§8. Ionization and Charge Transfer of Atomic Hydrogen in Collisions with Multiply-Charged Ions

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The close-coupling method has been applied successfully to ion-atom collisions and it has achieved a status of being one of the most reliable theoretical methods. Excitation and electron capture processes have been studied by this method extensively and good agreement with experimental data has been achieved. However, ionization processes have been studied mostly by treatments based on the perturbation theory, which breaks down in the intermediate or low energy region. The present project is the first systematic theoretical study of ionization processes of atomic hydrogen in collisions with multiply-charged ions (Z=2–8)

$$A^{Z+} + \mathrm{H} \rightarrow A^{Z+} + p + e, \qquad (1)$$

by the close-coupling calculations. We adopt the pseudostate-expansion method, which was recently developed for the nonperturbative study of the Thomas mechanism [1]. The time-dependent Schrödinger equation is expanded by a large number of two-center atomic orbitals which are constructed from Gaussian-type orbitals by the diagonalization of the atomic Hamiltonians of the target and the projectile. The relative motion of the heavy projectile is described by a classical rectilinear trajectory with a constant velocity.

We have coupled 168 states on the hydrogen atom and 154 to 320 states on the projectile ion increasing the number for higher nuclear charge Z. We show the ionization and electron capture cross sections for O^{8+}+H collisions in Fig. 1. No experimental cross section is available for the ionization process and we compare our results with other theoretical calculations. The circles are from the atomic-orbital close-coupling calculations by Fritsch and Lin [2] and the triangles are from the adiabatic superpromotion model by Janev, Ivanovski, and Solov'ev [3]. Our capture cross sections are larger than those of Fritsch and Lin at higher energies. This difference comes from the contribution of the n=7 and 8 states of O^{7+} which were not included in their calculations. The ionization cross sections of Janev *et al* decrease smoothly with decreasing collision energy while our cross section curve shows double-humped structure there. This structure exists commonly for other projectile ions though it becomes less remarkable for smaller charge Z.

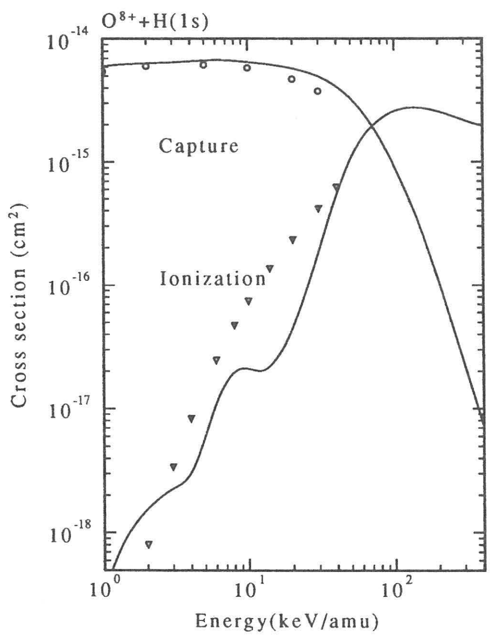

Figure 1. The ionization and electron capture cross sections for O^{8+} + H collisions. Solid lines are present results. The circles are from Fritsch and Lin and the triangles from Janev *et al.*

References
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3) R. K. Janev, G. Ivanovski, and E. A. Solov'ev, Phys. Rev. A**49**, 645 (1994).