Many-body theory of positronium-atom scattering and pickoff annihilation

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Synopsis We present a new method to describe low-energy Ps scattering and pickoff annihilation from many-electron atoms.

Many-body theory is very successful in describing low-energy positron scattering, annihiation rates and γ-ray spectra for noble-gas atoms [1], as well as electron scattering [2]. In this work we develop the many-body theory approach to describe the interaction between an electron-positron pair (positronium, Ps) and many-electron atoms.

Recent experiments on Ps scattering on noble-gas atoms revealed some unexpected trends, e.g., that the scattering cross section becomes very small at low Ps energies [3]. Overall, there is a large uncertainty in Ps-atom scattering data. Theoretically, Ps collisions have been difficult to describe because of the composite nature of both the target and projectile, and a significant cancellation between the repulsive static Ps-atom interaction and van der Waals-type attraction. An accurate calculation must account for virtual excitation of both objects during the collision, which until now has only been achieved for simple targets, e.g., hydrogen and helium.

In our approach, we confine the Ps-atom system within a hard-wall spherical cavity [4] with the atom at the centre. A B-spline basis is used to solve the Dyson equations $\left(H_0^{\pm}+\Sigma^{\pm}\right)\psi^{\pm}=\varepsilon^{\pm}\psi^{\pm}$ for the electron ($-$) and positron ($+$) in the field of the target atom. Here, $H_0^{\pm}$ is the Hamiltonian of the electron/positron in the static (Hartree-Fock) field of the atom and $\Sigma^{\pm}$ is the correlation potential. We calculate Σ^{-} and Σ^{+} in second order and also the electron-positron ladder series in Σ^{+} [1]. This yields the bases of electron/positron states $\psi^{\pm}$ with eigenenergies $\varepsilon^{\pm}$.

The Ps eigenstates $\Psi=\sum_{\mu,\nu}C_{\mu\nu}\psi_{\nu}^{-}\psi_{\mu}^{+}$ are found from $H\Psi=E\Psi$, where the total Hamiltonian includes the electron and positron parts $(H_0^{\pm}+\Sigma^{\pm})$, and the electron-positron interaction $V+\delta V$, V being the Coulomb interaction and δV the second-order screening contribution due to polarization of the atomic electrons. The boundary condition at the cavity wall enables the scattering phase shifts (and hence the cross section) to be found from the energies E. Figure 1 shows the cross section for Ar in the frozen-target approximation (i.e., without $\Sigma^{\pm}$ and δV), and with full many-body treatment. Despite the limited agreement with experiment, our calculations are the most reliable to date.

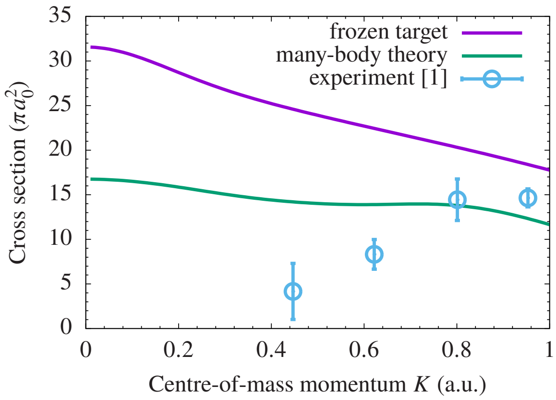

Figure 1. Ps-Ar scattering cross sections.

The Ps wave function can also be used to investigate *pickoff* annihilation, where the positron from Ps annihilates one of the atomic electrons. The pickoff annihilation rate λ is usually expressed in terms of the dimensionless quantity $^1Z_{\rm eff}$ defined by $\lambda = 4\pi r_0^2 cn\,^1Z_{\rm eff}$, where r_0 is the classical electron radius, c is the speed of light, and n is the gas density. Previous calculations [5] of $^1Z_{\rm eff}$ for noble gases have underestimated the experimental data [6] by as much as a factor of 10. By accounting for many-body corrections to the annihilation vertex, we expect to obtain a much more accurate description of this quantity.

References

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