§5. Ionization of Hydrogen by Low Energy Protons

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The proton-hydrogen-atom collision system has been extensively studied within various theoretical models and in several experiments, but discrepancies among theoretical calculations and among experimental measurements are still quite large. At the order of keV energies, the total ionization cross sections obtained by experimental studies of Pieksma *et al.* [2] are quite larger than the recent measurements of Shah *et al.* [3] (below 10 keV/amu), and to decrease much less rapidly with the energy decrease. At the lowest energy considered (1 keV/amu), the cross sections of Pieksma *et al* [2] exceed the values by Shah [3] by $\sim$ 4 times. Numbers from the precise experiments [4, 5] and the extensive theories [6, 7, 8] disagree by 20% at the peak of ionization cross section.

In this note, we report new accurate single differential and total ionization cross sections on proton-hydrogen collision system at 0.1-10 keV/amu. We use the close-coupling expansion with electron translation factors (ETF's) modified H_2^+ molecular states. It is the first calculation using this method for the ionization problem, based on the direct evaluation of all couplings between the bound and continuum states. Figure 1 shows the comparison of our total ionization cross sections and other theoretical calculations as well as experimental values. Our results are in an excellent agreement with the recent experiments of Shah *et al.* [3], but differ from the other measurements by Pieksma *et al.* [2].

From a methodological point of view, we show that the appropriate ETF's not only exactly cancel the spurious asymptotic behavior of nonadiabatic couplings, but also systematically reduce the size and effective range of most coupling matrix elements. With the ETF-corrected molecular basis, the accurate ionization cross sections can be obtained by a calculation in a small region of configuration space and coordinate space. For H_2^+ system in the range 0.1-10 kev/amu, a good convergence has been achieved with a basis including 10 bound states and 11 continuum partial waves.

In addition, we find that the upper levels play a completely different role in *gerade* and *ungerad* components. In case of g components, an excitation sequence via upper levels is the dominant mechanism for the ionization, which enhances the total ionization cross sections (as compared to the direct ionization process) by more than two times at the collision energy E =10 keV/amu. In case of u components, the excitation to upper levels reduces the total ionization cross section significantly, especially the excitation to $2p\pi_u$ molecular state. Since the total ionization cross section is mainly decided by u components, we conclude here that the upper levels are a "trap" on the way of electron going to ionization continuum, in contrast the general recognized "ladder". Using the ETF-modified MOCC method, we have a tool to examine the role of each molecular state in the ionization process in a systematic way. The present method is readily applicable to further physical systems of interest, such as He^{++}/H, p/He^+ or p/Li.

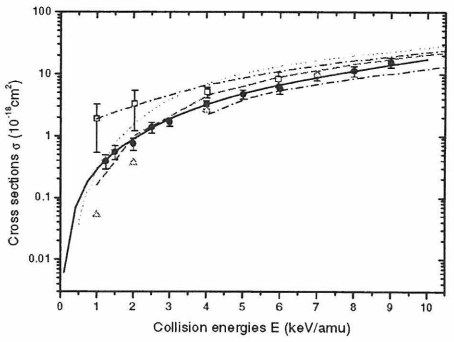

Figure 1: Total ionization cross sections of proton-hydrogen system: solid circles, measured cross sections of Shah *et al.* [3]; open squares, measured cross section of Pieksma *et al.* [2]; dash dotted lines, hidden crossing theory with S and T and radial decoupling promotion mechanisms [9]; dashed lines, hidden crossing theory with only S and T promotion mechanisms [2]; dotted lines, close-coupling triple-center calculations [3]; up triangles, two-center close-coupling calculations [7]; short dash dotted lines, two-center atomic orbitals plus pseudostates expansion [10]; solid lines, present calculation.

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