POSITRONIUM FORMATION FROM VALENCE AND INNER SHELLS IN NOBLE GAS ATOMS

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When recent experimental positronium (Ps) formation cross sections have been compared with the most up-to date theoretical studies, the agreement is qualitative, but not quantitative. In this paper we re-examine this process and show that at low energies Ps formation must be treated non-perturbatively. We also look at Ps formation with inner shell electrons.

Positronium (Ps) represents a bound state between a positron and an electron. It is formed in positron-atom collisions,

$$A + e^+ \longrightarrow A^+ + \mathrm{Ps}, \tag{1}$$

when the positron energy, $\varepsilon = k^2/2$, is above the Ps formation threshold,

$$\varepsilon > |\varepsilon_n| - |E_{1s}| \tag{2}$$

where ε_n is the energy of orbital n and $E_{1s} = -6.8$ eV is the energy of the ground-state Ps. In this work we will only consider Ps formation in the ground-state. Noble gas atoms have tightly bound electrons, making excited-state Ps formation much less probable.

Recently positronium formation in Ne, Ar, Kr and Xe has been determined by two experimental groups, in London[1] (UCL) and San Diego[2] (UCSD). The two sets of data are in fairly good agreement. However, recent distorted-wave Born approximation (DWBA) calculations[3] overestimate the cross sections by as much as three times (for Xe), although their overall energy dependence is reasonable. This is in contrast with earlier coupled-static calculations[4], which yield better magnitudes of the cross section maxima, but disagree on the energy dependence. In this paper we perform 1st-order and all-order calculations of Ps formation from valence and subvalence subshells. We also consider Ps formation from inner

shells. It produces inner-shell vacancies and can be important for positron-annihilation-induced Auger-electron spectroscopy.

In the lowest order of the many-body perturbation theory, the Ps formation amplitude is given by[5]

$$\langle\widetilde{\Psi}_{1s,\mathbf{K}}|V|n,\varepsilon\rangle = -\int \widetilde{\Psi}^*_{1s,\mathbf{K}}(\mathbf{r}_1,\mathbf{r}_2)\frac{1}{|\mathbf{r}_1-\mathbf{r}_2|}\psi_n(\mathbf{r_2})\varphi_\varepsilon(\mathbf{r_1})d\mathbf{r}_1 d\mathbf{r}_2, \quad (3)$$

where $\varphi_\varepsilon(\mathbf{r_1})$ is the incident positron wavefunction, $\psi_n(\mathbf{r_2})$ is the Hartree-Fock wavefunction of the initial electron state ("hole"), and $\widetilde{\Psi}_{1s,\mathbf{K}} = (1-\sum_{n'}|n'\rangle\langle n'|)\,\Psi_{1s,\mathbf{K}}$ is obtained from the wavefunction of the ground-state Ps with momentum $\mathbf{K}$,

$$\Psi_{1s,\mathbf{K}}(\mathbf{r}_1,\mathbf{r}_2) = e^{i\mathbf{K}\cdot(\mathbf{r}_1+\mathbf{r}_2)/2}\phi_{1s}(\mathbf{r}_1-\mathbf{r}_2), \quad (4)$$

by orthogonalising it to all electron orbitals n' occupied in the target ground state. The positron wavefunction is calculated in the field of the target. The Ps center-of-mass motion is described by a plane wave. The Ps formation cross section is found by integration over the directions of $\mathbf{K}$,

$$\sigma_{\rm Ps} = \frac{MK}{4\pi^2 k}\int \left|\langle\widetilde{\Psi}_{1s,\mathbf{K}}|V|n,\varepsilon\rangle\right|^2 d\Omega_{\mathbf{K}} \quad (5)$$

This approximation is equivalent to DWBA for a rearrangement collision.

The cross sections are found by summing over the positron partial waves from $l = 0$ to 10. Figure 1 shows the Ps formation cross sections for the valence np and subvalence ns orbitals in Ne, Ar, Kr and Xe. The present results for the np subshell agree with the Ps($1s$) formation cross section from DWBA[3]. Both calculations progressively overestimate the cross section near the maximum, compared to the experimental results[1,2] which were obtained by different methods. For Ne, Ar and Kr experiment and theory converge at higher energies, while in Xe the discrepancy persists.

