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Time-dependent studies of ionization of atoms and molecules

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The time-dependent close-coupling method has been a successful and efficient method of calculating cross sections for many fundamental atomic processes including electron-impact excitation and ionization, multiple photon ionization and heavy-ion impact collisions. In the past decade this method has been applied to the electron-impact ionization of many atoms and ions. Beginning with studies of the electron-impact ionization of hydrogen, the time-dependent method has also been applied to multi-electron systems such as He, Li, Be, C, and O, as well as many of their ions. Also, electron-impact excitation cross sections have been calculated for many of these systems. Recently a program of work was initiated to apply these time-dependent techniques to the electron-impact ionization of small diatomic molecules. This work was motivated by the need for accurate cross sections for these molecules, as well as complementary work on photoionization of light molecules. In this talk an overview will be given of our time-dependent method, especially as applied to molecular systems. Recent results will be presented for electron-impact ionization cross sections of various atomic ions, and very recent results will be presented for the electron-impact ionization of H_2^+ . Comparison will be made, where available, with previous theoretical and experimental results. This work is supported in part by grants to Auburn University from the U.S. Department of Energy. Work at Los Alamos National Laboratory is performed under the auspices of the U.S. Department of Energy. In collaboration with Michael Pindzola, Auburn University.