Mutual neutralization of atomic ions

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To theoretically investigate the low energy mutual neutralization reaction in collisions between oppositely charged atomic ions can be a challenge. The ion-pair channel formed by the colliding fragments is highly excited. The ion-pair state has a long-range attractive Coulomb potential. There are non-adiabatic interactions between the ion-pair state and covalent Rydberg states. Some of these interactions can take place at very large internuclear distances. These are the interactions driving the mutual neutralization process. Furthermore, for some molecular systems there are interactions between the neutral states and the ionization continuum. Hence the process of autoionization has to be included in the theoretical treatment. The nuclear dynamics for the coupled electronic states has to be described quantum mechanically including very high angular momentum for the colliding fragments. We will here discuss the theoretical framework we use to describe mutual neutralization of atomic ions. Results from studies on three different molecular systems will be presented.

Mutual neutralization in $H^+ + H^-$ collisions can be used as a model system to compare experiments with theory. The reaction is driven by the non-adiabatic interactions between the ion-pair state and the n=3 Rydberg states occurring at large internuclear distances. We have here calculated both the total and partial cross sections [1] as well as the cross section for double charge transfer [2].

In collisions between $H^+ + F^-$ there are non-adiabatic interactions at smaller distances that will cause resonant structures in the cross section for mutual neutralization. For the HF system we have also considered the effect of autoionization [3].

We have also started to investigate mutual neutralization in collisions of $He^+ + H^-$. Here the ion-pair state is embedded in the ionization continuum. The ion-pair state interacts with Rydberg states converging to an excited ionic core. Electron scattering calculations are needed to describe the energies and autoionization widths of electronic resonant states. Non-adiabatic interactions between these states will drive the mutual neutralization reaction.

References

[1] M. Stenrup, Å. Larson, and N. Elander, Phys. Rev. A **79**, 012713 (2009).

[2] J. Zs. Mezei, M. Stenrup, N. Elander, and Å. Larson, Phys. Rev A **82**, 014701 (2010).

[3] J. Zs. Mezei, J. B. Roos, K. Shilyaevam N. Elander, and Å. Larson, submitted to Phys. Rev. A (2011).

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