CALCULATIONS OF POSITRON AND POSITRONIUM SCATTERING

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ABSTRACT

Progress in the theoretical treatment of positron - atom and positronium - atom scattering within the context of the coupled - pseudostate approximation is described.

INTRODUCTION

Although I (HRJW) was well acquainted with the works of Aaron and Dick, it was some time before I actually met these giants of Atomic Physics in person. My first encounter with Aaron was in 1976. At that time I had already been impressed by the substantive section that had been devoted to his work in the famous text by Mott and Massey on "The Theory of Atomic Collisions" (ref. 1). Here I had read about "Temkin's Method" for treating the total S-wave electron - hydrogen problem (ref. 2) and his polarized orbital technique (refs. 3, 4). The former was later to be exploited by Poet (ref. 5) to create one of the most important benchmarks for electron scattering by atomic hydrogen, the latter became an ubiquitous approximation which is used to the present day. I had also read his edited compendium on "Autoionization" (ref. 6) and, in particular, his own article in that compendium which had done much to clarify my ideas on the topic. The occasion of the meeting was the local UK ATMOP conference which, in 1976, had come to Belfast. It was a very difficult time, for "The Troubles" were then in full swing. Fearful that attendance would be low, Phil Burke had organised a pre - ATMOP workshop that, as it turned out, was attended by a glittering array of international stars, amongst the foremost of whom was Aaron. We at Belfast shall be forever grateful for the support that we received from those who came at that risky time. It is David Thompson that I have to thank for my introduction to Aaron.

It was not until relatively late, 1987, that I met up with Dick. The occasion was the Positron Workshop satellite of ICPEAC which was then held at University College London. Our accommodation was arranged in one of the Halls of Residence of London University. In the mornings we would queue up outside the breakfast hall and, somehow, Dick and I were always first in the queue. It was during these moments that Dick regaled me, in his own inimitable way, with some fascinating anecdotes. It was there that I learnt that Dick's family had passed through London, a loss to British science but a gain to the US. One of the highlights of the London meeting was Dick's talk on "Theoretical aspects of positronium collisions". This can be read in ref. 7, it is a superb and insightful article which I strongly recommend. It was this talk more than anything that persuaded me that Positronic Atomic Physics was really an exciting area worthy of study. Perhaps a better title for the present article would be "The Drachman Programme" for I find that with each step I take I follow in a path already trodden by Dick. So let us begin that Programme.

POSITRON - ATOM SCATTERING

When a positron scatters off an atom, A, the following processes (assuming A contains enough electrons) are possible:

$e^+ + A$	$\longrightarrow$	$e^+ + A$	Elastic Scattering	$(1a)$
		$e^+ + A^*$	Excitation	$(1b)$
		$e^+ + A^{n+} + ne^-$	Ionization	$(1c)$
		$Ps(nlm) + A^+$	Ps Formation	$(1d)$
		$Ps^- + A^{++}$	Ps^- Formation	$(1e)$
		$Ps + A^{(n+1)+} + ne^-$	Transfer Ionization	$(1f)$
		$Ps^- + A^{(n+2)+} + ne^-$	Transfer Ionization with Ps^- Formation	$(1g)$
		$A^+ + \gamma$ rays	Annihilation	$(1h)$

Reactions (1a) to (1c) are also possible using electrons as a projectile. Reactions (1d) to (1h) are unique to the positron. It is these latter reactions which distinguish the positron as a more subtle projectile than the electron. Unlike the electron, the positron competes with the atomic nucleus for the "attention" of the electrons in the system, leading to a more correlated dynamics. Positronium formation is the most obvious manifestation of this competition while the annihilation process gives "pin - point" information on correlation in the system in that it measures the probability that the positron coincides with an electron.

Because of the competition between the positron and the atomic nucleus for electrons, positron - atom scattering is inherently a two - centre process, in contrast to electron - atom scattering where the whole dynamics is essentially centred on the atomic nucleus. It is this two - centre nature which makes the theoretical description of positron - atom scattering so much more difficult than that of electron - atom scattering. Considerable success has been achieved using the coupled - (pseudo)state approach to treat positron scattering by "one - electron" and "two - electron" atoms (refs. 8 - 17). To illustrate what is involved we shall describe the method as applied to positron scattering by atomic hydrogen. [1]

Let $\mathbf{r}_p$ ($\mathbf{r}_e$) be the position vector of the positron (electron) relative to the hydrogen nucleus, ie, the proton. While these coordinates are convenient for describing positron - atom channels, the natural set of coordinates for positronium channels is $\mathbf{R} \equiv (\mathbf{r}_p + \mathbf{r}_e)/2$ and $\mathbf{t} \equiv \mathbf{r}_p - \mathbf{r}_e$ which give the position vector of the positronium centre of mass relative to the proton and the positronium internal coordinate respectively. In the coupled - state approach the wave function for the collision system, Ψ, is expanded as

$$\Psi = \sum_a F_a(\mathbf{r}_p)\psi_a(\mathbf{r}_e) + \sum_b G_b(\mathbf{R})\phi_b(\mathbf{t}) \tag{2}$$

where the first sum is over atomic hydrogen states ψ_a and the second is over positronium states ϕ_b. In the first instance it will be assumed that ψ_a and ϕ_b are eigenstates. The expansion (2) clearly represents both positron - atom (first sum) and positronium - proton (second sum) channels explicitly. Since the states ψ_a and ϕ_b separately form complete sets, the expansion (2) is technically over - complete. However, in practical calculations complete sets of states are never actually used. Substituting (2) into the Schrödinger equation and projecting with $\psi_a(\mathbf{r}_e)$ and $\phi_b(\mathbf{t})$ gives coupled equations for the unknown functions $F_a(\mathbf{r}_p)$ and $G_b(\mathbf{R})$ of the form

$$\begin{aligned} \left(\nabla_p^2 + k_a^2\right) F_a(\mathbf{r}_p) &= 2\textstyle\sum_{a'} V_{aa'}(\mathbf{r}_p)F_{a'}(\mathbf{r}_p) + 2\textstyle\sum_{b'} \int K_{ab'}(\mathbf{r}_p, \mathbf{R})\, G_{b'}(\mathbf{R})\, d\mathbf{R} \\ \left(\nabla_R^2 + p_b^2\right) G_b(\mathbf{R}) &= 4\textstyle\sum_{b'} U_{bb'}(\mathbf{R})\, G_{b'}(\mathbf{R}) + 4\textstyle\sum_{a'} \int K^{\star}_{a'b}(\mathbf{r}_p, \mathbf{R})\, F_{a'}(\mathbf{r}_p)\, d\mathbf{r}_p \end{aligned} \tag{3}$$

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[1] We use atomic units (au) in which $\hbar = m_e = e = 1$ throughout this article.

where

$$E = \frac{k_a^2}{2} + \epsilon_a = \frac{p_b^2}{4} + E_b \tag{4}$$

E being the total energy and ϵ_a (E_b) being the energy of the state ψ_a (ϕ_b). The symbol $\star$ stands for complex conjugation. In (3) the local potentials $V_{aa'}(\mathbf{r}_p)$ and $U_{bb'}(\mathbf{R})$ come from the direct Coulombic interaction between the positron and the hydrogen atom and between the positronium and the proton respectively. From a computational viewpoint the really difficult objects in (3) are the non - local couplings $K_{ab}(\mathbf{r}_p, \mathbf{R})$ which represent positronium formation. In practice, the coupled equations (3) are reduced to partial wave form and the resulting radial equations are solved using some suitable technique such as the R - matrix method (ref. 18).

