POSITRON SCATTERING BY ATOMIC HYDROGEN USING OPTICAL POTENTIALS AND WITH POSITRONIUM FORMATION

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INTRODUCTION

We consider the scattering of positrons by H(1s) in a two-state model which incorporates optical potentials. The model explicitly describes elastic scattering, i.e.,

$$e^+ + H(1s) \rightarrow e^+ + H(1s) \qquad (1)$$

and Ps(1s) formation, i.e.,

$$e^+ + H(1s) \rightarrow Ps(1s) + p. \qquad (2)$$

The inelastic processes

$$e^+ + H(1s) \rightarrow e^+ + H^* \qquad (3)$$

$$Ps(1s) + p \rightarrow Ps^* + p \qquad (4)$$

where * stands for a state other than 1s, are implicitly taken into account through the optical potentials, which also allow for polarization of H(1s) and Ps(1s).

APPROXIMATIONS

Three levels of approximation are investigated which serve to illustrate the effects of polarization, absorption and positronium formation.

(i) Full Approximation (ELV2 + PSV2)

We start from the coupled static approximation. The wave function for the system in this approximation is

$$\Psi(\underline{r}_p, \underline{r}_e) = F(\underline{r}_p)\psi_{1s}(\underline{r}_e) + G(\underline{R})\phi_{1s}(\underline{r}) \qquad (5)$$

Here $\underline{r}_p$ and $\underline{r}_e$ are the coordinates of the positron and the electron relative to the proton as origin, $R \equiv (\underline{r}_p + \underline{r}_e)/2$, $\underline{r} \equiv \underline{r}_p - \underline{r}_e$, ψ_{1s} is the 1s wave function of atomic hydrogen, and ϕ_{1s} is that of ground state positronium. The approximation (5) leads, in the usual manner, to the pair of coupled equations (in atomic units)

$$(\nabla_p^2 + k_o^2)\, F(\underline{r}_p) = 2\, V_{oo}(r_p) F(\underline{r}_p) + 2 \int K(\underline{r}_p, \underline{R})\, G(\underline{R})\, d\underline{R} \qquad (6a)$$

$$(\nabla_R^2 + p_o^2)\, G(\underline{R}) = 4 \int K(\underline{r}_p, \underline{R})\, F(\underline{r}_p)\, d\underline{r}_p \qquad (6b)$$

where V_{oo} is the static potential of H(1s), $K(\underline{r}_p, \underline{R})$ is the positronium formation coupling kernel, k_o is the momentum of the incident positron, and p_o is the momentum of the positronium.

Our full approximation is obtained by adding second order optical potentials[1] $V_{oo}^{(2)}$ and $V_{pp}^{(2)}$ to the H(1s) and Ps(1s) channels of (6), i.e.,

$$(\nabla_p^2 + k_o^2)\, F(\underline{r}_p) = 2\, V_{oo}(r_p)\, F(\underline{r}_p) + 2\, V_{oo}^{(2)}\, F(\underline{r}_p) + 2 \int K(\underline{r}_p, \underline{R})\, G(\underline{R})\, d\underline{R} \qquad (7a)$$

$$(\nabla_R^2 + p_o^2)\, G(\underline{R}) = 4\, V_{pp}^{(2)}\, G(\underline{R}) + 4 \int K(\underline{r}_p, \underline{R})\, F(\underline{r}_p)\, d\underline{r}_p \; . \qquad (7b)$$

The real part of the potential $V_{oo}^{(2)}$ contains the polarizability of H(1s) while the imaginary part allows for the direct excitations (3). Similarly, $V_{pp}^{(2)}$ contains the polarizability of Ps(1s) in its real part while representing the inelastic processes (4) through its imaginary part. The construction of these potentials is described later. Thus, in the approximation (7) both H(1s) and Ps(1s) can be polarized and excited through the direct collisions (3) and (4).

(ii) Simpler Approximation (ELV2 + PS)

In this approximation $V_{pp}^{(2)}$ is dropped from (7b) but $V_{oo}^{(2)}$ is retained in (7a).