Ps formation thresholds for the inner shells lie at much higher energies, *e.g.*, at 242 and 320 eV for the $2p$ and $2s$ orbitals in Ar. Ps formation from inner shells is suppressed due to the positron repulsion from the nucleus. Figure 2 shows that Ps formation by the outer shells dominate near the inner-shell thresholds. At higher positron energies in Ar the various contributions become comparable, with $2p$ dominant above 550 eV.

Analysis of the lower partial-wave contributions which dominate near the cross section maximum ($l = 0$–3), shows that they become close to and even violate (for Kr and Xe) the unitarity limit for the inelastic processes, $\sigma^{(l)}_{\rm Ps} \le \pi(2l+1)/k^2$. This means that Ps formation cannot be treated perturbatively. In other words, one must take into account the effect of Ps

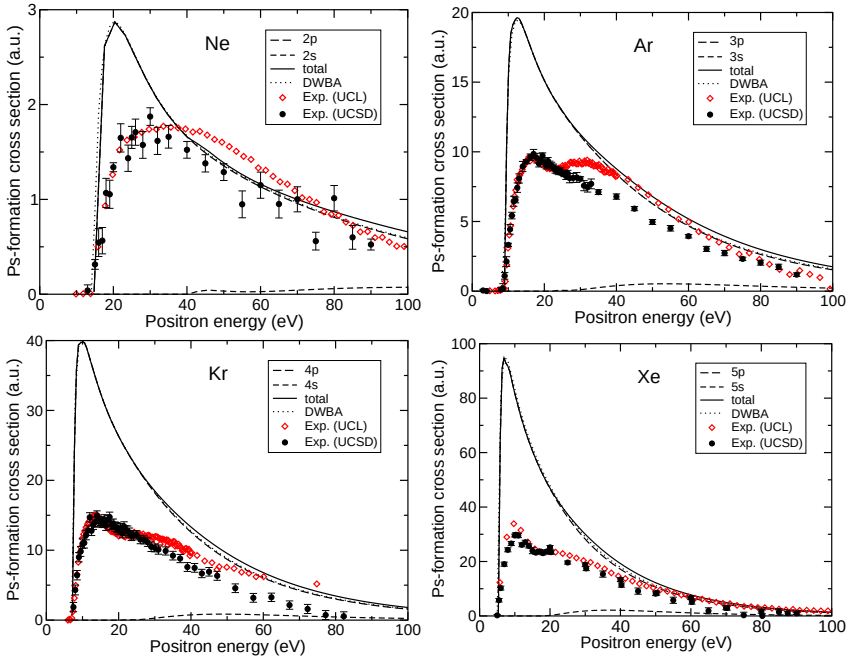

Figure 1. Total Ps-formation cross sections from Eq. (5) for the valence and subvalence subshells; DWBA[3] is only for the np subshell; experiment, UCL[1] and UCSD[2].

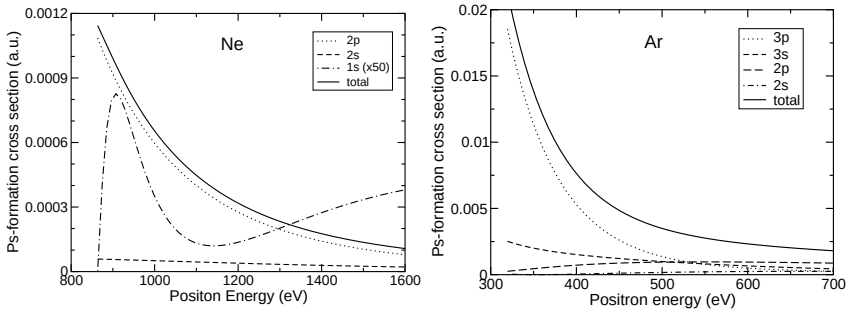

Figure 2. Inner-shell Ps formation cross sections in Ne and Ar.