The success of the coupled - state approach has in large part been due to the concept of pseudostates. A practical difficulty with using the expansion (2) is how to handle continuum states ψ_a and ϕ_b in the expansion. Such states correspond to the ionization channels of the system. In the pseudostate method the atom and positronium continua are replaced by discrete pseudostates $\overline{\psi}_a$ and $\overline{\phi}_b$ and so (2) becomes an expansion in terms of a finite number of discrete states. Some of these states will be true (discrete) eigenstates ψ_a (ϕ_b), the remainder will be pseudostates $\overline{\psi}_a$ ($\overline{\phi}_b$). The notation ψ_a (ϕ_b) will now be used to mean either an eigenstate or a pseudostate of this finite set. The pseudostates are constructed so that the set of states ψ_a (ϕ_b) diagonalizes the atom (positronium) Hamiltonian H_A (H_{Ps}):

$$\begin{array}{rclcrcl} \langle\psi_a|H_A|\psi_{a'}\rangle & = & \epsilon_a\delta_{a,a'} & & \langle\psi_a|\psi_{a'}\rangle & = & \delta_{a,a'} \\ \langle\phi_b|H_{Ps}|\phi_{b'}\rangle & = & E_b\delta_{b,b'} & & \langle\phi_b|\phi_{b'}\rangle & = & \delta_{b,b'} \end{array} \tag{5}$$

This means that the coupled equations for $F_a(\mathbf{r}_p)$ and $G_b(\mathbf{R})$ retain the form (3). The diagonalization (5) is normally achieved by using a basis of Slater orbitals (ref. 9) or Laguerre functions (refs. 9, 19, 20). We can think of pseudostates as being "clumps" or "distributions" of eigenstates with the clump being centred upon the energy ϵ_a (E_b). The distribution of a pseudostate over the eigenstate spectrum may be specified in terms of a function

$$f_n(\epsilon) = |\langle\chi_\epsilon \mid \chi_n\rangle|^2 \tag{6}$$

where $\chi_n \equiv \psi_a$ or ϕ_b, as appropriate, and χ_ϵ is an eigenstate of H_A or H_{Ps}, as appropriate, with energy ϵ and the same angular momentum quantum numbers as χ_n. If χ_ϵ is a bound state it is normalized to unity, if a continuum state to a delta function in ϵ, ie,

$$\langle\chi_\epsilon|\chi_{\epsilon'}\rangle = \delta(\epsilon - \epsilon') \tag{7}$$

The quantity $f_n(\epsilon)$ is just the probability that χ_n contains the eigenstate χ_ϵ. Figure 1 illustrates the distribution functions on the continuous part of the spectrum ($\epsilon \geq 0$) for some s - type atomic hydrogen pseudostates used in a 33 - state calculation of e^+ + H(1s) scattering by Kernoghan et al (ref. 14). Figure 2 shows results from the same calculation. The agreement with experiment is very good. Figure 3 demonstrates the power of the method. Here we see how the approximation can give a complete picture of all the main processes. In the coupled pseudostate approach we have a representation of all the main physical processes, ie, excitation of the atom, positronium formation, ionization, in effect a **complete dynamical theory**. How good this representation is, of course, depends upon the choice and number of pseudostates.

In figure 4 we show estimates of the cross sections for e^+ + H(1s) scattering made by Dick for use in an analysis of the annihilation of galactic positrons (ref. 23). These estimates were made in 1978. They are remarkably close to the numbers shown in figure 3 which were calculated 17 years later! But there is more, displayed also in figure 4 are estimates of the cross sections for positron scattering by molecular hydrogen. It will be a long time before such cross sections can be calculated by the sophisticated methods described here, but we would bet that, if they were, they would not be much different from Dick's estimates shown in figure 4, such is our confidence in his judgement.

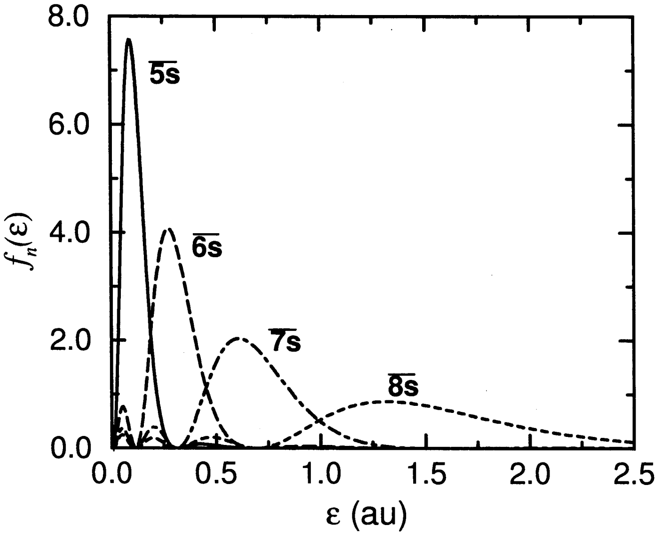

Figure 1: Distribution function f_n for $\overline{5s}$ to $\overline{8s}$ atomic hydrogen pseudostates used in the calculation of ref. 14.

Besides atomic hydrogen, coupled - state calculations have been performed on the alkali metals Li, Na, K, Rb and Cs (refs. 9, 10, 11, 13, 15, 16, 17) which have been treated as "one-electron" systems. An interesting prediction to come out of these calculations is the collapse in ground state positronium formation with a corresponding increase in excited state formation as we ascend the alkali metal series from Li to Cs, this is illustrated in figure 5.

When the atom contains more than one electron (N electrons, say) a new technical feature arises, namely, electron exchange between the formed Ps and the resultant atomic ion. We need now to label not only the states of the atom (a) and the Ps (b) but also the state of the ion (i). the coupled equations then generalise to

$$\begin{aligned}
\left(\nabla_p^2 + k_a^2\right) F_a(\mathbf{r}_p) &= 2\sum_{a'} V_{aa'}(\mathbf{r}_p) F_{a'}(\mathbf{r}_p) \\
&\quad +2N\sum_{i',b'} \int K_{a,i'b'}(\mathbf{r}_p, \mathbf{R}) G_{i'b'}(\mathbf{R}) d\mathbf{R} \\
\left(\nabla_R^2 + p_{ib}^2\right) G_{ib}(\mathbf{R}) &= 4\sum_{i',b'} U_{ib,i'b'}(\mathbf{R})\, G_{i'b'}(\mathbf{R}) \\
&\quad +4\sum_{a'} \int K^{\star}_{a'ib}(\mathbf{r}_p, \mathbf{R})\, F_{a'}(\mathbf{r}_p)\, d\mathbf{r}_p \\
&\quad +4\sum_{i',b'} \int L_{ib,i'b'}(\mathbf{R}, \mathbf{R}')\, G_{i'b'}(\mathbf{R}')\, d\mathbf{R}'
\end{aligned} \tag{8}$$

The non - local terms $L_{ib,i'b'}(\mathbf{R}, \mathbf{R}')$ describe the conversion of ion and Ps states ($i'b'$) into (ib) through electron exchange. Whereas the positronium formation kernels $K_{a,ib}$ are difficult to handle, the new terms $L_{ib,i'b'}$ are very much more difficult still. It is this new element which makes the generalisation of the "one - electron" case to many electron targets non - trivial. However, the new terms are fundamental to the study of Ps - atom scattering which we discuss in the next section. Missing from (8) is explicit allowance for other new channels that become possible with multi -

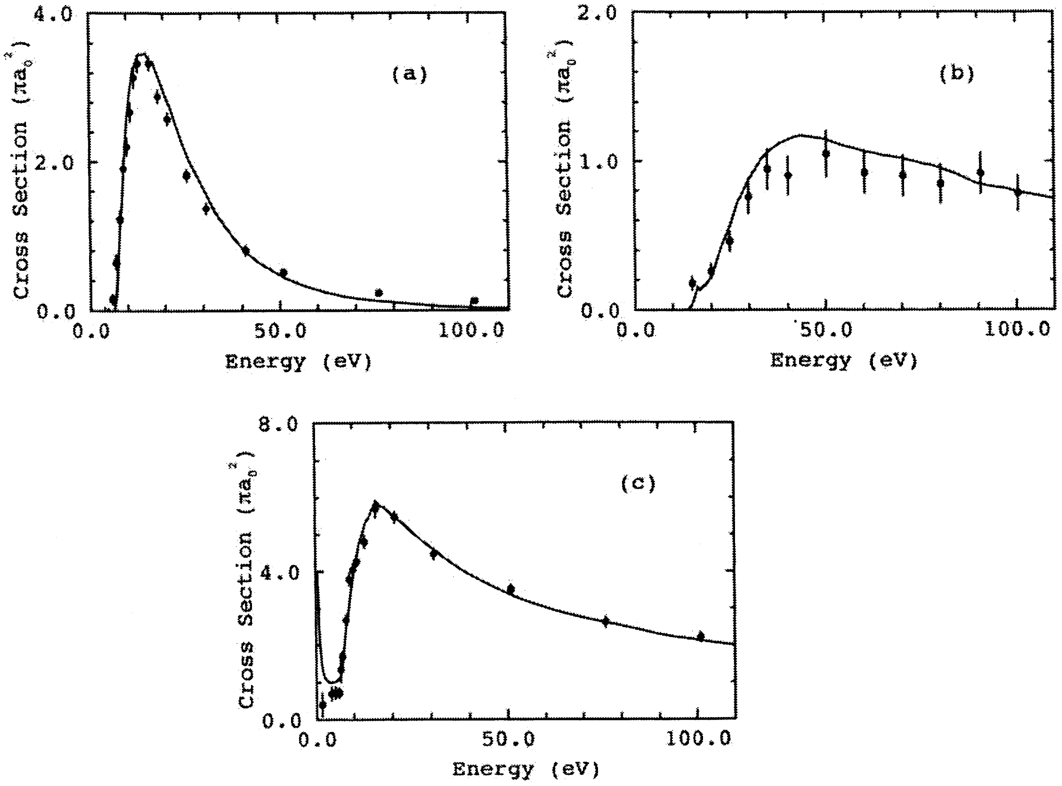

Figure 2: Positron scattering by H(1s): (a) total positronium formation; (b) ionization; (c) total cross section. Solid curve gives the 33-state results from ref. 14. Experimental data are from Zhou et al (ref. 21) and Jones et al (ref. 22).

