Electron Correlation in simultaneous electron transfer and excitation: Results of new 2eAOCC calculations and comparison to experiment in 50-500 keV $He^+ + H/H_2$ collisions

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Abstract

New two-electron semiclassical atomic orbital coupled channel calculations (2eAOCC) are compared to experimental data and to previous coupled channel calculations. Progress in these types of calculations is assessed in an effort to investigate the effect of electron correlations in this fundamental collision system.

The study of multi-electron processes occurring in ion-atom collisions is still a theoretical challenge due to the importance of static and dynamic correlation in these transitions. It is therefore interesting to investigate the dynamics of true two-electron systems, where the transfer of an electron and the excitation of another is likely. From this point of view, He^+ - H collisions, inducing transfer-excitation (TE) processes to autoionizing states of He, can be considered as a benchmark system.

Here, we present cross sections for such TE processes, especially

$$He^+ + H \rightarrow He(2l2l'\ ^1L) + H^+$$

for impact energies ranging from 50 to 500 keV. Results are obtained with a full configuration interaction (CI) close coupling semiclassical approach [1]: the two electrons are taken into account and the time-dependent Schrödinger equation is solved with an unprecedented large basis set to allow for convergence of the non perturbative scheme. These results are compared with three-decade old theoretical results [2], as well as with experimental data obtained with zero-degree Auger projectile spectroscopy for dihydrogen molecular target [3].

The discussion and interpretation of the results in terms of one-step mechanism, the so called resonant (correlated) transfer-excitation (RTE) [4], are particularly interesting when comparing with *ab initio* two-electron calculations, in which all mechanisms are described coherently. We present experimental and theoretical cross sections for production of $2p^2\ ^1D$ states in Fig. 1. Comparisons between the present calculations (including both basis set data) and previous theoretical work [2] are presented for $2p^2\ ^1D$, $2p^2\ ^1S$, $2s^2\ ^1S$ and $2s2p\ ^1P$ autoionising states in Fig. 2.

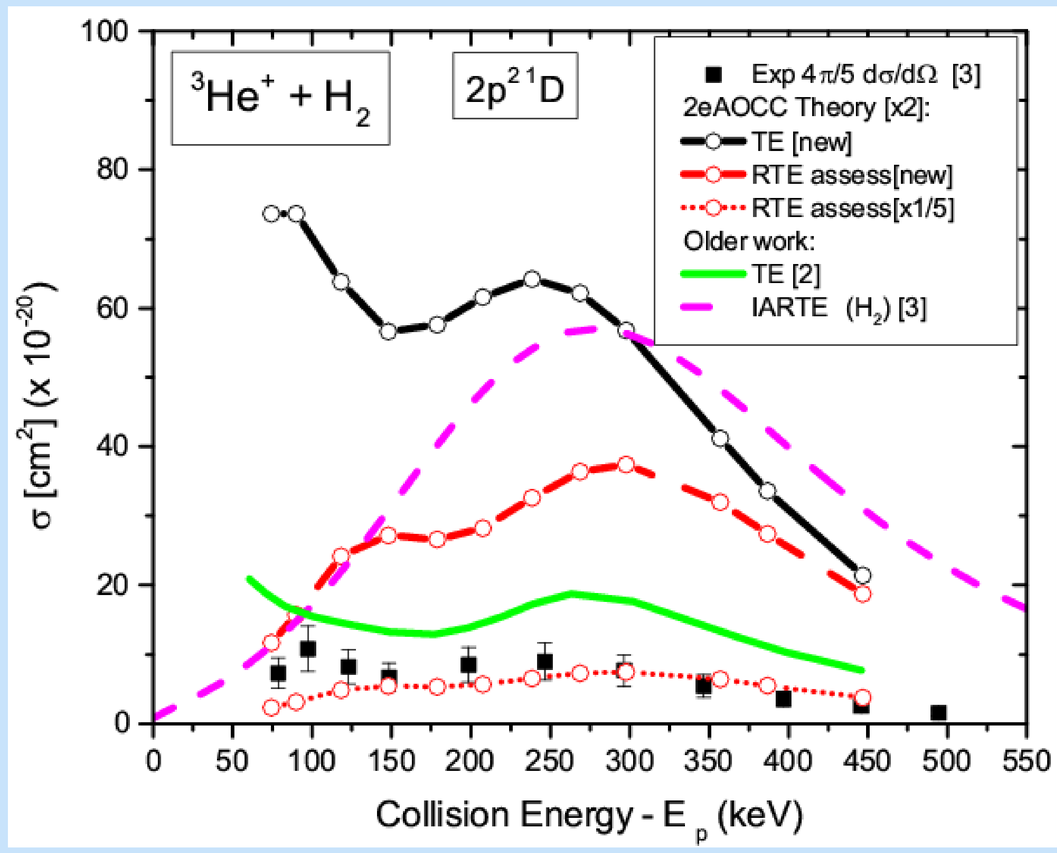

Figure 1. Comparison of cross sections for the production of the $He(2p^2\ ^1D)$ state in collisions with hydrogen. Theory: He^+ + H, 2eTE cross sections multiplied by two to account for H_2 target in experiment (squares) [3]. Impulse Approximation RTE (IARTE) (long dashes violet).

