the momentum of the Ps in the "ab" channel. The nonlocal coupling $L_{ab,a'b'}(\mathbf{R},\mathbf{R}')$ describes how the state $\phi_{a'}\psi_{b'}$ is converted into $\phi_a\psi_b$ by electron exchange between the Ps and the H atom; it is these terms which pose the major computational problem. It is easy to show that the direct potentials $V_{ab,a'b'}(\mathbf{R})$ are zero if the Ps states ϕ_a and $\phi_{a'}$ have the same parity. In particular, this means that the elements $V_{ab,ab'}$, which are diagonal in the Ps states, are zero, a property which enhances the importance of the exchange terms since $L_{ab,ab'}$ is nonzero. We convert the coupled equations (2) to partial wave form and solve using the R-matrix technique [17]. One useful feature of the R-matrix method is that it gives information

simultaneously on both the scattering states and the bound states of the system.

It is clear from (1) that the scale of the calculation escalates rapidly as the product of the number of Ps states ϕ_a times the number of H states ψ_b. We have therefore adopted the further approximation that the H atom is not excited in the collision, i.e., we retain only one H state ψ_b in (1), which is the ground state. We exhibit results from six approximations: (i) The classic static-exchange approximation (1ST) [6,18] in which only the Ps($1s$) and H($1s$) states are retained in (1); this approximation is driven solely by the exchange interaction since $V_{1s1s,1s1s} = 0$; (ii) a 3-state approximation (3ST) employing the $1s$, $2s$, and $2p$ eigenstates of Ps [7]; (iii) a 9-state approximation (9ST) which includes also $\overline{3s}$, $\overline{4s}$, $\overline{3p}$, $\overline{4p}$, $\overline{3d}$, and $\overline{4d}$ pseudostates of Ps [13,19]; (iv) a 22-state approximation involving the $1s$, $2s$, and $2p$ eigenstates as well as $\overline{3s}$ to $\overline{7s}$, $\overline{3p}$ to $\overline{7p}$, $\overline{3d}$ to $\overline{7d}$, and $\overline{4f}$ to $\overline{7f}$ pseudostates [5]. Approximations (i)–(iv) give a PsH bound state with binding energy of 0.263, 0.326, 0.543, and 0.634 eV, respectively; this should be compared with the best known value of 1.067 eV [11]. Approximations (v) and (vi) correspond to (iii) and (iv) but with the exchange terms in (2) dropped; they are labeled as 9STNE and 22STNE. Physically, (v) and (vi) correspond to scattering of the Ps by the frozen electrostatic field of the atom, an approximation that has been used to study Ps collisions with He and Ar [5].

From (2) we deduce, in the usual way, scattering amplitudes $f^{(S)}_{aa'}$ for electron spin singlet ($S = 0$) and triplet ($S = 1$) scattering and for transitions of the Ps from state ϕ_a to state $\phi_{a'}$.

Table I compares our results with the best S-wave elastic phase shifts available, those of Drachman and Houston (DH) [8,9]. Consistent with the variational lower bound principle, the phase shifts increase systematically on progression from 1ST to 22ST and converge towards the DH values. However, except at the lowest energy, the 22ST approximation overshoots the DH numbers for singlet scattering, which would seem to imply that it is giving more accurate answers in these cases. For triplet scattering there is a remarkable insensitivity of the phase shift to the approximation. This is similar to the situation encountered in triplet S-wave e^--H($1s$) elastic scattering (see Table I of Ref. [21]) and is probably explicable in terms of a Pauli exclusion mechanism analogous to that discussed by Walters [22]. We find that approximations (i)–(iv) remain in excellent agreement with each other for triplet S-wave Ps($1s$) elastic scattering right up to an impact energy of 15 eV. Such agreement does not obtain with the higher triplet partial waves. Also shown in Table I are the singlet and triplet scattering lengths a and effective ranges r_0. These follow the same pattern as the phase shifts. The agreement between 22ST and the results of DH is, perhaps, not so surprising. Thus, the trial wave function used by DH gives a PsH binding energy of 0.672 eV [23] which is comparable to the 22ST value of 0.634 eV; i.e., both approximations would appear to be of similar quality.