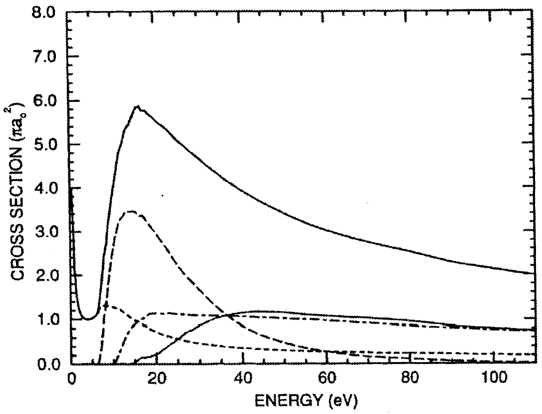

Figure 3: Cross sections in the 33-state approximation of ref. 14 for positron scattering from H(1s): upper solid curve, total cross section; long-dashed curve, total positronium formation; short-dashed curve, elastic scattering; dash-dot curve, H(2p) excitation; lower solid curve, ionization.

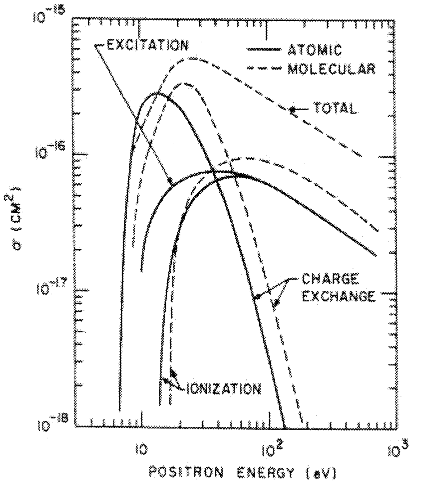

Figure 4: Ps formation (labelled "charge exchange"), ionization, discrete excitation, and total cross sections for e^+ scattering by H(1s) (solid curves) and H_2 (dashed curves), taken from ref. 23.

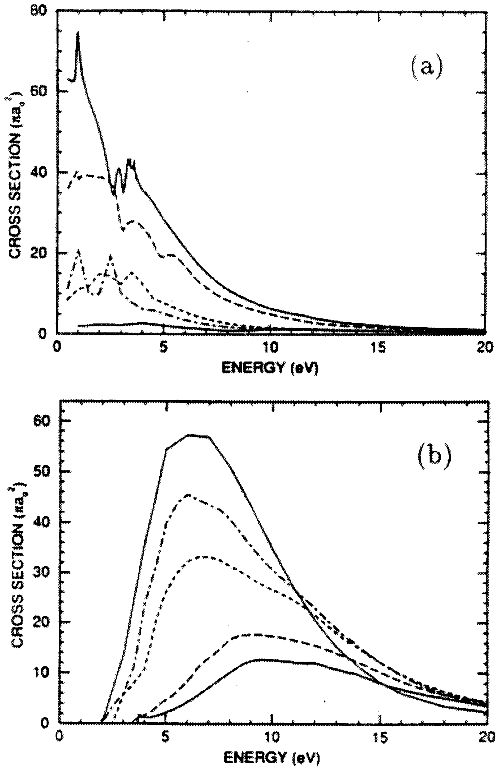

Figure 5: Positronium formation cross sections for Li, Na, K, Rb and Cs: (a) Ps(1s) formation; (b) positronium formation in excited states. Curves: upper solid in (a) and lower solid in (b), Li; long-dashed, Na; short-dashed, K; dash-dot, Rb; lower solid in (a) and upper solid in (b), Cs.

electron atoms, eg, Ps$^-$ formation, see (1). In principle, these could be incorporated into the coupled - state formalism as required. The formalism (8) has been applied to the "two - electron" targets He, Mg, Ca and Zn (refs. 17, 24), again, as for the "one -electron" targets, giving very good agreement with experiment where data exists (ie, He and Mg).

POSITRONIUM - ATOM SCATTERING

The development of monoenergetic Ps beams at University College London (refs. 25 - 28) has led to growing interest in Ps - atom collisions. Ps is the lightest neutral atomic projectile, being like a hydrogen atom but only 1/1000th of its mass, Ps collisions are therefore of considerable fundamental interest. It is important to specify the total spin state of the Ps which can be either singlet or triplet. Ps in the spin singlet state is called "para-positronium" (p-Ps), that in the triplet state "ortho-positronium" (o-Ps). The significance of this classification lies in the different lifetimes of these spin states against the annihilation of the electron and positron into photons. Thus p-Ps(1s) annihilates predominantly into two photons, each of 511 keV, with a lifetime of 0.125ns, while o-Ps(1s) annihilates predominantly into three photons with a much longer lifetime of 142ns. Because Ps has internal degrees of freedom, it is important in a collision experiment to define the electronic state of the beam. In the present state of the art, Ps beams consist essentially of o-Ps(1s) (ref. 27), the corresponding para species, p-Ps(1s), is too short - lived to be transportable as a beam. Experimental capability is at an early stage and measurements have, until recently, mostly been confined to total cross sections. In addition to the beam measurements there are also some cross section data at very low energies deduced from observations of the annihilation rate of o-Ps(1s) in various gases (refs. 25, 29 - 35). Providing that the atomic target is spin unpolarised and that the spins of the particles in the final state are not determined, the collision cross sections for o-Ps and p-Ps are the same (ref. 36). Under these assumptions, we can drop the "ortho" and "para" epithets and talk simply about Ps - atom cross sections.

The fact that Ps has internal degrees of freedom as well as the atom considerably complicates the theoretical description of Ps scattering. That the Ps centre of charge coincides with its centre of mass results in the direct Coulombic interaction between the Ps and the atom being very much weakened compared to the electron exchange interaction between the two particles. We have already met this exchange interaction in positron scattering by multi - electron atoms, see equation (8) where the exchange interaction between the formed Ps and the atomic ion is described by the non - local terms $L_{ib,i'b'}(\mathbf{R},\mathbf{R}')$. The exchange process is very difficult to calculate since it involves electron swapping between two different centres, the Ps and the atom. To illustrate what is involved, let us consider the most fundamental system, Ps scattering by H. For this system the Hamiltonian may be written as

$$\begin{aligned} H &= -\frac{1}{4}\nabla^2_{R_1} + H_{Ps}(\mathbf{t}_1) + H_A(\mathbf{r}_2) + V(\mathbf{R}_1,\mathbf{t}_1,\mathbf{r}_2) \\ &= -\frac{1}{4}\nabla^2_{R_2} + H_{Ps}(\mathbf{t}_2) + H_A(\mathbf{r}_1) + V(\mathbf{R}_2,\mathbf{t}_2,\mathbf{r}_1) \end{aligned} \tag{9}$$

where H_A and H_{Ps} are the atomic and positronium Hamiltonians given by

$$\begin{aligned} H_A(\mathbf{r}_i) &\equiv -\frac{1}{2}\nabla^2_i - \frac{1}{r_i} \\ H_{Ps}(\mathbf{t_i}) &\equiv -\nabla^2_{t_i} - \frac{1}{t_i} \end{aligned} \tag{10}$$

and V is the interaction between the Ps and the H atom,

$$V(\mathbf{R},\mathbf{t},\mathbf{r}) = \left(\frac{1}{|\mathbf{R}+\frac{1}{2}\mathbf{t}|} - \frac{1}{|\mathbf{R}+\frac{1}{2}\mathbf{t}-\mathbf{r}|}\right) - \left(\frac{1}{|\mathbf{R}-\frac{1}{2}\mathbf{t}|} - \frac{1}{|\mathbf{R}-\frac{1}{2}\mathbf{t}-\mathbf{r}|}\right) \tag{11}$$

