Positronium collisions with atoms and molecules

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Studies of positronium (Ps) collisions with atoms and molecules reveal interesting phenomena. In particular, when plotted as a function of velocity the total cross section for scattering of electrons and positronium (Ps) looks very similar for a variety of atomic and molecular targets [1]. Moreover, resonances have been observed in Ps-N_2 [2] and Ps-CO_2 [3] collisions that are similar to resonances in electron scattering by the same targets. In describing Ps collisions theoretically, the exchange interaction takes on a larger role than in the corresponding electron scattering problem due to the neutrality of Ps. At lower velocities correlation effects become more important. These correlation effects have often been modeled by using a van der Waals potential with a short-range cutoff which includes an adjustable parameter. While the long range correlation is included properly in this way, short-range correlations may be significantly underestimated.

In order to include exchange and correlation in an *ab initio* way we have calculated exchange and correlation energies and local potentials in a free-electron-gas model (FEG) [4,5]. We have applied this approach to Ps-N_2 scattering and found good agreement with experiment at velocities above the Ps ionization threshold. This agreement includes the presence of a resonance peak at a slightly lower velocity than experimentally observed. This discrepancy is probably due to the fixed-nuclei approximation employed in our calculations.

One deficiency of the local exchange and correlation potentials is that they do not properly take into account the antisymmetric character of the total wave function with respect to interchange of the projectile and target electrons. In order to incorporate this effect we have employed an orthogonalizing pseudopotential (OPP) that has been proposed for Ps-atom scattering by Mitroy et al. [6,7]. We have found that adding the OPP to the FEG potentials provides a good description of Ps-rare-gas scattering, especially for the heavier rare-gas atoms Ar, Kr and Xe [8].

Future work includes application of the FEG and OPP models to other atomic and molecular targets and inclusion of nuclear dynamics in Ps-N_2 scattering.

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