Figure 1 illustrates the singlet S-, P-, and D-wave cross sections for Ps($1s$) elastic scattering in the 22ST approximation. The most striking feature of these cross sections is the appearance of resonances in the vicinity of 5 eV. In the S- and P-wave cross sections these resonances are very sharp, but that in the D-wave cross section is noticeably wider. We also see resonances in the singlet F-, G-, and H-wave cross sections near 6.5, 8.3, and 10 eV, respectively, which become weaker and more diffuse with

TABLE I. S-wave phase shifts, scattering lengths a, and effective ranges r_0 for Ps($1s$) elastic scattering in various approximations.[a]

Singlet scattering

p_0^2 (a.u.)	1ST	3ST	9ST	22ST	DH, Ref. [8]	
0.1639	1.23	1.27	1.44	1.50	1.52	
0.2478	1.00	1.04	1.22	1.28	1.27	
0.3975	0.74	0.78	0.96	1.03	1.00	
0.5588	0.56	0.60	0.81	0.89	0.81	
a	7.25	6.70	5.51	5.20	4.5	Ref. [20]
r_0	3.07	2.98	2.63	2.52	2.2	Ref. [20]

Triplet scattering

p_0^2 (a.u.)	1ST	3ST	9ST	22ST	DH, Ref. [9]
0.0651	−0.620	−0.617	−0.611	−0.610	−0.591
0.0878	−0.714	−0.711	−0.704	−0.702	−0.6845
0.2315	−1.108	−1.102	−1.091	−1.086	−1.051
0.2898	−1.218	−1.212	−1.199	−1.191	−1.161
0.5064	−1.520	−1.510	−1.493	−1.486	−1.445
a	2.49	2.47	2.45	2.45	2.36
r_0	1.36	1.35	1.33	1.32	1.31

[a]$\mathbf{p}_0$ is the momentum of the incident Ps.

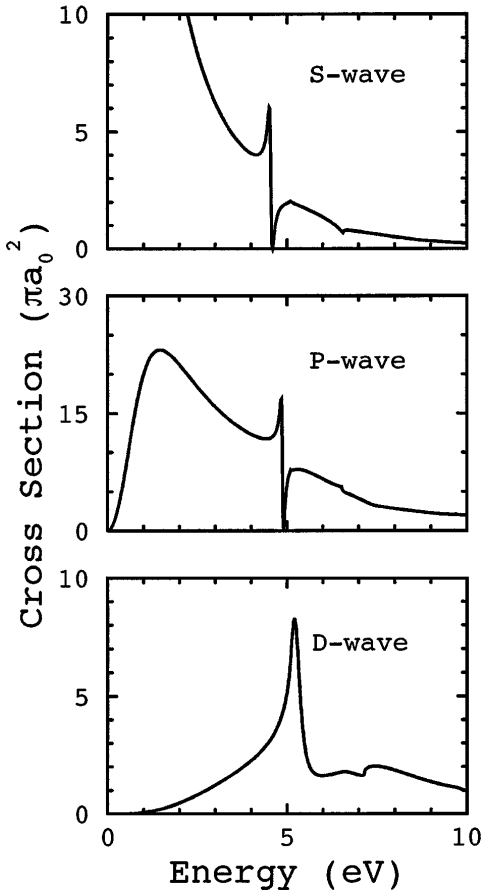

FIG. 1. Singlet partial wave cross sections in the 22ST approximation.

increasing angular momentum. The S-wave resonance was first predicted by Drachman and Houston [8,24] who calculated its position E_r as 4.455 ± 0.010 eV and its width Γ_r as 0.062 ± 0.015 eV. This compares well with our 22ST result $E_r = 4.55$ eV, $\Gamma_r = 0.084$ eV. However, more accurate calculations of Ho [12] give $E_r = 4.01 \pm 0.01$ eV and $\Gamma_r = 0.075 \pm 0.027$ eV. For the new P- and D-wave resonances we find $E_r = 4.88$ eV, $\Gamma_r = 0.058$ eV and $E_r = 5.28$ eV, $\Gamma_r = 0.47$ eV, respectively. We were unable to obtain satisfactory fits to the more diffuse F-, G-, and H-wave resonances. Drachman [25] has interpreted resonance formation in the Ps-H system as resulting from bound states of the positron about the H^- ion, these bound states becoming unstable due to coupling to the open Ps(1s) + H(1s) channel; higher resonances can also decay into excited Ps channels. Since H^- is in a spin singlet state, the resonances must have total electronic spin zero. Accordingly, we find no resonances in our triplet partial waves.

Figure 2 shows the spin averaged total cross section (i.e., the cross section for all possible outcomes averaged over the initial spin directions of the incident o-Ps) in our various approximations. In the energy range shown, 0 to 10 eV, there is excellent agreement between the two pseudostate calculations, 9ST and 22ST, which are very

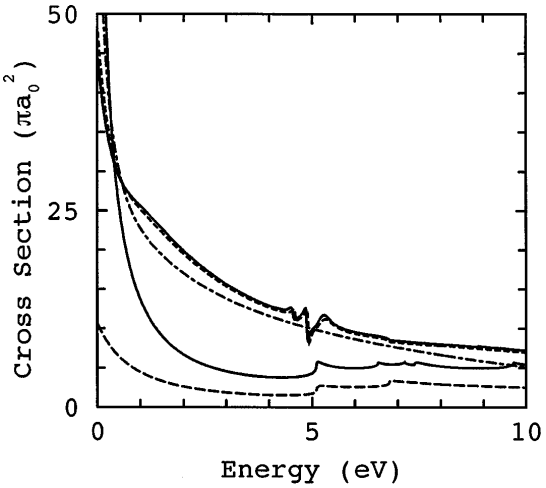

FIG. 2. Spin averaged total cross section. Curves: upper solid, 22ST; short-dashed, 9ST; lower solid, 22STNE; long-dashed, 9STNE; dash-dotted, 1ST.

