POSITRONIUM FORMATION FROM VALENCE AND INNER SHELLS IN NOBLE GASES

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Recently, positronium (Ps) formation in positron collisions with noble gas atoms has been determined by two experimental groups [1, 2]. The two sets of data are in fairly good agreement. However, when compared to recent theoretical results the agreement is qualitative but not quantitative [3]. In previous theoretical works only Ps formation with valence and subvalence electrons had been studied. We want to re-examine it and study Ps formation with the inner-shell electrons. The latter process can contribute to the production of inner-shell vacancies in positron-annihilation-induced Auger spectroscopy, a tool used to detect impurities on surfaces [4].

The 1st-order amplitude of the formation of Ps($1s$) by a positron of energy ε and an electron from the atomic orbital n is $\langle\tilde{\Psi}_{1s,\mathbf{K}}|V|n\varepsilon\rangle$, where V is the electron-positron Coulomb interaction and $\tilde{\Psi}_{1s,\mathbf{K}}$ is the wavefunction of the ground-state Ps atom with momentum $\mathbf{K}$, $\Psi_{1s,\mathbf{K}} = e^{i\mathbf{K}\cdot(\mathbf{r}+\mathbf{r}')/2}\varphi_{1s}(\mathbf{r}-\mathbf{r}')$. The tilde above $\Psi_{1s,\mathbf{K}}$ indicates that this wavefunction is orthogonalised to the electron orbitals n' occupied in the atomic ground state [5],

$$|\tilde{\Psi}_{1s,\mathbf{K}}\rangle = \Big(1 - \sum_{n'} |n'\rangle\langle n'|\Big)|\Psi_{1s,\mathbf{K}}\rangle \qquad (1)$$

The cross section proportional to $\left|\langle\tilde{\Psi}_{1s,\mathbf{K}}|V|n\varepsilon\rangle\right|^2$, is found by expansion in the positron partial waves (up to $l = 10$).

Figure 1 shows the Ps formation cross sections by the $3p$ and $3s$ electrons in argon and compares them with the experimental data. Our theoretical values (similiar to those of [3]) overestimate the experimental results, especially at low energies. We believe that this is primarily due to the limitation of the Born approximation for the low-l partial waves, e.g., the p- and d-wave contributions at positron momenta $k \approx 1$ au are at or above the unitarity limit, $\pi(2l+1)/k^2$.

Figure 2 shows Ps formation from all subshells in Ar. Around 500 eV the cross-sections are similar in magnitude and the inner-subshell contribution takes over at higher energies.

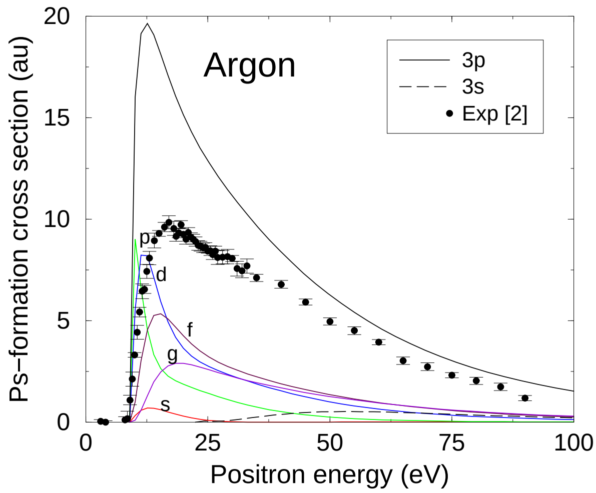

Fig. 1. Low-energy Ps formation in Ar, with partial wave contributions shown for the $3p$ subshell.

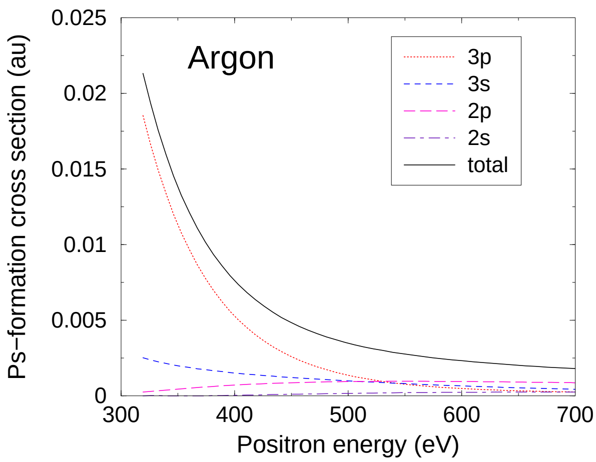

Fig. 2. Ps formation at higher energies.

References

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