Thus the Ps(1s) cannot be polarized or excited by the proton. Only H(1s) can be polarized and excited by the positron.

(iii) Simplest Approximation (ELV2)

Here we drop positronium formation completely and first look at the elastic scattering channel, i.e., we solve

$$(\nabla_p^2 + k_o^2)\, F(\underline{r}_p) = 2\, V_{oo}(r_p)\, F(\underline{r}_p) + 2\, V_{oo}^{(2)} F(\underline{r}_p) \qquad (8)$$

Construction of Optical Potentials[1]

The exact second order optical potentials $V_{oo}^{(2)}(\underline{r}_p,\underline{r}'_p)$ and $V_{pp}^{(2)}(\underline{R},\underline{R}')$ are non-local and energy dependent. Their plane wave matrix elements

$$-\frac{1}{2\pi} \int e^{-i\underline{k}_f\cdot\underline{r}_p}\, V_{oo}^{(2)}(\underline{r}_p,\underline{r}'_p) \times e^{i\underline{k}_o\cdot\underline{r}'_p}\, d\underline{r}_p\, d\underline{r}'_p \qquad (9a)$$

and

$$-\frac{1}{\pi} \int e^{-i\underline{p}_f\cdot\underline{R}}\, V_{pp}^{(2)}(\underline{R},\underline{R}')\, e^{i\underline{p}_o\cdot\underline{R}'}\, d\underline{R}\, d\underline{R}' \qquad (9b)$$

are equal to the second Born terms

$$f_{oo}^{B2}(k_o,q) \equiv -\frac{1}{8\pi^4} \sum_{n\neq 1s} \int d\underline{k} \langle \underline{k}_f\psi_{1s}|V|\underline{k}\psi_\pi\rangle \times \frac{\langle \underline{k}\psi_n|V|\underline{k}_o\psi_{1s}\rangle}{k_o^2 + 2(\varepsilon_o-\varepsilon_n) - k^2 + i\eta} \qquad (10a)$$

$$f_{pp}^{B2}(p_o,Q) \equiv -\frac{1}{2\pi^4} \sum_{n\neq 1s} \int d\underline{p}\, \langle \underline{p}_f\phi_{1s}|W|\underline{p}\phi_n\rangle \times \frac{\langle \underline{p}\phi_n|W|\underline{p}_o\phi_{1s}\rangle}{p_o^2 + 4(E_o - E_n) - p^2 + i\eta} \qquad (10b)$$

which describe elastic e^+ + H(1s) and Ps(1s) + p scattering respectively. In (10) $\underline{q} \equiv \underline{k}_o - \underline{k}_f$, $\underline{Q} \equiv \underline{p}_o - \underline{p}_f$, $\psi_n(\phi_n)$ is a hydrogen (positronium) eigenstate with energy $\varepsilon_n(E_n)$, $|\underline{k}\rangle \equiv e^{i\underline{k}\cdot\underline{r}_p}$, $|\underline{p}\rangle \equiv e^{i\underline{p}\cdot\underline{R}}$, $V \equiv \frac{1}{r_p} - \frac{1}{|\underline{r}_p - \underline{r}_e|}$, $W \equiv -\frac{1}{r_e} + \frac{1}{r_p}$ and the limit $\eta \to 0+$ is to be understood.

We use energy dependent local approximations[1] $V_{oo}^{(2)}(r_p)$ and $V_{pp}^{(2)}(R)$ which have the same on-energy-shell plane wave matrix elements as the exact potentials:

$$-\frac{1}{2\pi} \int e^{-i\underline{k}_f\cdot\underline{r}_p}\, V_{oo}^{(2)}(r_p)\, e^{i\underline{k}_o\cdot\underline{r}_p}\, d\underline{r}_p = f_{oo}^{B2}(k_o,q) \qquad (11)$$

where $|\underline{k}_f| = |\underline{k}_o|$. Then by simple Fourier inversion

$$V_{oo}^{(2)}(r_p) = -\frac{1}{\pi} \int_o^\infty \frac{\sin qr_p}{qr_p}\, f_{oo}^{B2}(k_o,q) \times q^2 dq \qquad (12)$$

Expressions similar to (11) and (12) hold for $V_{pp}^{(2)}(R)$.