different from their nonexchange counterparts, 9STNE and 22STNE. Also, the agreement between 9ST and 22ST stands in stark contrast to the differences between 9STNE and 22STNE. Clearly, inclusion of exchange reduces the sensitivity to the choice of pseudostates, a useful note for future work, as well as being very important in its own right at the lower energies. In Fig. 2 we also show the simplest approximation, 1ST, which provides a useful benchmark for judging the importance of coupling to Ps states other than Ps(1s).

Figure 3 exhibits the cross section for o-Ps(1s) to p-Ps(1s) conversion [6]. Most noticeable are the pronounced minimum and maximum at 0.23 and 1.30 eV predicted by the pseudostate approximations, as well as the structures near 5 eV coming from the resonances in the singlet partial waves discussed earlier.

Finally, in Fig. 4 we show, over an extended energy range (0 to 40 eV), the spin averaged total cross section

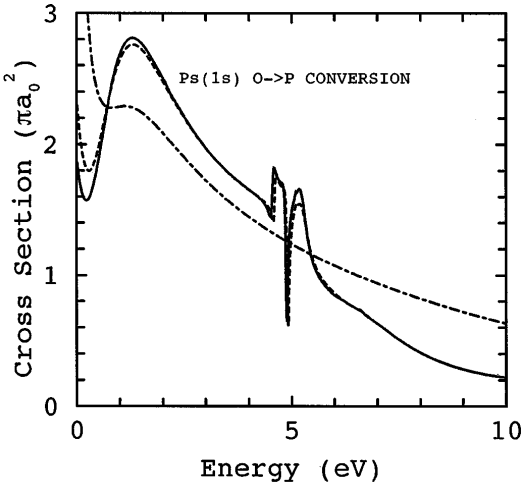

FIG. 3. Cross section for o-Ps(1s) to p-Ps(1s) conversion. Curves: solid, 22ST; short-dashed, 9ST; dash-dotted, 1ST.

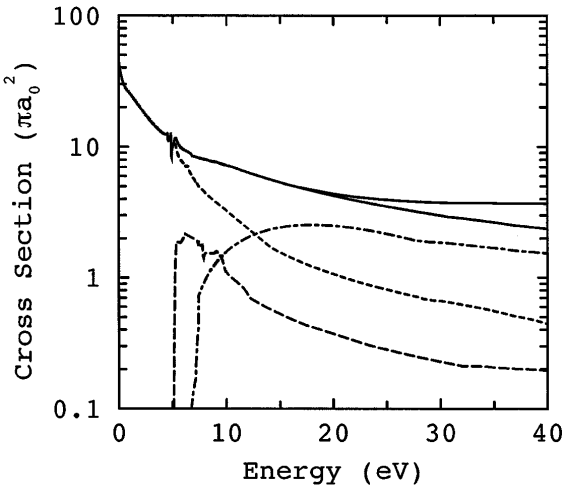

FIG. 4. Spin averaged total cross section and its components in the 22ST approximation. Curves: lower solid, total cross section; upper solid, total cross section with first Born estimate from Ref. [5] for H target excitation and ionization added; short-dashed, Ps($1s$) elastic scattering; long-dashed, Ps($n = 2$) excitation; dash-dotted, Ps ionization.

and its components in the 22ST approximation. Some small scale pseudostructure has been removed from the cross sections in this figure by smoothing [13]. The ionization cross section has been calculated using the usual pseudostate prescription [13,14]. Figure 4 shows that elastic scattering decreases rapidly above 5 eV, that Ps($n = 2$) excitation is not very important, and that the main result of a collision at the higher energies in Ps ionization. To allow for excitation and ionization of the H target we have added to the 22ST cross section the first Born estimate of Ref. [5] for these processes. The growing importance of target excitation and ionization above about 20 eV is to be noted. By 40 eV this amounts to more than 50% of the 22ST total cross section and is continuing to rise while the latter falls.

In conclusion, we have presented extensive new calculations of o-Ps($1s$) scattering by H($1s$) which significantly advance our knowledge of this fundamental system. While our approximation is limited by the restriction of the hydrogen atom to its ground state, our impression from comparison with other work [8,9] is that this may not be so serious at the lower energies, say $\leq$10 eV. Beyond about 20 eV, however, there is a clear need to take into account excitation and ionization of the atom. Although this would be a very major undertaking, within the coupled-pseudostate framework, we believe, from the technical experience gained here, that it may be possible within the not so distant future.

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