In the above equations $\mathbf{R}_i \equiv (\mathbf{r}_p + \mathbf{r}_i)/2$ is the position vector of the Ps centre 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), where all position vectors are referred to the atomic nucleus as origin. Under the Hamiltonian (9) the spin of the positron, s_p, and the total electronic spin, S, of the two electrons are separately conserved. The spatial part of the collision wave function, Ψ^S, for scattering in the electronic spin state S is then expanded as

$$\Psi^S = \sum_{a,b} \left[G^S_{ab}(\mathbf{R}_1)\psi_a(\mathbf{r}_2)\phi_b(\mathbf{t}_1) + (-1)^S G^S_{ab}(\mathbf{R}_2)\psi_a(\mathbf{r}_1)\phi_b(\mathbf{t}_2)\right] \tag{12}$$

where, as before, ψ_a (ϕ_b) is a H (Ps) state satisfying (5), either an eigenstate or a pseudostate. Substituting (12) into the Schrödinger equation and projecting with $\psi_a(\mathbf{r}_2)\phi_b(\mathbf{t}_1)$ leads to coupled equations of the form

$$\left(\nabla^2_R + p^2_{ab}\right) G^S_{ab}(\mathbf{R}) = 4\sum_{a'b'} \left[V_{ab,a'b'}(\mathbf{R})G^S_{a'b'}(\mathbf{R}) + (-1)^S \int L_{ab,a'b'}(\mathbf{R},\mathbf{R}')G^S_{ab}(\mathbf{R}')d\mathbf{R}'\right] \tag{13}$$

where the total energy, E, is given by

$$E = \frac{p^2_{ab}}{4} + \epsilon_a + E_b \tag{14}$$

and

$$V_{ab,a'b'}(\mathbf{R}) \equiv \langle\psi_a(\mathbf{r})\phi_b(\mathbf{t})\,|V(\mathbf{R},\mathbf{t},\mathbf{r})|\,\psi_{a'}(\mathbf{r})\phi_{b'}(\mathbf{t})\rangle \tag{15}$$

As before, the non-local couplings $L_{ab,a'b'}(\mathbf{R},\mathbf{R}')$ describe how the state $\psi_{a'}\phi_{b'}$ is converted into the state $\psi_a\phi_b$ by electron exchange between the Ps and the H. It is clear from (11) that

$$V(\mathbf{R},\mathbf{t},\mathbf{r}) = -V(\mathbf{R},-\mathbf{t},\mathbf{r}) \tag{16}$$

From this it follows that the direct potentials $V_{ab,a'b'}$ are zero unless the Ps states ϕ_b and $\phi_{b'}$ have opposite parity. The electron exchange terms do not share this symmetry with the result that exchange is enhanced relative to direct scattering. Indeed, in the simplest coupled - state approximation, static - exchange, where only one atom and one Ps state are retained in (12), the equations (13) reduce to a single equation

$$\left(\nabla^2_R + p^2_{ab}\right) G^S_{ab}(\mathbf{R}) = (-1)^S 4 \int L_{ab,ab}(\mathbf{R},\mathbf{R}')G^S_{ab}(\mathbf{R}')d\mathbf{R}' \tag{17}$$

which contains no direct potential and so is driven solely by the exchange interaction.
It is clear from (12) that the scale of the coupled - state calculation will escalate rapidly as the product of the number of atom states ψ_a times the number of Ps states ϕ_b. For this reason the first calculations adopted a “frozen target” approximation, ie, retained only one atom state in the expansion (12). In figure 6 we show the results of a 22 - state frozen target calculation of Ps(1s) + H(1s) scattering (ref. 37). The 22 states are Ps states and 19 of theses are pseudostates. We see from this figure that, at the higher energies, the main outcome of a collision is ionization of the Ps, hence the importance of including ionization channels (pseudostates) in the coupled - state approximation. Figure 6 shows that elastic scattering “dies” once ionization switches on and that discrete excitation of the Ps(1s) to Ps(n=2) is small at all impact energies, at least in this approximation. Also shown in figure 6 is a first Born estimate (ref. 38) of the contribution to the total cross section coming from collisions in which the H atom is excited or ionized, this suggests that target excitation/ionization is only important above about 20 eV. However, what the first Born approximation cannot tell us is how the solutions to the coupled equations (13) would be changed, for example, for elastic scattering at very low energies, if excited or ionized states of the atom were added to the expansion (12). The inclusion of these states would permit processes in which, for instance, the atom could be “virtually” excited/ionized and then de - excited/de - ionized back to its initial state, the overall result being no change in the observed state of the atom. Such processes, which are really just an interpretation of

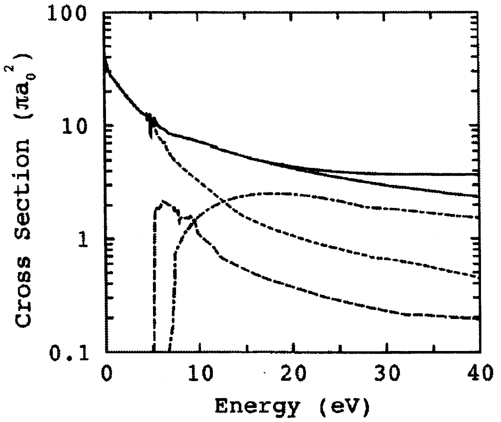

Figure 6: Frozen target total cross section, and its components, for Ps(1s)+H(1s) scattering (ref. 37). Curves: lower solid, total cross section; upper solid, frozen target total cross section with first Born estimate from ref. 38 for H target excitation and ionization added; short-dashed, Ps(1s) elastic scattering; long-dashed, Ps(n=2) excitation; dash-dotted, Ps ionization.

how the coupled equations "work", are referred to as "virtual" excitations[2] and are to be distinguished from real observable excitations which are represented by the first Born approximation in figure 6.

A noticeable feature in figure 6 is the structure near 5eV. A careful analysis of the partial wave contributions to the elastic cross section of figure 6 reveals that this structure corresponds to resonances in the electronic spin singlet partial waves. This is illustrated in figure 7 for the S-, P- and D-waves. However, no resonances appear in the triplet partial waves (see figure 12). What can be the origin of this? We shall return to this point later.

Unfortunately, experimental measurements on an atomic hydrogen target will not be feasible for some time yet. The targets most amenable to experimental study are the noble gases. In figures 8 to 10 we show some experimental results compared with frozen target calculations analogous to that of figure 6 (refs. 39, 40). We begin with figure 8 which compares the frozen target results for He (ref. 39), Ne and Ar (ref. 40) with cross sections deduced from annihilation measurements at very low energies (refs. 29-35). The experimental cross sections correspond to the momentum transfer cross section

$$\sigma_{mom} = \int (1 - \cos\theta) \frac{d\sigma_{el}}{d\Omega} d\Omega \tag{18}$$

where $d\sigma_{el}/d\Omega$ is the elastic differential cross section and θ is the scattering angle of the Ps. At these low energies only elastic scattering is possible. Figure 8 shows two theoretical cross sections, one the total elastic cross section, the other the momentum transfer cross section. We first note the importance of distinguishing between these two cross sections even at such low energies. Secondly, we see that the agreement between theory and experiment on the momentum transfer cross section is not particularly good, especially in the region of the most recent measurements (ref. 33) near 1eV. Figure 9 compares frozen target calculations (refs. 39, 40) with beam measurements of the total cross section for He and Ar (refs. 26, 27, 28) at impact energies of 10eV and above. Except at the lowest energy, the frozen target theory now underestimates the measured cross sections. An exciting new experimental development has been the first measurement of the fragmentation cross section for

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[2] Henceforth we shall use the term "excitation" to mean both discrete excitation and ionization.

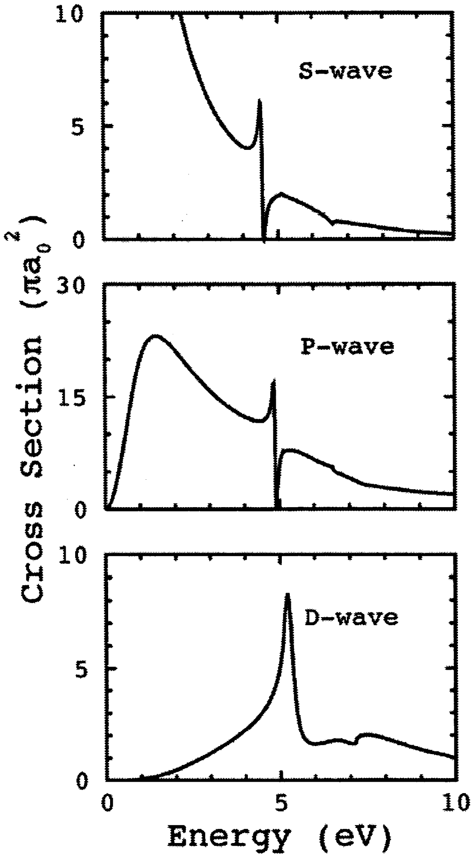

Figure 7: Electronic spin singlet elastic partial wave cross sections in the frozen target 22-state approximation of ref. 37.