The second Born amplitude f_{oo}^{B2} is calculated using an orthonormal pseudostate basis $\overline{\psi}_n$ of 1s, 2s $\overline{3s}$, $\overline{4s}$, 2p, $\overline{3p}$, $\overline{4p}$, $\overline{3d}$ and $\overline{4d}$ states. Normally this is the basis of Fon et al[2], but a similar second basis is also employed to avoid problems with pseudostate thresholds. The pseudostates diagonalize the atomic Hamiltonian:

$$\langle\overline{\psi}_n|H_{atom}|\overline{\psi}_m\rangle = \overline{\varepsilon}_n\, \delta_{nm} \quad . \qquad (13)$$

The pseudostate approximation to f_{oo}^{B2} is given by the same formula (10a) but with ψ_n and ε_n replaced by $\overline{\psi}_n$ and $\overline{\varepsilon}_n$.

A positronium pseudostate basis $\overline{\phi}_n$ is similarly used to evaluate f_{pp}^{B2}. This basis is derived from the $\overline{\psi}_n$ basis by taking

$$\overline{\phi}_n(\underline{r}) = \frac{1}{2\sqrt{2}}\, \overline{\psi}_n\,(\underline{r}/2) \quad . \qquad (14)$$

It immediately follows that

$$\langle\overline{\phi}_n|H_{positronium}|\overline{\phi}_m\rangle = \tfrac{1}{2}\, \overline{\varepsilon}_n\, \delta_{nm} \qquad (15)$$

Because of symmetry only the p pseudostates, i.e., 2p, $\overline{3p}$, $\overline{4p}$, give a non-zero contribution to f_{pp}^{B2} .

RESULTS

Our results for e^+ + H(1s) elastic scattering, Ps(1s) formation, and the total and total inelastic e^+ + H(1s) cross sections are shown in figures 1 to 4. Comparison is made with the accurate variational[3] calculations of Brown and Humberston[3] in the Ore gap (our ELV2 + PSV2 approximation has been used to extend their partial cross sections beyond the d-wave), with a new double-continuum R-matrix calculation[4] in the intermediate energy region 13 eV to 50 eV, and with the coupled pseudostate results of Walters[5] at higher energies. Also shown are corresponding electron scattering cross sections[6].

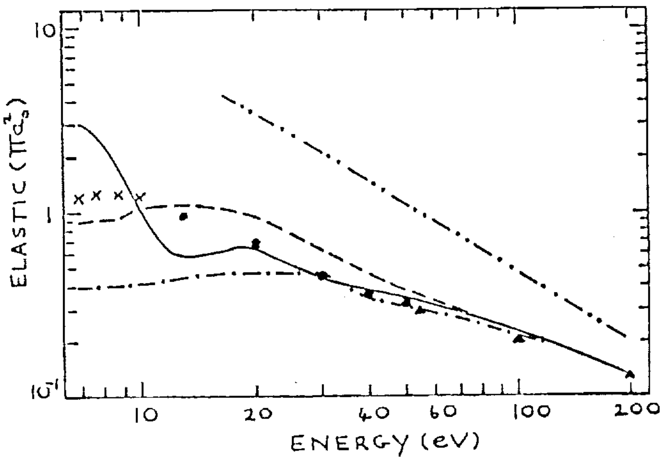

Figure 1. e^+ + H(1s) elastic cross section. Symbols: ———— Full Approximation ELV2 + PSV2; – – – –, Simpler Approximation ELV2 + PS; —·—·—, Simplest Approximation ELV2; —··—··—, electron cross section; X, variational results of Brown and Humberston[3]; ●, double-continuum R-matrix[4]; ▲, coupled pseudostates[5].

