Single- and multiple-particle dynamics in three-electron ion-atom collision systems

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Synopsis Recent progress in the theoretical description of the He^{+}-He and the O^{8+}-Li collision systems will be reported.

Studying atomic collisions to shed light on the fundamental few-body problem in physics is not a new research objective, but it remains a valid one and is indeed the driving force for the work to be presented in this talk. I will report on our recent progress in understanding electron dynamics in two somewhat different three-electron ion-atom collision systems: (i) the He^{+}-He system at intermediate impact energies, in which one has to deal with active target and projectile electrons; and (ii) the O^{8+}-Li system at high impact energy, in which one has to deal with active inner- and outer-shell (target) electrons.

The He^{+}-He system is addressed within the spin-density functional theory framework on the exchange-only level. The Krieger-Li-Iafrate (KLI) approximation is used to calculate the exchange potentials for spin-up and spin-down electrons, which ensures that self-interaction effects are avoided and the total Kohn-Sham (KS) potential exhibits the correct asymptotic behaviour [1]. Orbital propagation is accomplished with the two-center basis generator method [2]. The computationally challenging part is to feed the orbitals into the KLI functional at each time step in order to calculate the KS potential, which, in turn, is used to generate the orbitals at the next time step. An approximate yet reasonably accurate solution to this problem will be discussed and total cross section results for a variety of outcome processes presented in the 20 to 1000 keV/amu impact energy regime.

O^{8+}-Li collisions at 1.5 MeV/amu were recently studied experimentally using the magneto-optical-trap reaction microscope (MOTReMi) technique [3, 4, 5]. For this problem, a simplified *no response* approach can be used, but a nontrivial combination of perturbative and nonpertubative methods was required to extract the observables of interest, namely singly- and doubly-differential cross sections for single-electron emission [6, 7]. A careful analysis demonstrates that (i) two-electron excitation-ionization processes play a leading role in inner-shell vacancy production; and (ii) neither single-active-electron calculations, nor the independent-electron model are sufficient to explain the experimental data.

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References

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