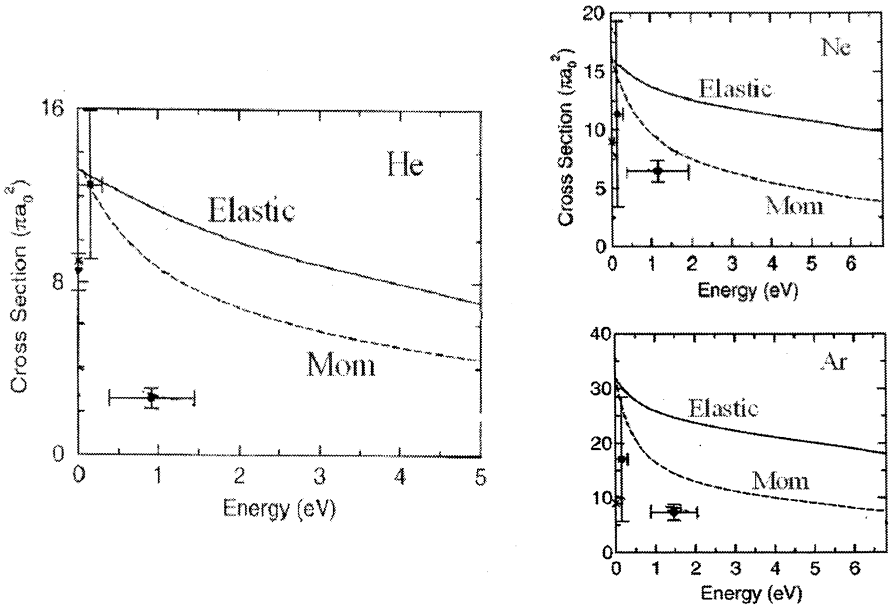

Figure 8: Total elastic and momentum transfer cross sections for Ps(1s) + He, Ne, Ar scattering in the frozen target approximation (refs. 39, 40). Experimental data: triangle, Canter et al (ref. 29); cross, Coleman et al (ref. 31); square, Nagashima et al (refs. 32, 34); circle, Skalsey et al (ref. 33).

Ps (refs. 41, 42) This is shown for a He target in figure 10 where comparison is also made with frozen target results (ref. 39). The agreement between theory and experiment is very satisfactory and contrasts with the difference on the total cross section shown in figure 9. Clearly, there is much still to be understood here. But, even more impressive is the newly acquired experimental capability to measure the Ps fragmentation cross section differential in the longitudinal energy of the ejected positron. The measurements for a He target (refs. 41, 42), which are absolute, are shown in figure 11. It is seen from this figure that, with increasing impact energy E, the differential cross section starts to exhibit a peak near $((E - 6.8)/2)$eV. Also shown in figure 11 are theoretical cross sections calculated in a frozen target approximation, not in this case using a coupled pseudostate approximation but an impulse approximation (ref. 43). Overall, the agreement between theory and experiment, both in shape and magnitude, is, all things considered, remarkably good. From the theory it is clear that the development of the peak arises from the desire of the Ps to fragment into the forward direction with roughly equal energies for the ejected electron and positron.

Let us now move on from the frozen target approximation and see what happens when excited target states are included in the expansion (12). Figure 12 shows elastic partial wave cross sections for Ps(1s) + H(1s) scattering calculated in the frozen target approximation and in an approximation in which target excitation is taken into account (ref. 36). In all of the cases shown we see a substantial difference between the two approximations. It is clear that at these energies target excitation, which is virtual in this energy range, is very important for both electronic singlet and triplet scattering. From the singlet cross sections of figure 12 we see that the resonance structure that was observed in the frozen target approximation (figure 7) is preserved but moved down in energy slightly. Figure 13 shows the total cross section in the energy range 0 to 6eV in the two approximations. From this we see that target excitation reduces the very low energy cross section substantially (by about 30%) although giving a slightly higher cross section, in the form of a bump,

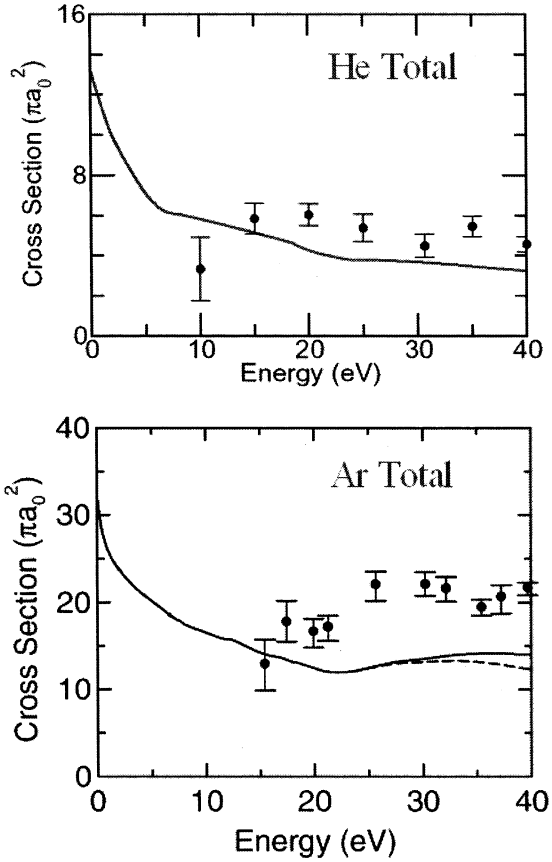

Figure 9: Total cross section for Ps(1s) + He (ref. 39) and Ps(1s) + Ar (ref. 40) scattering in the frozen target approximation: solid curve includes first Born estimate for target excitation (negligible for He in the energy range shown), dashed curve is pure frozen target result. Experimental data are from refs. 26, 27, 28.

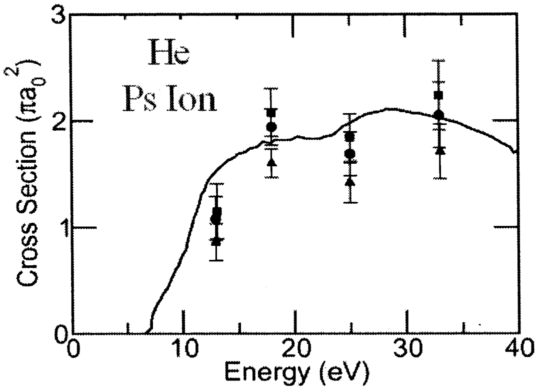

Figure 10: Cross section for fragmentation of Ps in Ps(1s) + He(1^1S) collisions. Curve, frozen target approximation of ref. 39. Experimental data from ref. 42.

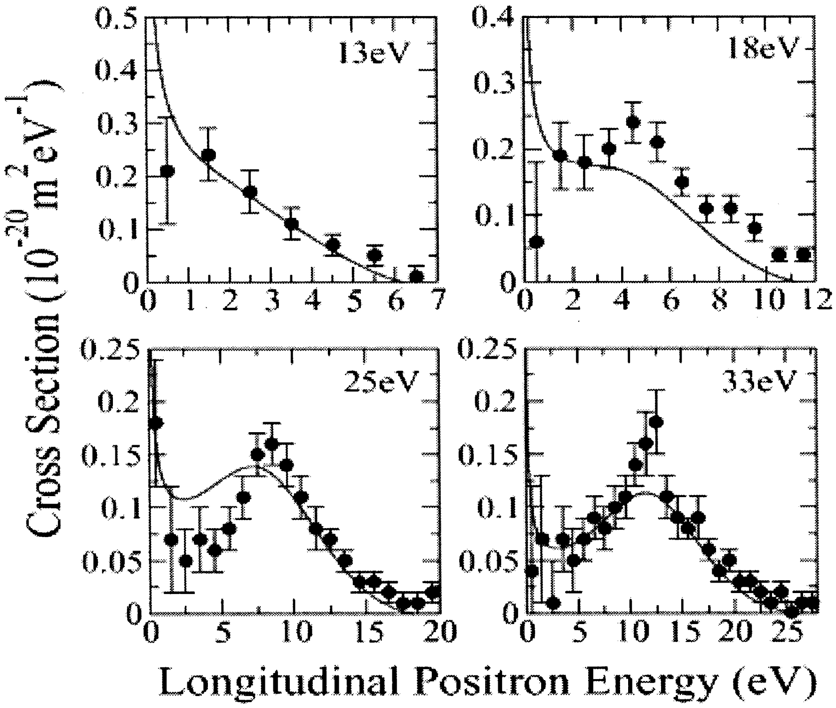

Figure 11: Cross sections differential in the longitudinal energy of the ejected positron for Ps(1s) fragmentation in He(1^1S) at Ps impact energies of 13, 18, 25 and 33eV: curve, impulse approximation calculation of ref. 43; experimental data from refs. 41, 42.

