Double-electron capture in low-energy $H^+ + H^-$ collisions

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Synopsis In this talk, I shall present our latest work [1] on the double-electron capture process in the H^+-H^- collision in the low energy range, from 60 eV to 20 keV. A fully correlated two-active-electron semi-classical atomic-orbital close-coupling approach (AOCC) is employed, using a large basis set ensuring a reasonable convergence in the whole energy domain. Our results reproduce well the experimental data for the first time in both magnitude and shape. Furthermore, the oscillation structures phenomenon observed in the experiments has been interpreted as coherence effects between double electron capture and the transfer-excitation processes.

In ion-atom/molecule collisions, one-electron processes for systems such as $H^+ + H$ [2] and $He^{2+} + H_2^+$ [3], have been fairly well understood [4], while the knowledge on multi-electron ones is still far from complete. As a benchmark of double electron collision system, $H^+ + H^-$ collision has been extensively investigated for more than five decades. Up to now, a complete description of the electronic dynamics of this system remains a challenge due to the predominant role of the electronic correlation.

In the present work, low energy H^+-H^-collision has been studied using a fully correlated two-active-electron AOCC method. In order to obtain convergent results, a large basis set of 45 Gaussian-type orbitals (GTOs) (11 for l=0, 8 × 3 for l =1, and 2 × 5 for l = 2) is employed and totally 1977 states are included in our calculation, describing elastic, single electron capture (SEC) and double-electron capture (DEC) channels, as well as ionization through the inclusion of 1446 pseudostates of energy lying up to 1 a.u. above ionization thresholds. Comparing the present results with those from other two basis sets, the convergence was evaluated to be about 10% for impact energies above 0.2 keV and smaller than 30% for lower energies.

In Fig.1, our calculated DEC cross sections are compared with available experimental [5-7] as well as theoretical [5, 7-10] results. Although slightly higher than the experimental ones at the lowest collision energy, our cross sections are in good agreement with experiments over the whole collision energy range; they are the first ones to reproduce well the experimental data in both magnitude and shape. Furthermore, the cross section shows a clear oscillatory structure whose period increases with increasing impact energies. It is demonstrated to be stem from coherence effects between double electron capture and other two-electron inelastic channels (transfer-excitation). From the view of a molecular picture, the oscillation period can be well estimated by a Rosenthal-like model [11].

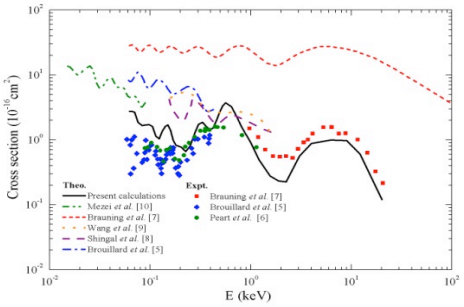

Figure1. Double electron capture cross sections as function of the impact energy. The present results are shown as a black line. Experimental and theoretical results are reported as points and lines, respectively.

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