Non perturbative treatment of atomic and molecular collisions: valence and inner shell processes in keV H^+-Li collisions

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Abstract We present a new approach to describe electronic processes occurring in ion-atom and ion-molecule collisions at impact energies ranging from 50 eV.u^{-1} to 1 MeV.u^{-1}. The treatment is based on the semiclassical approximation in which the time-dependent Schrödinger equation is solved non perturbatively, taking into account all the electrons of the collision system. This allows to describe exactly multielectronic processes and also, at the same footing, processes involving valence and inner shell electrons. We apply this model to describe electron transfer in a genuine three-electron system, H^+-Li.

The description of multielectronic processes is a complex task in atomic and molecular collisions. This is especially challenging in the intermediate energy region where electron transfer, excitation and ionization are likely and should be described in a coupled way [1].

We present a new semiclassical approach in which the time dependent Schrödinger equation is solved with the exact Hamiltonian operator, i.e. for ion-atom collisions

$$H_e = \sum_{i=1}^{N_e}\left[-\frac{1}{2}\Delta_i - \frac{Z^t}{r_i^t} - \frac{Z^p}{r_i^p} + \sum_{j>i}^{N_e}\frac{1}{r_{ij}}\right]$$

where the $\vec{r}_i^{\,t/p}$ are the coordinates of the N_e electrons with respect to target (T) or projectile (P) and $\vec{r}_i^{\,p} = \vec{r}_i^{\,t} - \vec{R}(t)$. The time-dependent wavefunction is then expressed in terms of a linear combination of products of states centered around T and P, depending on the considered processes. The 2-, 3-, ... electron states are found by diagonalizing the T or P Hamiltonian on a basis of spin adapted linear combination of products of Gaussian-type orbitals. To insure both the correct spin multiplicity and spatial symmetry we use the permutation group theory together with Young diagrams [2] instead of combinations of Slater determinants.

We applied this approach on a three-electron system, H^+-Li($1s^2 2s^1$), which has been studied extensively, both experimentally and theoretically, in a wide energy domain. It therefore presents the advantages (i) to able to check the model and its implementation and (ii) to provide an interesting simple system where processes involving inner- and valence shell electrons can be coupled. Figure 1 shows cross sections of electron transfer processes leaving the target as ^{1}S $Li^+(1s^2)$ or ^{1}S/^{3}S $Li^+(1s^1 2s^1)$ after the collision. Further details and data for various processes will be presented in the conference.

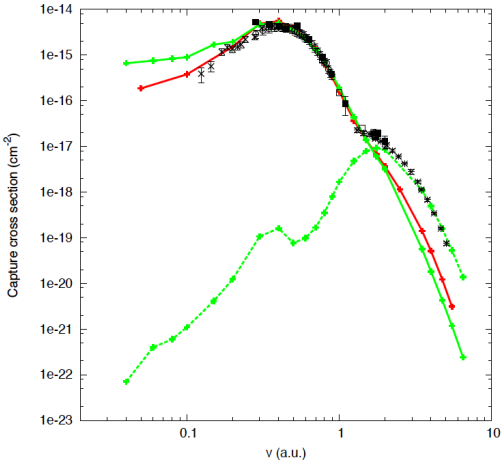

Figure 1. Cross sections of electron transfer vs. impact velocity in H^+-Li(2s) collisions. The green/red line shows three-/one-electron results. The green solid/dotted line shows transfer from the valence/inner shell. Symbols are experimental data [3-7].

References

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