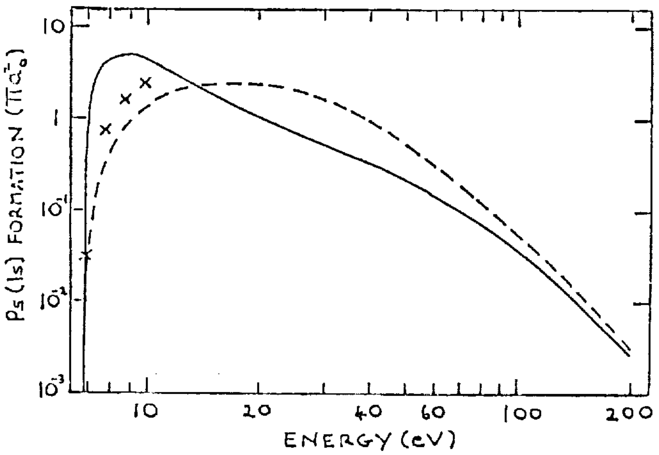

Figure 2. Ps(1s) formation cross section. Symbols as in figure 1.

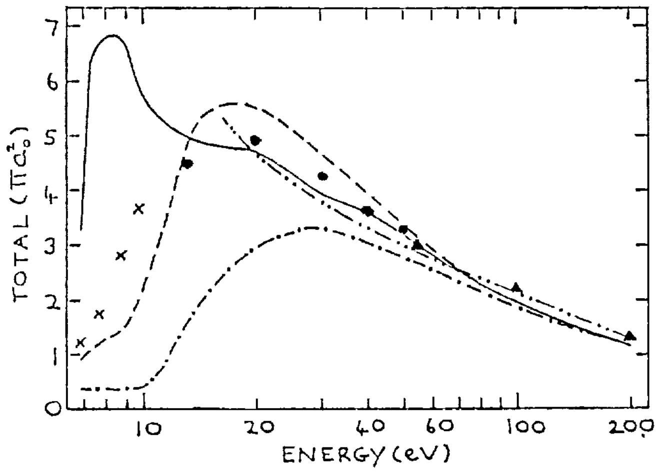

Figure 3. Total cross section. Symbols as in figure 1.

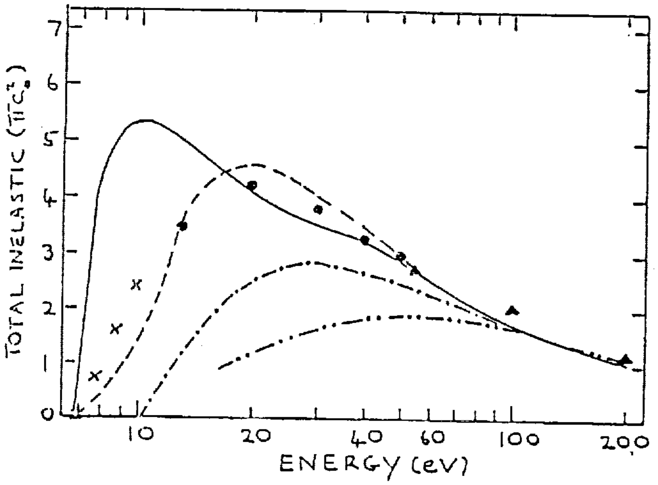

Figure 4. Total inelastic cross section. Symbols as in figure 1.

The following points are worth highlighting:

(i) At 20 eV and above the Full Approximation ELV2 + PSV2 appears to be performing well.

(ii) Polarization and absorption effects in the Ps(1s) channel can reduce the Ps(1s) formation cross section by a factor of three at intermediate energies.

(iii) Except at high energies: the elastic cross section for electron scattering substantially exceeds that for positron scattering; the total inelastic cross section for electron scattering is substantially lower than that for positron scattering; yet the (best) total cross sections for positron and electron scattering are in good agreement above 20 eV.

(iv) The simpler ELV2 + PS approximation gives cross sections which are generally too large at intermediate energies.

(v) Except for elastic scattering above 30 eV the simplest approximation ELV2 tends to produce cross sections which are too small.

References

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