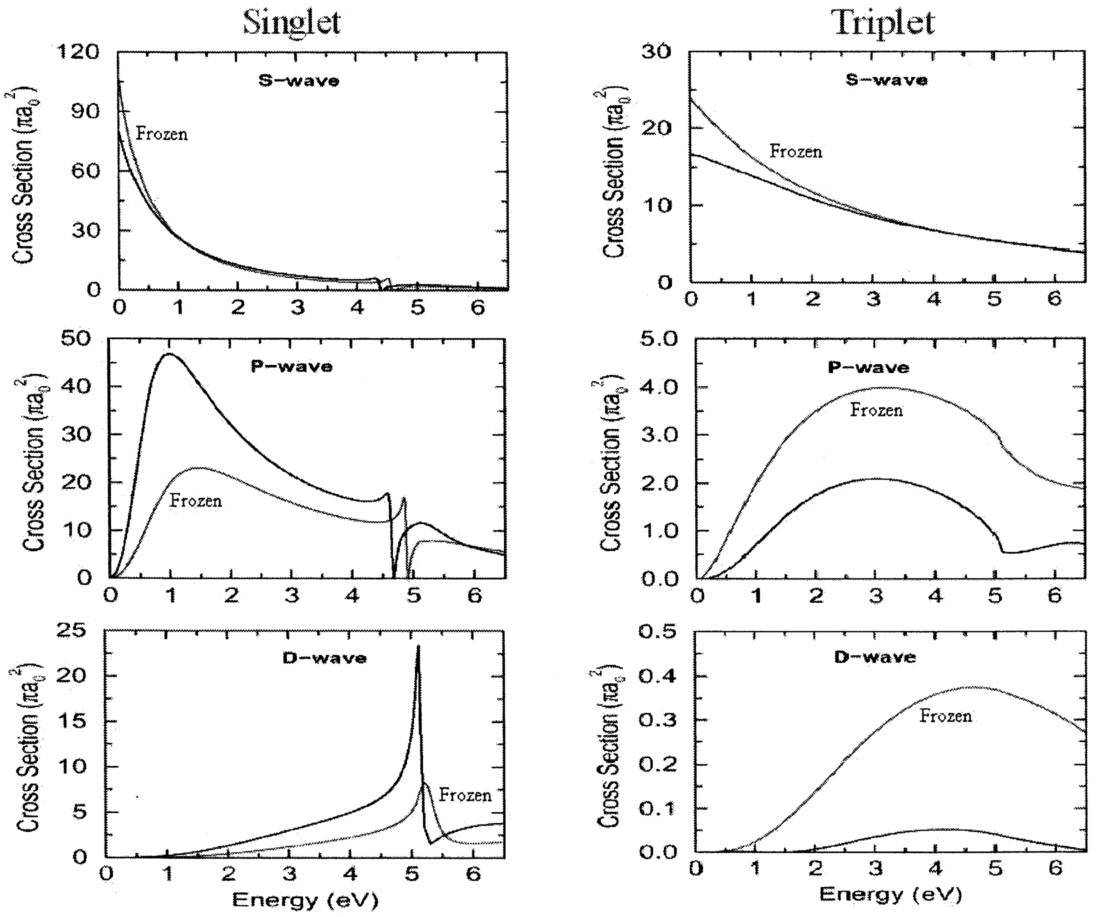

Figure 12: Elastic partial wave cross sections for Ps(1s) + H(1s) scattering in the frozen target approximation (Frozen) and in an approximation including target excitation (ref. 36).

at more elevated energies. Allowing for target excitation also seems to enhance the resonance structure near 5eV somewhat. Could virtual target excitation explain the discrepancies we are seeing between the frozen target theory and experiment in figure 8?

It has been suggested that Ps + He scattering should bear a similarity to Ps + H electronic spin triplet scattering since in both cases the Ps electron is prevented from occupying the same space as an atomic electron by the Exclusion Principle. Figure 14 shows S and P partial waves for Ps(1s) + He(1^1S) elastic scattering both in a frozen target approximation and in an approximation allowing for target excitation (ref. 44). Consistent with the suggestion, we note a clear similarity between figures 14 and 12. However, the differences between the two approximations is smaller for He. This is to be expected since He is less easily excited than H. Figure 15 now shows the consequences for the momentum transfer cross section in He. Allowing for target excitation does move the cross section towards the experiments of Canter et al, Rytsölä et al and Skalsey et al but there is still substantial disagreement. However, as Di Rienzi and Drachman (ref. 45) have most pertinently pointed out, the theoretical situation is obscured by uncertainty about the sensitivity of results to the use of approximate He target wave functions. This issue needs to be resolved.

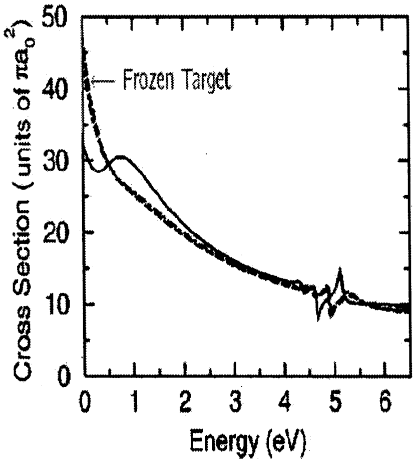

Figure 13: Total cross section for Ps(1s) + H(1s) scattering. Curves: dashed, frozen target results; solid, approximation including target excitation (ref. 36).

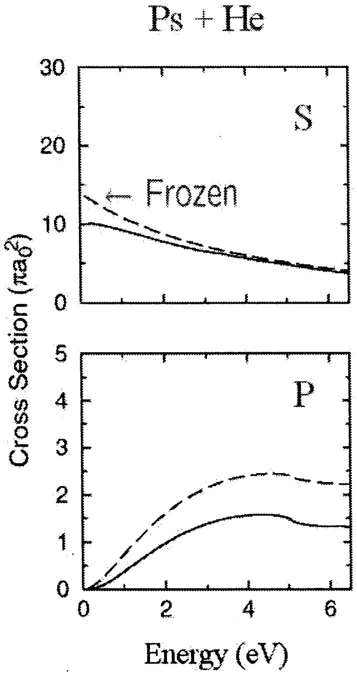

Figure 14: Partial wave cross sections for Ps(1s) + He(1^1S) elastic scattering in the frozen target approximation (dashed curve) and in an approximation allowing for target excitation (from ref. 44).

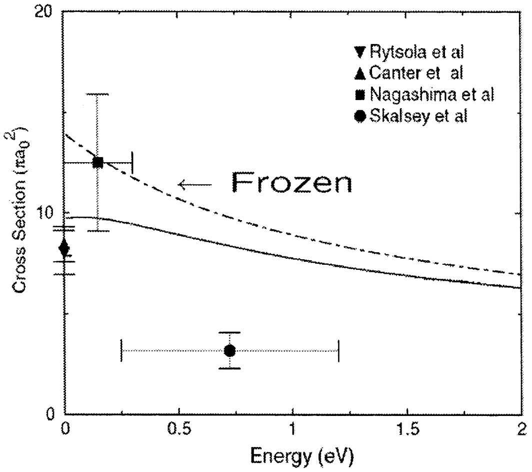

Figure 15: Momentum transfer cross section for Ps(1s) + He(1^1S) scattering. Theory (from ref. 44): dashed curve, frozen target approximation; solid curve, approximation allowing for target excitation. Experiment: square, Nagashima et al (ref. 32); up triangle, Canter et al (ref. 29); down triangle, Rytsölä et al (ref. 30); circle, Skalsey et al (ref. 35).