formation on the positron scattering. We achieve this by considering the Ps formation contribution to the positron-atom correlation potential[5],

$$\langle \varepsilon' | \Sigma_E^{(\mathrm{Ps})} | \varepsilon \rangle = \int \frac{\langle \varepsilon', n | V | \widetilde{\Psi}_{1s,\mathbf{K}} \rangle \langle \widetilde{\Psi}_{1s,\mathbf{K}} | V | n, \varepsilon \rangle}{E + \varepsilon_n - E_{1s} - K^2/4 + i0} \frac{d^3K}{(2\pi)^3}. \qquad (6)$$

The potential is complex above the Ps-formation threshold. The corre-

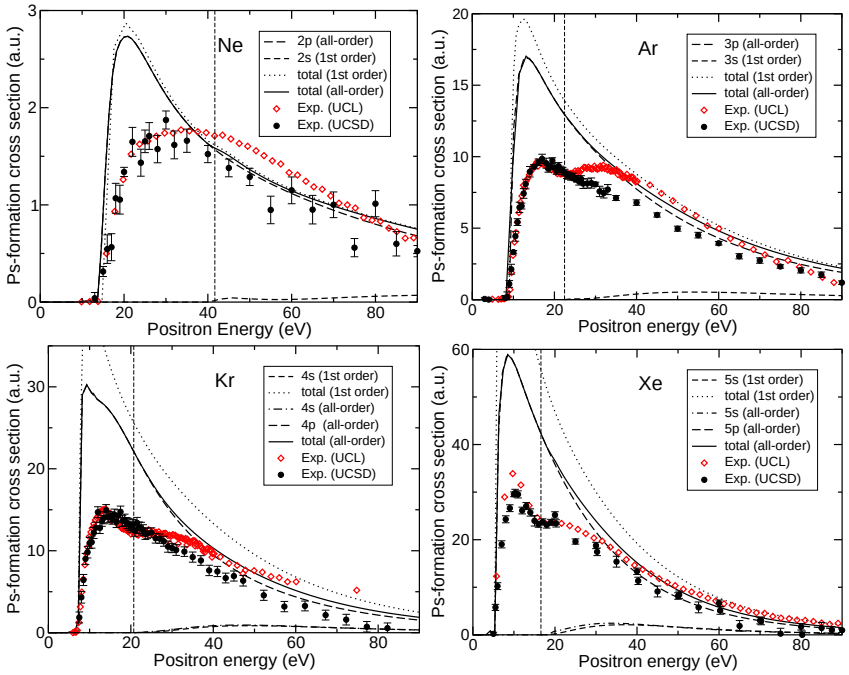

Figure 3. Ps formation cross sections obtained nonperturbatively using $\Sigma^{(\mathrm{Ps})}$. Vertical lines show ns Ps formation thresholds.

sponding scattering phaseshifts, $\delta_l = \delta_l' + i\delta_l''$ are used to determine the cross section as $\sigma_{\mathrm{Ps}} = \pi/k^2 \sum_{l=0}^{\infty}(2l+1)(1-e^{-4\delta_l''})$. This leads to noticeable reduction of the cross sections, especially for Kr and Xe, Fig. 3.

Figure 3 shows that the subvalence ns subshell gives a small but detectable contribution. The cross section maximum is still overestimated. A better calculation must include a more accurate positron-atom correlation potential, and account for the interaction between the Ps and residual ion.

References

1. G. Laricchia, P. Van Reeth, M. Szłuińska and J. Moxom *J. Phys. B: At. Mol. Opt. Phys.* **35**, 2525 (2002).
2. J. P. Marler, J. P. Sullivan and C. M. Surko, *Phys. Rev. A* **71**, 022701 (2005).
3. S. Gilmore, J. E. Blackwood and H. R. J. Walters *Nucl. Instrum. Methods B* **221**, 129 (2004).
4. M. T. McAlinden and H. R. J. Walters, *Hyperfine Interactions* **73**, 65 (1992).
5. V. A. Dzuba, V. V. Flambaum, G. F. Gribakin and W. A. King, *J. Phys. B: At. Mol. Opt. Phys.* **29**, 3151 (1996).