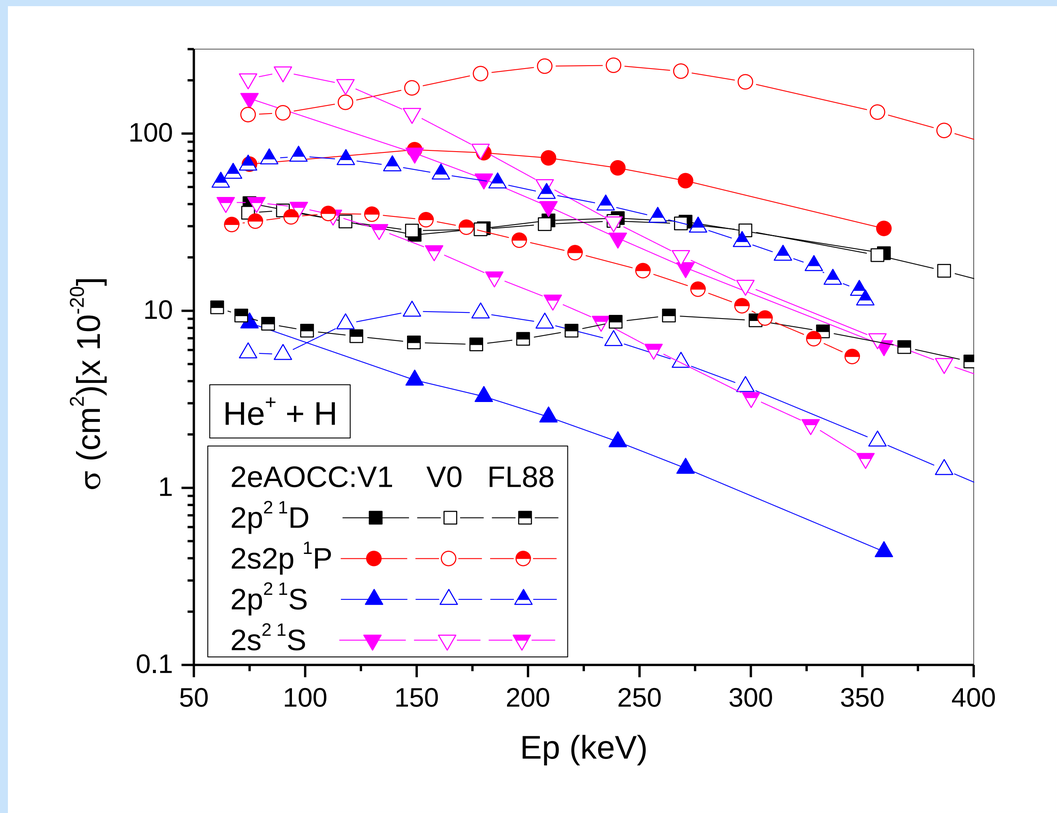

Figure 2. Comparison of TE cross sections for the production of the He $2p^2\ ^1D$, $2s2p\ ^1P$, $2p^2\ ^1S$ and $2s^2\ ^1S$ states in collisions with H. Three different 2eAOCC calculations are presented: V1 basis and V0 basis (this work) and FL88 (Fritsch and Lin 1988 Ref. [2]).

V0 basis: 7 GTO "s" on H (1s,2s,3s and 4 "s" pseudo states of positive energy) and 18 GTO on He^+ (10 "s" + 3*3 "p") and 60 2e-states on He (good $1s^2$, 1s2s, 1s2p some pseudo states, $2s^2\ ^1S$, $2p^2\ ^1D$, $2s^2\ ^1P$, $2p^2\ ^1S$ then pseudo states)

V1 basis: 8 "s" and 6*3 "p" GTOs on H and 10 "s" + 8*3 "p" GTO on He^+ and 138 states on He with more real states and more pseudostates.

FL88 basis: see Ref. [2]

References

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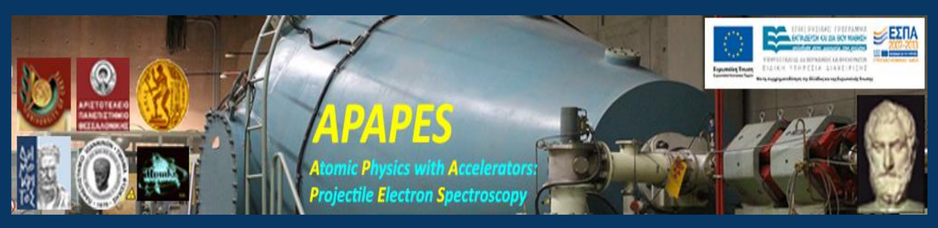

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