Let us now return to Ps + H scattering and list the processes that are possible. They are

$$
\begin{aligned}
Ps(1s)+H(1s) &\longrightarrow Ps(nlm)+H(NLM) && (19a)\\
&\longrightarrow e^+ + e^- + H(NLM) && (19b)\\
&\longrightarrow Ps(nlm)+p+e^- && (19c)\\
&\longrightarrow e^+ + e^- + p + e^- && (19d)\\
&\longrightarrow e^+ + H^- && (19e)\\
&\longrightarrow Ps^- + p && (19f)
\end{aligned}
$$

where nlm (NLM) labels any bound state of Ps (H). Using pseudostates, the approximation (12) takes account of (19a) to (19d). In the sense that, in principle, the sets of states ϕ_a and ψ_b could be taken to completeness, (19e) and (19f) are also implicit in (12). However, in practice we need to add (19e) and (19f) explicitly if we want to calculate these processes. The expansion (12) then has to be modified to

$$
\begin{aligned}
\Psi^S &= \sum_{a,b} [G^S_{ab}(\mathbf{R}_1)\psi_a(\mathbf{r}_2)\phi_b(\mathbf{t}_1) + (-1)^S G^S_{ab}(\mathbf{R}_2)\psi_a(\mathbf{r}_1)\phi_b(\mathbf{t}_2)]\\
&\quad + F(\mathbf{r}_p)\psi^-(\mathbf{r}_1,\mathbf{r}_2)\delta_{S,0} + H\left(\frac{\mathbf{r}_1+\mathbf{r}_2+\mathbf{r}_p}{3}\right)\phi^-(\mathbf{r}_1-\mathbf{r}_p,\mathbf{r}_2-\mathbf{r}_p)\delta_{S,0} \qquad (20)
\end{aligned}
$$

where ψ^- (ϕ^-) is the H^- (Ps^-) wave function. The new terms only contribute to the electronic spin singlet wave function since H^- and Ps^- are electronic singlets. So far, calculations have only been made including the H^- term (refs. 46, 44). The results for the elastic partial waves are shown in figure 16. We see that at the lower energies (below 3.5eV) adding the H^- term does not radically alter the results obtained with inclusion of target excitation, however, in the resonance region between 3.5 and 6.05eV there is a spectacular change in the resonance structure. Whereas the approximation without the H^- term produced only one prominent resonance in each partial wave

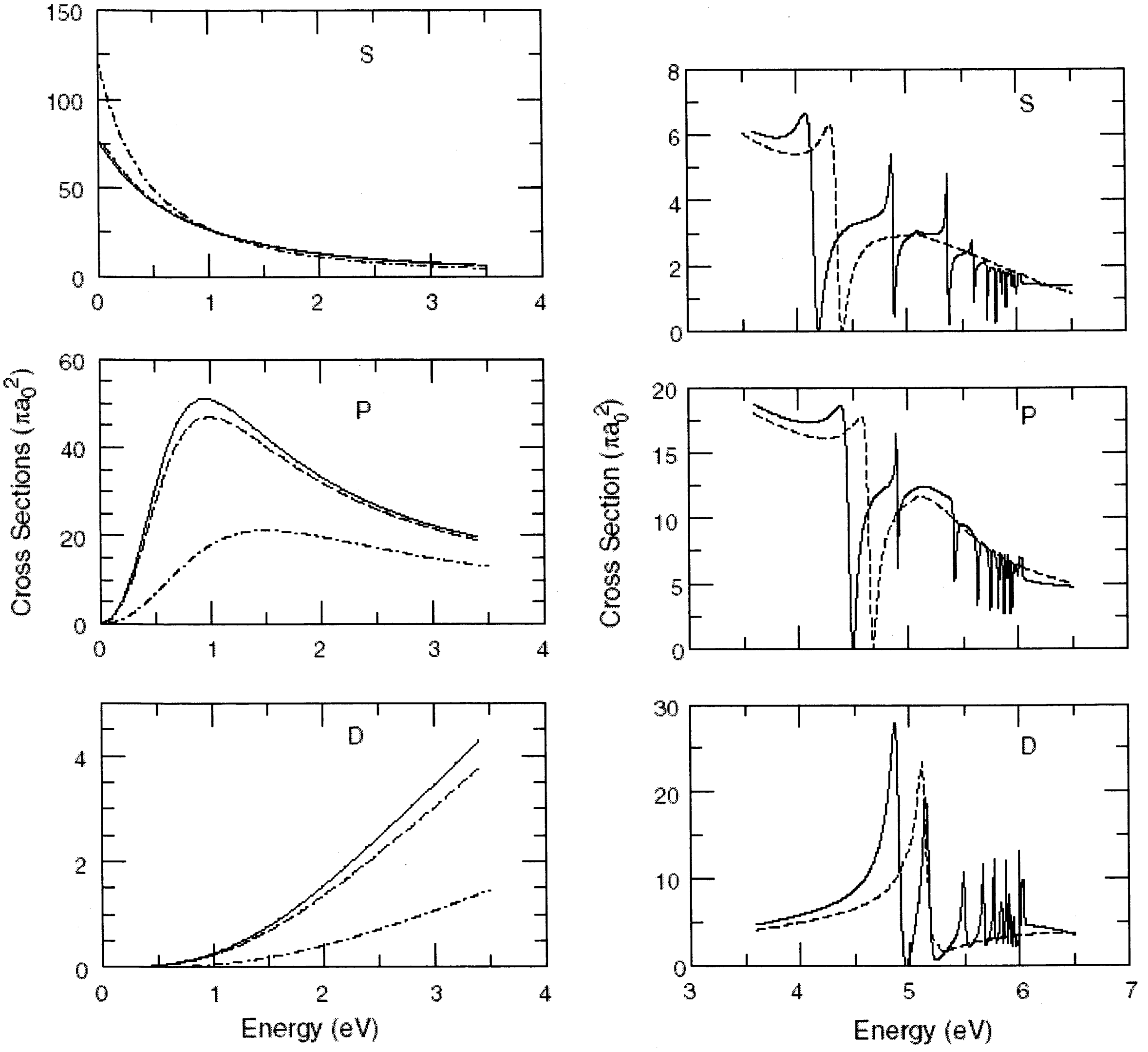

Figure 16: Electronic spin singlet partial wave cross sections for Ps(1s) - H(1s) elastic scattering (ref. 44). Curves: dash - dot, frozen target approximation; dashed, approximation allowing for target excitation; solid, approximation allowing for target excitation and also including the H^- channel.

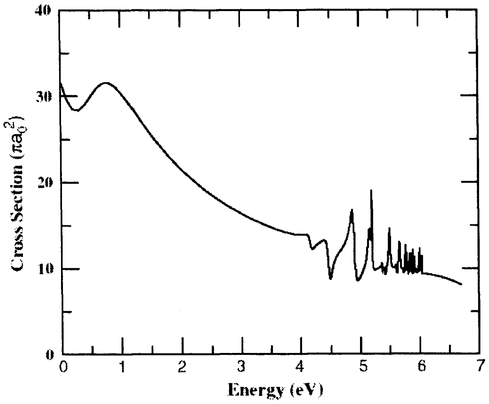

Figure 17: Total cross section for Ps(1s) + H(1s) scattering (from ref. 44).

Table 1: PsH Binding Energy

Approximation	Energy (eV)
Frozen Target	0.634
Target Excitation	0.994
Target Excitation + H^-	1.03
Exact (ref. 50)	1.067

(figures 7 and 12), the addition of the H$^-$ term gives a much richer resonance structure in each partial wave. We now understand the origin of the resonances, they are unstable states of the positron attached to the H$^-$ ion. What we have in each partial wave is an infinite sequence of Rydberg resonances converging on to the H$^-$ formation threshold at 6.05eV. Should this be a surprise? No. As long ago as 1975 Dick and Ken Houston found the first of these resonances in S-wave scattering (ref. 47), and in an insightful paper of 1979 (ref. 48) Dick had already given the correct interpretation. What we see in figure 16 is a visual realisation of his foresight. At this time we do not know the effect of adding the Ps$^-$ channel. That is an interesting new direction for future investigations.

At this point it is useful to summarise where we presently stand with the Ps - H system. In figure 17 we show the latest results (ref. 44) for the total cross section. This calculation allows for target excitation and includes the H$^-$ channel. Also shown in figure 18 is the first realistic calculation of the H$^-$ formation cross section (ref. 46). Note that this cross section is finite at threshold since the final state involves two charged particles, the positron and the H$^-$. However, everything is not completely settled in the low energy region. The Ps + H system has one true bound state, first predicted by Ore in 1951 (ref. 49). In table 1 we show the energy of this bound state as calculated in the various coupled state approximations. We see that the frozen target approximation can only account for about 60% of the energy. Allowing for target excitation gets us to about 93%. Further addition of the H$^-$ channel brings us to 96.5% which is 3.5% short of very accurate variational results (ref. 50). What is the cause of this discrepancy? Is it the missing Ps$^-$ channel?

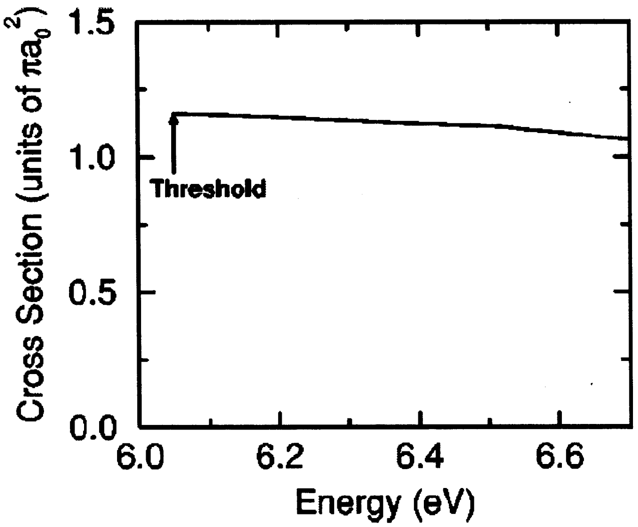

Figure 18: H^- formation cross section for Ps(1s) colliding with H(1s) (from ref. 46).

Finally, It is interesting to compare the early pioneering calculations of Dick and Ken Houston on Ps(1s) + H(1s) scattering (refs. 47, 51) with the most up-to-date results (Van Reeth and Humberston, ref. 52). In table 2 we show the scattering length and effective range for this system. The agreement between the early work and the most recent is remarkably good. Considering how restricted computing facilities were in the 1970s, Dick and Ken had done a really good job.

Table 2: Scattering Lengths and Effective Ranges (in au) for Ps(1s) + H(1s) Scattering

	Van Reeth and Humberston (2003) (ref. 52)	Drachman and Huston (1975, 1976) (refs. 47, 51)
Singlet Scattering Length	4.311	4.5
Triplet Scattering Length	2.126	2.36
Singlet Effective Range	2.27	2.2
Triplet Effective Range	1.39	1.31

POSITRON SCATTERING BY H^-

In 1991 Jack Straton and Dick published an heroic attempt to get a handle on the very difficult problem of positron scattering by H^- (ref. 53). It seems that this process is of Astrophysical importance. They looked at a series of approximations based on the Fock - Tani/Coulomb Born formalism with the purpose of calculating Ps formation. Because $e^+ + H^-$ is such a difficult system, they restricted their calculations to the case where both the Ps and the residual H atom were left in the 1s ground state. Now, $e^+ + H^-$ scattering is just the inverse of the reaction

$$\mathrm{Ps} + \mathrm{H} \longrightarrow e^+ + \mathrm{H}^- \tag{21}$$

and so must be contained within the approximation (20). Inspired by the work of Dick and Jack, McAlinden et al (ref. 54) decided to see what (20) would yield. Like Dick and Jack, they decided to restrict themselves to reactions in which the H atom would be left in the 1s state, ie, they included only the H(1s) state in the sum of (20). Their approximation amounted to a frozen target calculation with the addition of the H^- channel. [3] However, because they used Ps eigenstates and pseudostates in the expansion (20) they were able to take account of Ps formation in excited states, Ps(nlm), and, through the Ps pseudostates, ionization. Some of their results are shown in table 3 where they are compared with Dick and Jack's calculation.

Table 3: Ps Formation Cross Sections (in πa_0^2) for $e^+ + H^-$ Scattering

	Straton and Drachman (ref. 53)	McAlinden et al (ref. 54)		
Energy (eV)	Ps(1s)	Ps(1s)	Ps(2s)	Ps(2p)
0.1	904	567	715	2702
0.5	178	116	134	651
1.0	82.5	57	48	290
5.0		13	4.7	22
10.0		5.0	1.0	3.5

Dick and Jack obtained a range of values for the Ps(1s) formation cross section depending upon the approximation used, the numbers shown in table 3 correspond to their smallest values. Taking account of what a difficult problem this is, it is fair to say that Dick and Jack's results are in the same "ball park". However, the results of McAlinden et al show that, at the lower energies, Ps formation in the $n = 2$ states is much more important than Ps(1s) formation. Ps formation in the $n = 1$ and $n = 2$ states are exothermic processes, the cross sections diverging as $1/E$ as the impact energy, E, tends to zero (ref. 54). It was Dick who brought this to our attention at the Positron Satellite of the Santa Fe ICPEAC in 2001. At the time we were under the impression that the divergence was $1/\sqrt{E}$. In figure 19 we show aggregate Ps formation cross sections from McAlinden et al in the impact energy range 0 to 10eV. Interestingly, we see that Ps($n \geq 3$) formation is comparable to Ps(1s + 2s + 2p) formation at energies above 2eV. However, as figure 20 shows, ionization of the H^- soon starts to dominate with increasing impact energy.

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[3] The Ps^- channel was also omitted from (20).

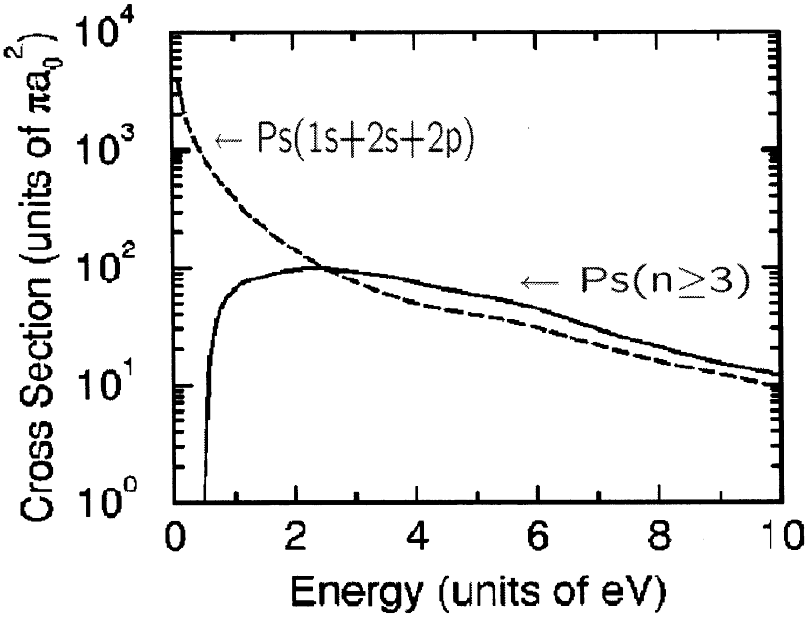

Figure 19: Aggregate Ps formation cross sections from McAlinden et al (ref. 54).

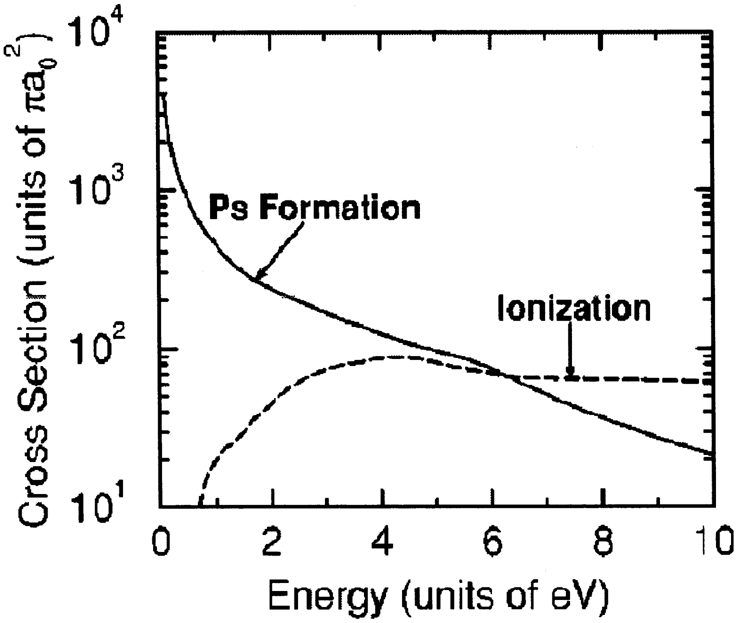

Figure 20: Direct ionization and total Ps formation cross sections from McAlinden et al (ref. 54).

CONCLUDING REMARKS

We are reminded of a remark by Isaac Newton (ref. 55): “If I have seen further it is by standing on ye shoulders of Giants”. If we have seen further it is by standing on the shoulders of giants like Dick and Aaron!

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